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MetaboNews

This month in metabolomics

September, 2025 Vol 15, Issue 8

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





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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

Message from Warwick (Rick) Dunn, President

Dear Metabolomics Society Members and metabolomics friends,

I have some sad news. Professor Steven Gross from Cornell University passed away on September 1st. Steve was known to many of us and further online discussions will follow I am sure as well as an obituary in the journal Metabolomics. I have known Steve's work for decades but was lucky enough to meet him in his role as GRC cochair in 2019 and more recently. One quote has always stuck with me 'I was the luckiest man alive because I never had to work, my job is my passion and I love doing scientific research'. Thanks, Steve, for everything.

It is a busy time of the year for the Board of Directors. Metabolomics 2026 planning, working to a new financial year, identifying potential locations for Metabolomics 2027 and the election of new Directors being some of the major activities.

As previously announced, Metabolomics 2026 will be hosted in late June in Buenos Aires. We hope to announce the accurate dates in the coming weeks; the delay in this announcement is due to the board ensuring the financial aspects of the conference

are appropriate for the society long-term. We have also received three proposals to host the Metabolomics 2027 conference which will be reviewed by the board in the coming weeks.

It is both a sad and exciting time. I am sad because we have five Directors who have supported and significantly contributed to the society during the last five years standing down – Stacey Reinke, Natasa Giallourou, Kati Hanhineva, Michael Witting and Matej Oresic. The EMN chair, Silvia Radenkovic, has also come to the end of her term. It is a significant commitment to be a Director or EMN chair and both the officers and myself would like to thank all of these individuals, you will be missed! It is exciting that we will have five new Directors joining the board from October 1st and I look forward to welcoming them in the coming weeks when the election is closed.

Stacey has kindly provided some thoughts below of her time as a Director.

When I started the role of Chair (Training Committee) in 2020, there was a lot of appetite for learning support in metabolomics. Novice metabolomics researchers faced a few difficult challenges. First, the multi-disciplinary nature of metabolomics meant that researchers either had to have broad expertise or work as part of a multi-disciplinary team. For many early-career researchers, the latter wasn't an option.

Second, the diversity and complexity of metabolomics meant that researchers couldn't follow standardised workflows. Instead, they had to make context-dependent evaluative judgements. In some cases, it was easier to follow the footsteps of those before, but this didn't always lead to the best outcomes. Finally, teaching in metabolomics was still mainly limited to training courses. While there was ample opportunity to enhance one's skills in specific areas, developing a deep understanding to underpin those skills was more difficult.

The Training Committee members were eager to fill these gaps and support learning in the community. The big question was 'How?'. In volunteer committees, time is a very finite resource. We knew we that developing and delivering content was well beyond the scope of what we could achieve. We also knew that metabolomics was expanding into the formal education space and that we need to lean into that. We spent the first few months brainstorming and working through various options.

One of the first things we did was change the committee's name to the Education & Training Committee. This recognised the important role that both forms of learning had to support the field. We also developed a mission statement to make it clear to the community (and ourselves when we got distracted) what we aimed to do. Shortly thereafter, we really got to work. Our two main successes were publishing a white

paper titled <u>Providing metabolomics education and training: pedagogy and considerations</u> and the launch of a podcast-style webinar series. The podcast provided us an opportunity to fill the evaluative judgement gap – we could discuss questions and challenges with experienced researchers and hear how they would approach tasks or solve problems.

Over the last 5 years, there have been many people who have generously donated their time to this cause. I would like to extend a thank-you to all of them. The EMN Committee joined forces with us by having a couple of members sit on the Education & Training Committee (ETC). We also had several community members join the committee, bringing their enthusiasm and diverse perspectives. Finally, I would like to offer a special thank-you to two people. First, a huge thank-you to Catherine Winder who championed the pedagogy paper. At the time, Cate wasn't an official committee member, but she did an enormous amount of work on the paper. Second, I'd like to thank Nik Rattray for enthusiastically taking the baton from me. I look forward to seeing where the ETC will be in another 5 years.

Finally, mQACC is currently performing a survey on the reporting of concentration data in metabolomics. Please complete the survey below which mQACC assembled to gather data on the processes scientists are currently using to generate and report concentration data.

https://www.surveymonkey.com/r/KP8QZH6

YOU TOO CAN BE A PART OF DEFINING THE FUTURE!

All the very best, Warwick (Rick) Dunn, University of Liverpool, UK President, Metabolomics Society

Early-career Members Network

EMN Elections

We are happy to announce that Breanna Dixon has been elected as the new chair for the EMN 2025-2026 committee and Nicholas Rattray has been elected EMN advisor!

In addition, we are happy to welcome newly elected EMN 2025-2026 committee

members- Renata Garbellini Duft (UK), Maria Llambrich (Spain), Shauni Loopmans (Belgium), Luciana Ribeiro da Silva Lima (Brazil), Dakshat Trivedi (UK), and Carolina Thomaz dos Santos D'Almeida (Brazil)! We extend our gratitude towards our outgoing EMN members Aleš Kvasnička, Loic Mervant, Diana Pinto, Daniela Ramirez, Monique Ryan, Thomas Vial and Simone Zuffa, and wish them all the best in their next endeavors!

We thank once again all the applicants and encourage the unsuccessful candidates to apply next year!

Conference Workshop

The EMN, strengthened by new and highly motivated members, is already back in action to design the EMN Workshop 2026! The success of the recent round tables at the Metabolomics 2025 conference provides a solid basis for defining a key topic for early-career researchers which we hope to further expand into workshop at the next conference!

