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# MetaboNews

### This month in metabolomics

August, 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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## 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**

**Board of Directors Election – Voting Now Open!** 

All members of the Metabolomics Society are welcomed and encouraged to participate in the 2025 Board of Directors election. Voting is open now through **September 17, 2025** at 11:59pm USA CST.

There are (6) open positions on the Board this year, making your votes very important. Please ensure your votes represent geographical and gender diversity to ensure the Society represents all continents and genders.

#### **HOW TO VOTE:**

- You must be a current member of the Society.
- If you have not signed up for membership in 2025, sign up here: 2025 Membership.
- If you are currently a member, proceed directly to the <u>election poll</u> and enter your membership credentials.

This is a crucial election year, you can place (6) votes as there are (6) open positions.

You're encouraged to review the nominee biographies. Your voice counts! Please contribute to shaping the future of our Society by voting.

### TASK GROUPS CORNER

### **Diversity, Equity and Inclusion Task Group**

The DEI survey is still open, and we want to hear from you!

We're working toward a more diverse, inclusive, and equitable metabolomics community, and your input is essential.

Please take a few minutes to complete our survey and help shape our future initiatives: <a href="https://docs.google.com/forms/d/e/1FAlpQLSdKrVc8xfYCSycYgr9fmEtCJNR63IzEKB2F-vRIROg-YO29YQ/viewform?usp=header">https://docs.google.com/forms/d/e/1FAlpQLSdKrVc8xfYCSycYgr9fmEtCJNR63IzEKB2F-vRIROg-YO29YQ/viewform?usp=header</a>

Your voice matters. Let's continue building a stronger, more inclusive community—together.

Thank you to everyone who has already shared their voice through the DEI survey. We truly appreciate your input!

### **International Affiliates' Corner**

### Metabolomics Association of North America (MANA)

Visit <a href="https://metabolomicsna.org">https://metabolomicsna.org</a>

email <u>mana@metabolomicsna.org</u>

LinkedIn @MANA (Metabolomics Association of North America)

X @MetabolomicsANA

MANA is gearing up for its <u>7th Annual Conference</u> that will take place September 2-5, 2025, at the Banff Centre for Arts and Creativity, Alberta, Canada! The event is sold out! Looking forward to interacting with our membership.

In other news, the MANA NMR IG has been working on a standardized reporting manuscript which will be published soon!

A warm congratulations also our **Early Career Member Awardees**:

- Early Career Scientist Awardees: Drs. Prasanna Vadhana Kumaar Ashok (Buck Institute for Research on Aging), Mauricio Caraballo (MSCollaboratory, UC San Diego)
- Postdoctoral Fellow Awardees: Drs. Courtney Christopher (University of Tennessee, Knoxville), Maribel Okiye(Harvard Medical School), Mengyuan Ren (Emory University), and Helena Mannochio Russo (UC San Diego);
- Graduate Student Awardees: Hannah Heath (University of Illinois Urbana-Champaign), Sathya A. Amarasena(Memorial University), and Youran Tan (Emory University).

As always, please check the <u>MANA website</u> for the latest details and <u>our job board</u> for open positions and scientists looking for job opportunities in metabolomics.

### **Polish Society of Metabolomics**

Visit <a href="https://ptmet.pl/">https://ptmet.pl/</a>



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

11<sup>th</sup> Conference of Polish Metabolomic Society

Metabolomics Circle 2025 & 5<sup>th</sup> Poznan Scientific Conference

'Modern Pharmaceutical and Biomedical Analytics in Health Care'

### Held in Poznan, Poland, on November 5-7<sup>th</sup>, 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: <a href="https://metabolomics2025.bok-ump.pl/">https://metabolomics2025.bok-ump.pl/</a>

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

Warm regards,
Organizing Committee

### **Thailand Metabolomics Society (TMS)**

Visit <a href="https://thailand-metabolomics.org/">https://thailand-metabolomics.org/</a> Sakda Khoomrung (sakda.kho@mahidol.edu)

### **Upcoming Conference Announcement**

The 3rd Thailand Metabolomics Association Conference November 10–12, 2025 Khon Kaen University Science Park, Khon Kaen, Thailand

Theme: Metabolome-Microbiome in Health & Diseases for One Health

This international conference will bring together leading scientists and young investigators to discuss the latest advances in metabolomics, microbiome research, and their integration for precision medicine and One Health.

### Plenary Speakers include:

- **Prof. Jeremy Nicholson** (Murdoch University, Australia)
- **Prof. Ron Heeren** (Maastricht University, The Netherlands)
- **Prof. Hiroshi Tsugawa** (Tokyo University of Agriculture and Technology)
- Prof. Jianhong Ching (Shanghai Jiao Tong University, China)
- Prof. Jia Li (Imperial College London, UK)
- Prof. Zhigang Liu (Shanghai Jiao Tong University, China)
   ...and many more.