International Affiliates' Corner

Réseau Français de Métabolomique et Fluxomique (RFMF)

Visit http://www.rfmf.fr/



First Edition of RFMF thematic school: an unforgettable meeting in Sète

It is with great enthusiasm that we look back on the first edition of the Thematic School of the French-Speaking Network of Metabolomics and Fluxomics (#ET01RFMF), held in 2025 in Sète, France. Under the Mediterranean sun, this event brought together around fifty participants in a warm and friendly atmosphere, fostering both learning and collaboration.



A focus on plant metabolome annotation. This inaugural thematic school was dedicated to the annotation of the plant metabolome, a topic of growing importance for the metabolomics community. Through lectures, case studies, and discussions, participants explored strategies, tools, and best practices for tackling one of the key challenges in plant metabolomics: transforming raw spectral data into meaningful biological knowledge.

A rich and inspiring program. The program featured stimulating contributions from experts such as Nicolas Sommerer, Isabelle Schmitz, Alessandra Maia-Grondard, Aécio Luís De Sousa Dias, Massimiliano Corso, David Touboul, Guillaume Marti, Ludovic Cottret, François Perreau, Jean Chrisologue Totozafy, Patricia Homobono, among many others. Their insights and perspectives sparked lively exchanges and inspired new ideas within the community.

Teamwork behind the success. The success of this first edition was also made possible thanks to the dedication of the organising team. We warmly thank our sponsors for their valuable support: Hubert Latappy (LECO), Société Française de Biologie Végétale (SFBV), Saclay Plant Sciences (SPS) and MetaboHUB-Bordeaux Metabolome Facility. Their contribution provided an excellent environment for scientific exchange and strengthened ties within the plant community.

Looking ahead to 2026. This inaugural edition of ET01RFMF, organised by Pierre Pétriacq, has laid the foundations for a rich tradition. The next edition will be organised by Audrey Le Gouellec, and we are already looking forward to continuing this exciting momentum. Until then, RFMF wishes everyone a productive and inspiring scientific

year ahead!

19th Edition of the BBBS Webinar Series – Fluxomics and Isotopy in the Spotlight

The 19th BBBS Webinar Series, organised by RFMF and RFMF Junior, will be held on October 9th, 2025 (3:00–4:30 pm, GMT+1). This edition will spotlight fluxomics and isotopy, with keynote speaker Jean-Charles Portais alongside talks from Audrey Carrière, Denis Jallet, and Koloina Rabemanantsoa.

Free access, no registration required <u>Join here</u> Full program available on the flyer below.



Join the 19th RFMF webinar! 9th October 2025, 3-4:30pm (GMT+1) Fluxomics & Isotopy

Chaired by Lindsay Peyriga & Amandine Rocher
To join the webinar: https://meet.goto.com/381388357

03.00 pm





« Fluxomics : metabolism in action »

Jean-Charles Portais MetaboHUB-MetaToul RESTORE - TBI Toulouse (France)



« Modeling metabolic fluxes to unveil trophic interactions within the drosophila gut microbiota »

Koloina Rabemanantsoa
PhD student, TOXALIM
Team Metabolism and Xenobiotics
Toulouse (France)

4.00 pm



« Bacterial micro-compartements: the tiny wonders of Escherichia Coli »

Toulouse Biotechnology Institute - Team MetaSys
Toulouse (France)

4.15 pm



« Using in vivo isotopic tracing experiments to characterize lactate metabolic fate according to brown/beige adipose tissues activity »

Audrey Carrière

RESTORE – Team METABOLINK

Toulouse (France)

Polish Society of Metabolomics

Visit https://ptmet.pl/



It is our great pleasure to invite you to participate in the

11th Conference of Polish Metabolomic Society[:] Metabolomics Circle 2025 and 5th Poznan Scientific Conference[:] 'Modern Pharmaceutical and Biomedical Analytics in Health Care'

Held in Poznan, Poland, on November 5-7th, 2025

Both Symposia are recognized for a high scientific level. The connection of these two conferences gives a unique opportunity to exchange experiences in the field of metabolomics and its application in biomedical research. The conferences' subject matters will concern new trends in bioanalysis, pharmaceutical and clinical analytics, and the analysis of raw materials of natural origin. The proposed combination of topics will bring together experts, innovators, and leaders from omic sciences.

Our invitation is especially directed to life scientists, pharmacists, physicians, analysts, clinicians, pharmacologists, biochemists, pharmacognostists, and chemists specializing in the use of the modern omics methods in current medicine and pharmacy, with particular emphasis on health prevention and treatment activities.

We are also excited to host high-level lectures, panel discussions, and poster sessions. The event will offer ample opportunities for networking, knowledge exchange, and collaboration with researchers and professionals.

Please save the date in your calendars. You may also follow our website: https://metabolomics2025.bok-ump.pl/

We would be honored by your participation and look forward to welcoming you to Poznan.

Warm regards,
Organizing Committee

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Metabolnterview

Devanshi Pandit



Devanshi Pandit is a researcher with a passion for metabolomics and the gut microbiome. She first became interested in the field during her undergraduate studies, where she worked on biomarker discovery for chronic diseases. That experience opened her eyes to the potential of metabolites as powerful indicators of health and disease. Currently, she is focused on developing an artificial gut system to simulate gastrointestinal conditions in a controlled environment, with the goal of studying how new drugs, diets, and diseases affect microbial activity and metabolite production. Her

long-term vision is to bridge the gap between bench research and patient care by using metabolomics tools to accelerate discoveries in personalized medicine.

1. Could you share your journey into metabolomics and what initially sparked your interest in this field?

My journey into metabolomics really began during my undergraduate years. I was working on research focused on biomarkers for chronic diseases, and that was the first time I was introduced to the world of metabolites and their role in health. What struck me was how metabolites aren't just tiny molecules floating around but they tell a story about what's happening inside the body at any given moment. From there, I started seeing how metabolomics touches almost every part of biology: organ function, immunity, the microbiome, even disease progression. That realization is what pulled me in. It felt like opening a door into a whole new way of understanding the human body and its connections to health and disease.

2. What inspired you to focus on metabolomics in the context of gut microbiota?

The gut has always fascinated me because it's not just an isolated system, it's deeply interconnected with the rest of the body. The gut—brain axis is a perfect example as it shows how what happens in your gut can influence mood, cognition, and overall mental health. Beyond that, the gut plays a huge role in immunity and metabolic health. What inspired me was realizing that metabolomics gives us a way to actually measure and understand these interactions. By looking at metabolites, you can see how microbes and the host "talk" to each other, and that's such a powerful tool for figuring out how the gut impacts our broader health.

3. What other key metabolomics projects are you currently pursuing or look forward to pursuing in the future?

Right now, my biggest focus is building an artificial gut system. The goal is to create a controlled environment that mimics the human gastrointestinal system so we can test

and study things in a way that would be impossible in humans directly. I'm really excited about the applications! For example, seeing how new drugs interact with the microbiome, or how diseases shift microbial metabolism. Looking ahead, I'd love to use this system to explore organ-to-organ communication through metabolites, like how gut-derived molecules affect the brain or liver. It's one of those projects that feels like it could keep expanding the more you think about the possibilities.



Artificial Gut

4. What are some common challenges you've faced working with metabolomics data, and how have you addressed them?

Since I haven't directly analyzed metabolomics datasets yet, I can't say I've personally run into those challenges but I've seen how tricky it can be. From talking to colleagues and reading in the field, a couple of things stand out. First, the datasets are massive and very complex, which makes them hard to interpret without strong computational tools. Second, there's often a reproducibility challenge making sure results are consistent across labs and platforms. For me, the way I'm preparing to tackle these challenges is by building collaborations with people who have that data expertise, and also making sure I'm familiar with the workflows that connect sample preparation to data interpretation. Even though I'm not knee-deep in the data yet, I see myself as building the systems and tools, like the artificial gut, that generate high-quality samples for those analyses.

5. How does metabolomics help in identifying new metabolites or biomarkers relevant to gut health and disease?

I think this is one of the most exciting aspects of metabolomics. It's basically like having a window into the chemical language of the gut. Metabolites tell you what the microbes are producing, how the host is responding, and what might be shifting in disease. This means metabolomics can pick up on subtle signals that other techniques might miss. For gut health specifically, those metabolites can act as biomarkers of dysbiosis, inflammation, or even treatment success. In the bigger picture, metabolomics isn't just about identifying markers but it's about helping us connect biology to clinical outcomes in a very concrete way.

6. What technological advancements do you believe will shape the future of metabolomics?

I think automation and artificial intelligence are going to completely change the landscape. Automation is important because metabolomics is still very hands-on, and sample preparation in particular can slow things down. Having more automated platforms will make the process faster, more reproducible, and easier to scale up. On the other side, Al is going to be huge for data interpretation. These datasets are massive, and Al has the potential to pick up subtle, complex patterns that humans wouldn't be able to find on their own. Together, these technologies will make metabolomics more powerful and more accessible, opening it up to labs that don't currently have the bandwidth to take it on.

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

In the near term, I see the artificial gut being used in research labs to speed up discoveries about gut health. It could be used to test how certain drugs interact with the microbiome before moving to clinical trials, or to study how diseases alter microbial activity in a way that affects the host. Longer term, I'd love to see systems like this being used for personalized testing. Imagine being able to predict how your

own microbiome might respond to a diet, a probiotic, or a medication before you even try it. That's the kind of future application I think metabolomics can help make possible.

8. What resources or tools have you found most helpful in your metabolomics studies?

A mix of tools and collaborations has been really important. On the technical side, platforms like LC–MS and NMR are essential for capturing metabolites, and databases like HMDB are incredibly useful for identifying them. But honestly, I've found the most valuable resource to be collaboration. Metabolomics is such a cross-disciplinary field that you need engineers, biologists, and computational experts all working together. Having access to mentors and colleagues who can fill in the gaps has been just as helpful as any instrument or software.

9. What excites you most about the intersection of engineering and biology in your artificial gut project?

What excites me is how engineering allows us to take something as complex as the human gut, a system we can't directly control or fully observe in real time, and recreate its conditions in the lab. By building an artificial gut, I get to bring engineering precision into biology, which means we can test hypotheses in a much more controlled way. I love that it's not just one discipline driving this project, but a blend of biology, chemistry, and engineering all working together. That intersection is where the most innovative discoveries happen.

10. How do you hope your work will contribute to the future of personalized or precision medicine?

My hope is that the artificial gut becomes a tool that can help bridge the gap between research and patient care. For example, in precision medicine, one of the big challenges is predicting how different people will respond to a drug or even a diet. By modeling gut conditions outside the body, we could test those responses in advance

and generate metabolomics data that guide treatment decisions. Long-term, I'd love to see systems like this being used to design more personalized therapies where medicine isn't one-size-fits-all but tailored to each person's unique microbiome and metabolic profile.