Highlights include plenary lectures, workshops, poster sessions, and networking opportunities with global leaders in metabolomics and microbiome science.

Conference Website & Registration: conference.thailand-metabolomics.org



# Siriraj Launches "SiMPC Services": A Premier Biomolecular and Phenomics Research Facility in Thailand

16 July 2025 – The Faculty of Medicine Siriraj Hospital, Mahidol University, officially launched **SiMPC Services**, a state-of-the-art research unit under the Siriraj Metabolomics and Phenomics Center (SiMPC) and the Department of Biochemistry. This initiative strengthens Thailand's biomolecular research capacity and positions it as a regional hub with global impact.

**SiMPC Services** offers comprehensive analysis of small biomolecules from clinical specimens (blood, urine, stool) and bioactive compounds from natural products, herbal medicines, dietary supplements, and crops. The platform supports precision medicine,

novel compound discovery, host-microbe interaction studies, and translational innovation.

At the opening ceremony, an **MOU** was signed with DKSH, Waters Pacific, and Agilent Technologies (Thailand) to advance metabolomics research using cutting-edge mass spectrometry platforms, including Ion Mobility–MS, LC-MS/MS, and GC-MS/MS. Highlights included:

- Keynote lecture: "From Discovery to Applications: Siriraj and the Growth of Metabolomics in Thailand" by Dr. Sakda Khoomrung.
- Exhibitions on high-resolution ion mobility imaging, Metabox 2.0 (Metabolomics and multi-omics data analysis), SiMD (spectral library of >800 biomolecules), and a zebrafish screening platform for efficacy and safety testing.

SiMPC's research spans chronic kidney disease, lung and liver cancers, dermatology, natural products, and host–microbe interactions, emphasizing both precision medicine and industrial translation. The launch brought together leaders from academia, industry, and government, underscoring SiMPC's pivotal role in advancing biomedical innovation in Thailand.

Learn more: Siriraj Metabolomics and Phenomics Center



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### Metabolnterview

## **Zachary Kroezen**



Zach obtained his Honours B.Sc. in Chemistry at McMaster University in 2019. From 2019 until 2025 he worked alongside Dr. Philip Britz-McKibbin and Dr. Meera Shanmuganathan at the McMaster node within TMIC. Here Zach was involved in collaborative works with colleagues from McMaster, other academic institutions and industry partners, performing metabolomic analyses on a variety of biological samples including: urine, serum, plasma, cord blood, intestinal fluid, tissue, stool, cecum, saliva, dried blood spots, and cell extracts. Since 2019, Zach has co-authored 15 peer-reviewed publications and provided 5 oral presentations at domestic scientific conferences. This January Zach started his PhD studies within the Britz-McKibbin research group. Based on his ambitious attitude, proven dedication and research experience Zach was awarded a Vanier Canada Graduate Scholarship.

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

I was introduced to metabolomics from my appreciation of analytical chemistry. At first, metabolomics was more of an afterthought. To a greater extent I appreciated the analytical tools and the quality control/assurance procedures required to generate high

quality data. At the time, I was working in the McMaster node within TMIC meaning all my research was metabolomics based. It was when I started to recognize the plethora of applications that existed in my work, that the research became much more tangible and my true appreciation of metabolomics began. In time I have recognized metabolomics' revolutionary impact on diverse fields, including disease etiology, biomarker discovery, drug development/pharmacokinetics, microbiome research, environmental monitoring, and more.

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

Recently I have finished the analysis of two large-scale studies. In both, we analyzed over 70 unique metabolic signatures where in total, 17,000 serum samples were analyzed. The first project was completed in collaboration with the Population Health Research Institute (PHRI) at McMaster University. Specifically, samples from the Prospective Urban and Rural Epidemiological (PURE) study were analyzed to assess the influences of CVD, diabetes, lung disease, cancers, kidney disease, brain health, and injuries. The second analysis evaluated the impacts of breastfeeding and dietary intake in Brazilian children through the Estudo Nacional de Alimentação e Nutrição Infantil (ENANI) study.

My ongoing research aims to elucidate the impact of dietary exposures on the metabolic health of children from Mexico. Childhood obesity has well-established links to metabolic syndrome (MetS) which includes a cluster of risk factors (i.e. elevated blood pressure, abdominal adiposity, insulin resistance and dyslipidemia) associated with cardiovascular disease and type 2 diabetes. Early detection of children at risk for MetS could revolutionize healthcare and allow for more personalized lifestyle interventions for disease prevention that also improves metabolic health.