11. If you had unlimited resources, what experiment or study would you love to do?

If I had unlimited resources, I would love to run a large-scale, longitudinal study that connects the artificial gut to real-world patient data. Imagine being able to take samples from individuals, recreate their gut conditions in the lab, and then test how their unique microbiome responds to different drugs, diets, or environmental exposures. Pairing that with metabolomics and AI analysis could give us an unprecedented level of insight into how gut metabolism influences human health over time. It would be a massive undertaking, but it could completely transform how we approach personalized medicine.

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MetaboReads

Methodological Advances in Metabolomics and Data Integration

High-quality measurement and synthesis methods continue to set the pace for discovery. The papers collected here extend NMR sensitivity with hyperpolarization, formalize meta-analysis for compositional microbiome data, and push nontarget HRMS toward confident elemental patterning using machine learning. They also illustrate how to combine molecular networking with multivariate statistics to read complex botanical pharmacology in vivo. Collectively, these studies reduce technical bias, raise detection ceilings, and make heterogeneous datasets interoperable, which is precisely what the field needs to translate signal into mechanism.

Semi-Targeted Nuclear Magnetic Resonance Metabolomics via Parahydrogen-Induced Hyperpolarization for Enhanced Sensitivity to Metabolic Composition

Posthumus and colleagues in JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

showed that non-hydrogenative parahydrogen-induced polarization (nhPHIP) can be used in a semi-targeted NMR workflow to quantify metabolites in human urine with submicromolar sensitivity. They extended prior nhPHIP work on α-amino acid motifs by applying 2D nhPHIP to patients with pyridoxine-dependent epilepsy, a setting where diagnostic biomarkers are dilute. The signal enhancement, coupled with 2D spectral resolution, delivered superior sensitivity to metabolic composition relative to conventional ^1H NMR. The approach enabled detection and quantification of multiple metabolite classes in complex mixtures that would otherwise be below NMR limits. The study positions nhPHIP-NMR as a practical addition to metabolomics for low-abundance biomarkers.

Melody: meta-analysis of microbiome association studies for discovering generalizable microbial signatures

Wei and colleagues in GENOME BIOLOGY developed Melody, a meta-analysis framework that harmonizes study-specific summary statistics to identify robust microbial signatures across heterogeneous cohorts. Through realistic simulations, they demonstrated superior true-positive prioritization and stability compared with existing microbiome meta-methods. Applications to five colorectal cancer datasets and eight gut metabolome studies showed that Melody-derived signatures generalize and predict better across studies. The framework explicitly respects compositional constraints and reduces instability from batch and protocol differences. This provides a reproducible path to cross-study microbial markers suitable for translation.

Interpreting metabolic profiling of YIV906 in vivo: A Synergistic strategy combining LC-HRMS-based molecular networking and metabolomics thought integration

Li and colleagues in JOURNAL OF CHROMATOGRAPHY A showed that feature-based molecular networking integrated with multivariate metabolomics resolves complex in vivo metabolism of the botanical candidate YIV906. By coupling a self-built prototype compound database and the Biotransformation module in Compound Discoverer with GNPS networking, they identified 63 parent components and 180 metabolites across rat plasma and tissues. The strategy clarified chemical families spanning flavonoids, organic acids, monoterpenoids, triterpenoids, and alkaloids, and mapped tissue distributions. The workflow overcame typical interference from endogenous backgrounds that confound herbal mixture studies. This generalizable pipeline should aid pharmacokinetic deconvolution of multicomponent therapeutics.

Machine Learning-Assisted Recognition of Environmental Sulfur-Containing Chemicals in Nontargeted Mass Spectrometry Analysis of Inadequate Mass Resolution

Low and colleagues in ACS ENVIRONMENTAL AU found that machine learning applied to HRMS spectra at resolutions as low as 25,000 can accurately recognize sulfur isotope patterns and predict sulfur atom counts. Trained on 200 sulfur standards spiked into complex matrices, the models achieved 87–95% accuracy for recognition and 86–97% for count prediction in both ESI polarities. Deployed as the SulfurFinder R program, the method recovered all previously reported 2-mercaptobenzothiazole disinfection byproducts in an external dataset and tentatively identified 169 sulfur features in wastewater, confirming

several pharmaceuticals. By upgrading elemental patterning at routine resolutions, the approach expands exposomics coverage without hardware changes.

Host–Microbiome Metabolic Interactions and Environmental Physiology

These studies chart how symbionts, parasites, and environmental stress remodel host energy budgets and physiology. From gut bacteria that supply glycolytic intermediates in cold bees to parasites that impose subtle but compounding energetic debts in mussels, metabolism proves to be the shared currency. Human-relevant physiology also appears, with intermittent hypoxia linking taxa, lipids, and clinical indices. Across systems, coordinated shifts in carbohydrate, lipid, and organic acid pathways emerge as the proximate mechanisms of adaptation or cost.

Honeybee-Gilliamella synergy in carbohydrate metabolism enhances host thermogenesis in cold acclimation

Tang and colleagues in NPJ BIOFILMS AND MICROBIOMES found that the gut symbiont Gilliamella enriches carbohydrate fluxes that bolster thermogenesis in cold-adapted honeybees. Comparative metagenomics showed enrichment of Gilliamella in Apis mellifera and A. cerana from colder climates, with genomic capacity favoring glucose, pyruvate, lipid, and glucuronate processing. Mono-colonization experiments increased activity, body temperature, and fat storage under cold exposure, with saccharide metabolomics revealing higher hindgut glucose and coordinated utilization of glucose and pyruvate. Transporter repertoires suggested preferential ascorbate uptake and conversion to xylulose-5-phosphate, promoting lipogenesis while limiting competition for host glucose. The work reveals a complementary host–microbe division of labor that supports energy acquisition during cold stress.

Correlation between gut microbiota and metabolomics under intermittent hypoxic conditions

Zeng and colleagues in BMC MICROBIOLOGY showed that chronic intermittent hypoxia associated with obstructive sleep apnea correlates with distinct gut microbial and metabolite signatures linked to disease severity. Mouse and human data indicated increased Firmicutes and Tenotrophomonas, decreased Bacteroidota and Ligilactobacillus, and elevations of nervonic and erucic acids with lower arachidonic acid. Clinical indices such as apnea—hypopnea index and blood cell differentials tracked with specific taxa and lipids. Targeted metabolomics and 16S data converged on associations between hypoxia, membrane lipid remodeling, and inflammation. These correlations nominate microbiome—lipid axes as candidate biomarkers for OSA assessment.

<u>Transcriptomics and Metabolomics Analyses Reveal How Rhizobacteria Acinetobacter</u> <u>calcoaceticus Enhance the Growth and Stress Tolerance in Lespedeza davurica</u>

Liang and colleagues in AGRONOMY-BASEL found that inoculation with the phosphatesolubilizing rhizobacterium Acinetobacter calcoaceticus DP25 substantially improved growth and stress tolerance of Lespedeza davurica in saline-alkali soils. Field-relevant gains included 48% taller plants, 103–132% higher biomass, and large increases in root architecture metrics. Antioxidant capacity rose while malondialdehyde and proline decreased, indicating lower oxidative stress. Integrated omics highlighted enrichment in carotenoid biosynthesis, ABC transporters, pentose and glucuronate interconversions, and coordinated increases in secondary metabolites. The data support a multi-pathway mechanism by which DP25 enhances nutrient mobilization, photoprotection, and stress resilience.

Physiological costs of infection by the invasive parasitic copepod Mytilicola intestinalis accumulate across temporal scales in the blue mussel Mytilus edulis

Demann and colleagues in JOURNAL OF INVERTEBRATE PATHOLOGY showed that sublethal energetic costs of Mytilicola intestinalis infection compound over time to impair fitness in Mytilus edulis. Stable isotope analyses across seasons evidenced direct parasite consumption of host tissue, while elevated heart rates and amino acid metabolism shifts measured by ^1H NMR reflected increased repair demands. Laboratory and field follow-up connected these short-term changes to lower body condition over months and slower growth over one year. With regional prevalences exceeding 70%, the parasite's cumulative energetic draw can scale to population impacts. The study exemplifies how small metabolic reallocations integrate into meaningful life-history consequences.

Metabolomics in Neurology and Aging

The nervous system remains a proving ground for metabolomics, from genotype-conditioned bioenergetics to multi-omic markers of frailty and botanical interventions in stroke. These papers link acylcarnitine ratios, branched-chain amino acid utilization, and inflammatory proteo-lipoprotein profiles to resilience and risk. They also explore how complex mixtures may act through vascular and trophic signaling. The throughline is energy management under stress and the value of convergent markers across species and cohorts.

APOE genotype influences on the brain metabolome of aging mice – role for mitochondrial energetics in mechanisms of resilience in APOE2 genotype

Borkowski and colleagues in MOLECULAR NEURODEGENERATION found that APOE genotype shapes brain metabolomic trajectories with aging, implicating mitochondrial energetics and BCAA utilization in APOE2-linked resilience. Targeted metabolomics across humanized APOE mice showed age-related shifts in acylcarnitines, amino acids, and lipids, with decreased medium-to-long-chain acylcarnitine ratios suggesting impaired β-oxidation. Aging APOE2/2 mice displayed altered BCAA profiles and increased C5 acylcarnitine, consistent with enhanced anaplerosis into the TCA cycle. Human dorsolateral prefrontal cortex data mirrored lower markers of impaired BCAA catabolism in APOE2/3 carriers. The work ties protective genotype to flexible substrate use as fatty acid oxidation declines.

Extreme MetaboHealth scores in three cohort studies associate with plasma protein markers for inflammation and cholesterol transport

Bizzarri and colleagues in IMMUNITY & AGEING showed that extreme values of a mortality-risk metabolomics score co-vary with plasma proteins marking inflammation and HDL remodeling. Across individuals from the Leiden Longevity and Rotterdam studies and discordant monozygotic twins, high (poor-health) scores aligned with elevated cytokines (GDF15, IL-6, MIG), increased inflammatory proteins (CRP, LBP, HPT), and reduced HDL-related proteins (APOA1/2/4, TETN). Twin analyses indicated moderate heritability of the score ($h^2 \approx 0.4$), but many protein associations persisted within monozygotic pairs, limiting a genetic explanation. The pattern supports a mechanistic link between metabolic frailty, sterile inflammation, and impaired cholesterol transport. These markers could refine risk stratification beyond metabolite panels alone.

Multi-omics reveals Fuyuan Xingnao Decoction's therapeutic mechanism in cerebral infarction via gut microbiota and JAK2-STAT3 pathway

Wan and colleagues in JOURNAL OF ETHNOPHARMACOLOGY found that the traditional formula FYXN reduces infarct size and improves neurological outcomes in rodent stroke, potentially through gut-derived short-chain fatty acids and activation of JAK2–STAT3 signaling. Metabolomics, network pharmacology, transcriptomics, and proteomics converged on targets including JAK2, STAT3, and EGFR, with increased p-STAT3 and VEGF and reduced caspase-3 in treated brains. 16S profiling showed stroke-associated declines in microbial diversity, while butyrate levels correlated inversely with neuronal damage and tracked improvements in functional scores. In vitro, FYXN enhanced proliferation of brain microvascular endothelial cells. These results motivate controlled clinical evaluation of vascular and microbiota-mediated mechanisms.

Plant and Algal Stress Metabolism and Agronomic Interventions

Plant and algal systems in these studies illustrate how redox control and carbon flow govern both growth and defense. Micronutrient inputs such as selenium, along with signaling molecules like melatonin, reshape photosynthesis, antioxidant capacity, and lipid-derived hormone pathways to rebalance resources under stress. Macroalgae accommodate salinity extremes by adjusting energy metabolism, pigment and carotenoid biosynthesis, and transporter activity, maintaining performance despite large osmotic shifts. Across species, these interventions impose recognizable trade-offs, including delayed flowering when immunity is prioritized, but they also reveal practical levers for cultivation and crop protection. The common message is that targeted tuning of sugar metabolism, lipid signaling, and antioxidant networks can convert environmental stress into manageable operating conditions.

Effects of organic selenium on metabolic responses and disease resistance in rose plants

Bian and colleagues in JOURNAL OF HAZARDOUS MATERIALS found that organic selenium augments disease-resistance signaling in roses while constraining flowering. Integrated physiological, transcriptomic, and metabolomic analyses showed elevated ABA and jasmonate in flowers with rising Se, along with upregulation of pentose phosphate cycle

genes and metabolites such as D-gluconate and glucose that prime induction. Se application remodeled linoleic and α-linolenic acid pathways via LOX2S and AOS, linking fatty acid oxidation to JA synthesis. Low Se doses improved photosynthesis through enhanced electron transport components and ATP synthase subunits. The data reveal an immunity–flowering trade-off, suggesting careful dose control for green agriculture.

Physiological, transcriptomic, and metabolomic analyses reveal the adaptation mechanism of Gracilaria tenuistipitata var. liui under long-term salt stress

Li and colleagues in ENVIRONMENTAL AND EXPERIMENTAL BOTANY showed that the macroalga Gracilaria tenuistipitata tolerates a wide salinity range via coordinated regulation of energy metabolism, photosynthesis, and antioxidant defenses. Growth and photosynthetic capacity shifted with both hypo- and hypersaline exposure, with stronger tolerance under hypo-salinity. Transcriptomics identified thousands of DEGs, with enrichment in nitrogen metabolism, amino acid biosynthesis, betalain and carotenoid pathways at low salinity, and ABC transporters at high salinity. Metabolomics detected 25 key metabolites and showed S5 profiles more similar to control than S60, aligning with physiological resilience in dilute conditions. These mechanisms explain the species' ecological range and inform cultivation.

Systemic role of melatonin in enhancing temperature stress tolerance in fenugreek

Gharanjik and colleagues in BMC PLANT BIOLOGY found that exogenous melatonin, particularly at 60 ppm, improves fenugreek performance under heat and cold by tuning antioxidant systems, hormones, and energy status. Treatments increased photosynthetic pigments, lowered electrolyte leakage and malondialdehyde, and boosted total protein, indicating reduced oxidative damage. Cross-talk with nitric oxide, hydrogen sulfide, and cysteine pathways maintained redox potential and water balance. Energy metabolism improved through higher ATP content, cellular energy charge, and ATPase activity, while hormonal balance shifted toward ABA and auxin. Upregulation of diosgenin pathway genes linked stress mitigation to valuable secondary metabolite production.

Foodomics and Natural Products: Composition, Traceability, and Flavor Formation

Food systems research is increasingly multi-omic and systems-aware. This set ranges from regulatory-aware traceability frameworks to metabolomic dissection of traditional foods and high-value fungi and medicinal fruits. The common contribution is a move from lists of compounds to pathway-level understanding that can guide quality control, segment-specific harvesting, and authentication across complex supply chains.

Agri-food traceability today: Advancing innovation towards efficiency, sustainability, ethical sourcing, and safety in food supply chains

Rossi and colleagues in TRENDS IN FOOD SCIENCE & TECHNOLOGY showed that robust traceability depends on harmonizing regulatory frameworks with analytical and digital technologies spanning proteomics, metabolomics and volatilomics, stable isotopes, AI,

blockchain, IoT, and food contact materials. They propose a taxonomy by technological maturity and data granularity, mapping tools to use-cases across supply chains. Case studies in wine, garlic, and coffee illustrate combined chemical and digital fingerprints for authentication and provenance. The review emphasizes best practices for end-to-end efficiency that supports consumer trust and public health. It offers a roadmap for technology selection and integration under real regulatory constraints.

<u>Unveiling the formation mechanism of characteristic components in steam pot chicken soup</u> with sanchi-ginseng based on HPLC, GC-MS combined with metabolomics

Du and colleagues in FOOD CHEMISTRY-X found that the combined chicken—ginseng preparation produces distinctive flavor chemistry through fatty acid release and specific metabolite shifts. HPLC and GC-MS showed reduced ginsenoside levels in the combined soup relative to ginseng alone, while free fatty acids rose compared with either component alone. UHPLC-Q-Exactive metabolomics identified 13 shared differential metabolites and implicated amino acid and fatty acid metabolism as key pathways. The integration explains how protein–lipid interactions and herbal constituents shape sensory attributes. These findings provide actionable levers for process control in traditional foods.

<u>Wide-target metabolomics and network pharmacology reveal metabolic regulation and targets of bioactive compounds in antler-shaped Ganoderma lucidum</u>

Luo and colleagues in FOOD BIOSCIENCE showed that antler-shaped Ganoderma lucidum exhibits region-specific metabolite distributions that can guide segmented harvesting. UPLC-MS/MS identified 1,016 metabolites and 615 differentials across cap, stalk, and base, with KEGG assigning 353 pathways. The undifferentiated cap accumulated triterpenes, while the base was richer in polysaccharides. Network pharmacology linked saccharide and terpenoid differentials to 41 key human targets, supporting rational extraction for nutraceuticals. The study connects developmental anatomy to bioactive yield optimization.

Multi-omics dissection of metabolic and transcriptional regulation underlying fruit maturation in Panax ginseng

Bian and colleagues in BMC PLANT BIOLOGY found stage-specific waves of ginsenosides, phenolics, and progressively rising flavonoids and anthocyanins during ginseng fruit maturation. Integrated metabolome—transcriptome maps delineated primary and secondary metabolic shifts along with ABA, GA, and brassinosteroid signaling modules. MYB, bHLH, and ERF transcription factors coordinated these transitions, as revealed by co-expression network modules tied to metabolite clusters. The atlas provides targets for breeding or process interventions to enhance nutritional and medicinal quality. It serves as a template for developmental metabolomics in other medicinal fruits.

Clinical Biomarkers and Immune-Vascular Interfaces

Two studies illustrate how targeted and nontargeted metabolomics can yield clinically actionable signatures in toxicology and complex autoimmunity in pregnancy. Both emphasize careful statistical modeling, orthogonal validation, and pathway-level interpretation. The arc

runs from discovery to diagnostic potential, with a focus on immune and vascular pathways that translate to practice.

<u>Identifying Metabolic Signatures of Bisphenol Analog Exposure: Implication for Rapid Toxicity Screening of New Alternatives</u>

Kuang and colleagues in ENVIRONMENTAL SCIENCE & TECHNOLOGY found that plasma metabolomics combined with molecular docking can identify robust biomarkers of exposure to bisphenol substitutes. Across BPAF, BPB, and BPAP exposures, hundreds of metabolites shifted, with kynurenine and histidine serving as shared signatures. A composite histidine/kynurenine ratio achieved an AUC of 0.937 and accuracy of 0.820 for classifying exposure, outperforming either metabolite alone. Docking suggested that metabolic disruption scales with receptor binding of parent compounds versus detoxified transformation products, linking biotransformation to effect modulation. The study proposes a rapid screen for the safety evaluation of emerging bisphenols.

<u>Untargeted metabolomics reveals the metabolic characteristics and biomarkers of obstetric antiphospholipid syndrome and undifferentiated connective tissue disease</u>

Li and colleagues in FRONTIERS IN MOLECULAR BIOSCIENCES showed that LC-MS serum metabolomics discriminates OAPS, UCTD, their overlap, and healthy controls with ion-mode-specific signatures. From 1,227 detected metabolites, PLS-DA in positive mode yielded the best group separation, with candidates including 17(S)-HpDHA, 4-methyl-5-thiazoleethanol, and 3-hydroxybenzoic acid depending on the comparison. Enrichment analyses highlighted immune-linked pathways and lipid mediators aligned with vascular and inflammatory biology. The work nominates several metabolites as early diagnostic markers and frames an immunity-metabolism-vasculopathy axis for obstetric disease. Future validation should standardize ion modes and control for treatment effects to move toward clinical assays.

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The Metabolomist Podcast



New episode

Bacterial metabotypes & the medicine of tomorrow

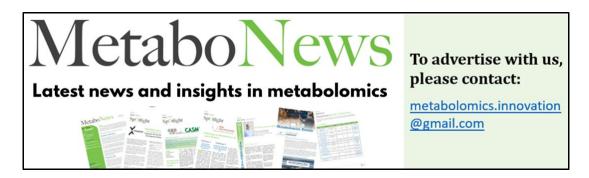
For me, the central dogma needs to be revisited. We think that everything comes from genes, but maybe everything comes from metabolites!

Because without certain pools of metabolites, we couldn't have transcription and translation.

- Audrey Le Gouellec

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Metabolomics Events

DGMet Annual Meeting 2025

October 1 - 2, 2025

Venue: Hanover, Germany

The DGMet Annual Meeting 2025 will take place at the Fraunhofer Institute for Toxicology and Experimental Medicine Fraunhofer ITEM in Hanover.

Key Topics:

Metabolomics and Nutrition
Exercise & Muscle Metabolism

Computational Metabolomics
Plant Metabolomics
Metabolomics and Lipidomics in Health and Disease

Visit the website for more details

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Bits & Bites #6: Using MetaboAnalyst for Metabolomics Statistics and Data Visualizations October 9, 2025

Venue: Online

The short course is taught by Dr. Jeff Xia from McGill University. This introductory-level session requires basic knowledge of computer skills, and no programming experience is necessary.

Short description of the course:

They 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.

Check for more details

2025 World Critical Care and Anesthesiology Conference

October 10 - 11, 2025

Venue: Singapore/Hybrid Online

The 9th World Critical Care & Anesthesiology Congress (2025 WCAC) will take place in Singapore, offering both physical and virtual participation options. Speakers and delegates will have the chance to meet international faculty members, enjoy extensive networking sessions and explore the city's landmarks. The congress invites submission of speaker proposals as well as oral and poster presentations on the latest topics in critical care and emergency medicine, anesthesiology and pain medicine, trauma, pediatrics, neurocritical and cardiac critical care, COVID-19 and related subjects.

Check for more details

MANA SODAMeet

October 14, 2025

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

Frontiers in Metabolomics & Metabolomic Imaging in Medicine: Challenges & Opportunities

October 16 - 18, 2025

Venue: Italy

This inaugural Metabolomics and Metabolomic Imaging (MMI) workshop is designed for scientists, clinicians, and trainees from academia, healthcare, and industry, who seek to learn and discuss the frontiers of metabolomics in medicine. The central focus of this workshop is medical metabolomics and metabolomic imaging, a burgeoning field with enormous potential for medical applications, particularly in the context of malignant and neurodegenerative diseases, which can present heterogenous systematic metabolic alterations that can only be collectively evaluated by metabolomics.

Learning Outcomes

- Identify technologies used in metabolomics and metabolomic imaging
- Understand the challenges and potential of metabolomics and metabolomic imaging for malignant and neurodegenerative disease studies
- Become familiar with advanced metabolomic data analysis using Al and machine learning

Check for more details

Bits & Bites #7: GNPS2 for Metabolomics Analysis, Annotation Propagation, and Visualization

October 23, 2025

Venue: Online

The short course is taught by Dr. Mingxun Wang, UC Riverside. This intermediate-level session requires GNPS Account, and no programming experience.

Check for more details

Introduction to Applying GC-MS in Untargeted Metabolomics

October 27-29, 2025

Venue: Liverpool, United Kingdom

Join the hands-on course offering practical training in GC-MS for untargeted metabolomics. Participants will gain foundational knowledge of metabolomics, explore experimental design, learn best practices for sample preparation and apply hands-on data acquisition using the LECO Pegasus BT 4D GC x GC-ToF MS, data processing and analysis. Designed for small groups to maximize instructor interaction and laboratory experience, the course equips attendees with the confidence and skills to apply GC-MS in their own research.

Visit the website for more details

EBRAINS Summit 2025

December 8 - 11, 2025

Venue: Brussels

The EBRAINS Summit 2025 will feature scientific talks with leading experts, a public day, a science slam, poster sessions, and a science market exhibition - all focused on advancing digital neuroscience. This year's programme includes a special joint day with the International Neuroinformatics Coordinating Facility (INCF).

Exhibitors will have the opportunity to showcase their work and engage with Europe's neuroscience and brain tech community.

Visit the website for more details

Metabolomics in Life Science 2026

January 27 - 28, 2026

Venue: Vävenscenen, Umeå, Sweden

Umeå University invites participants to explore the latest NMR- and MS-based metabolomics research from Sweden, the Nordics, and beyond. The conference will cover topics such as clinical and precision medicine, plant metabolomics, spatial and single-cell metabolomics, multi-omics, and computational/AI applications.

The program features six keynote speakers from leading institutions and an industry exhibition showcasing cutting-edge technologies and services in metabolomics research.

Learn more and register here

World Critical Care & Anesthesiology Conference 2026 (WCAC26)

March 6 - 7, 2026

Venue: Bangkok, Thailand

The 10th WCAC brings together professionals from around the globe to advance knowledge and expertise in Critical Care Medicine and Anesthesiology. Hosted in partnership with leading societies, this hybrid event offers an essential platform for multidisciplinary exchange, case discussions, and research in critical care and perioperative medicine. The conference's theme, "Advancing Patient Care in a Rapidly Evolving Field," reflects its commitment to sharing impactful insights and innovative solutions to complex clinical challenges. The event rotates worldwide and fosters collaboration among surgical and medical teams dedicated to improving patient outcomes.

Visit the website for more details

2026 Prague Metabolism and Signaling Symposium

June 24 - 27, 2026

Venue: Prague, Czech Republic

Discover the latest breakthroughs at the intersection of metabolism and signal transduction research. This international meeting in Prague features sessions on energy and metabolite sensing, organellar signaling, autophagy, aging, cancer, immune and stem cell metabolism, and host-pathogen interactions. Expect a diverse lineup of about 30 speakers, including two keynote addresses, covering topics from human studies to structural biology. The event also offers networking opportunities and the chance to experience beautiful Prague.

Check for more details

Metabolomics Jobs

Metabolomics Jobs

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Job Title	Employer	Location	Source
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Research Associate II - Metabolomics	Broad Institute of MIT and Harvard	Cambridge, MA, USA	Broad Institute

Senior Research Scholar - Mass Spectrometry Metabolomics	North Carolina State University	Raleigh, NC, USA	North Carolina State University
Research Associate Principal	Berkeley Lab	Berkeley, CA, USA	Lawrence Berkeley National Laboratory
Post Doctoral Fellow Research - American Elderberry Metabolomics (Dr. Lloyd Sumner's Lab)	University of Missouri- Columbia	Columbia, MO, USA	<u>University of</u> <u>Missouri-Columbia</u>
Manager, Quantitative Metabolite Analysis Center	University of California, San Francisco	San Francisco, CA, USA	UC San Francisco
Postdoctoral Fellow – Metabolomics, Proteomics, Exposomics, and Biology	Metabolomics & Department of Chemistry,	University of British Columbia, Vancouver, BC, Canada	University of British Columbia
Post-Doctoral Research Fellow	MITACS and Nova Medical Testing Inc	University of Alberta, Edmonton, AB, Canada	<u>University of</u> <u>Alberta</u>

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