# 3. How do you see metabolomics changing the way we approach chronic disease prevention and population health?

Quite simply, metabolomics provides an intriguing avenue for personalized medicine. The saying "an ounce of prevention is worth a pound of cure" couldn't be truer. Consider the newborn screening approach, which has been adopted throughout North America. This may be the greatest contribution metabolomics has established to date. By identifying individuals most at-risk, healthcare interventions and public policies can be tailored to them. Not only does this lead to improved health outcomes but it also

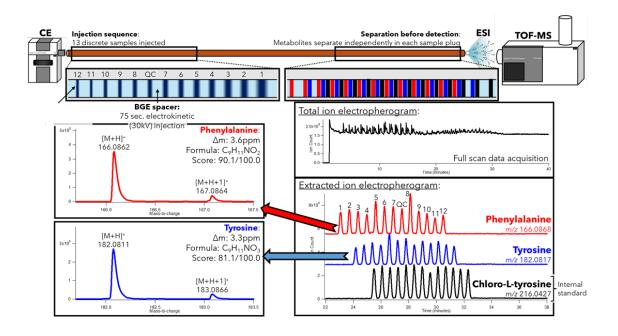
alleviates the burden on public/private healthcare systems.

### 4. What advantages do you see in using urine metabolomics over traditional selfreported data in large-scale epidemiological studies?

I'm not convinced that self-reported data, like questionnaires, will ever be fully eliminated. Despite their limitations, their simplicity, clinical relevance, and cost effectiveness makes them necessary tools, especially for large-scale epidemiological studies. However, I do believe urinary metabolomics offers a less subjective approach which enhances and complements self-reported data. It provides the opportunity to validate or correct self-reported data and identify likely misreports.

# 5. Could you explain why multisegment injection-capillary electrophoresis-mass spectrometry (MSI-CE-MS) was chosen for your study, and how it compares to other metabolomics techniques?

Multisegment injection-capillary electrophoresis-mass spectrometry (MSI-CE-MS) was an analytical technique developed in the Britz-McKibbin research group in 2013. MSI-CE-MS differs from conventional CE-MS where only a single sample is analyzed in each experiment. Given the isocratic separation conditions employed by CE, MSI-CE-MS allows up to 13 samples to be analyzed in every analytical run, increasing the throughput capabilities of CE without the need for additional costly infrastructure. For large-scale analyses where thousands of samples are analyzed, this multiplexed approach reduces analysis times by up to an order of magnitude when compared to LC and GC methods. Like any analytical platform used for metabolomics, none can analyze the entire metabolome. Specifically, MSI-CE-MS is well suited for ionic/polar analytes. This includes amino acids, short chain acylcarnitines, and organic acids. CE is also a relatively inexpensive separation tool. Instruments are a fraction of the cost of LC and GC systems and consume very little reagent during analysis.



# 6. What are the strengths and limitations of using untargeted versus targeted metabolomics in epidemiological research?

Most of my research opportunities have applied untargeted workflows, which are well suited for hypothesis generation. Untargeted workflows allow for a more comprehensive analysis of the metabolome, but sensitivity is often sacrificed as a result. Stringent quality control/assurance procedures are also necessary when performing untargeted analyses since many features are often artifact/redundant signals from in-source fragmentation, adduct formation, and/or isotopic peaks.

Besides a boost in sensitivity, targeted approaches are clinically translatable.

Downstream processes in the workflow, like data preprocessing are also simpler given the limited coverage/scope included in targeted work.

# 7. What have you found most rewarding or challenging as an early-career researcher working on large-scale metabolomics projects?

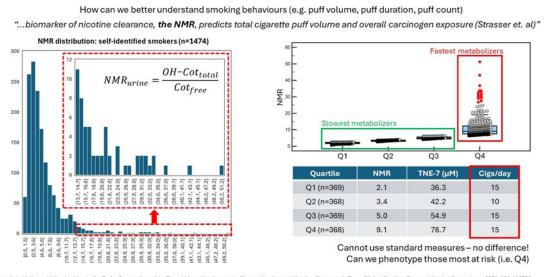
Collaborating with other researchers has been the biggest reward. Having provided metabolomic analyses on over 25,000 human samples, I have worked beside many collaborators from diverse backgrounds, including biologists, clinicians, and epidemiologists. Although I only support the metabolomic experiments for these large-scale studies, it has been through these collaborations where I have learned the most. By combining everyone's expertise, our discoveries have become much more impactful as a result!

## 8. What advice would you offer to early-stage scientists interested in applying metabolomics to their research?

Given my appreciation of analytical chemistry, I would remind new students and scientists of its importance in metabolomics research. You cannot expect highly impactful results without high quality data. Generating this data can be tedious, but it is necessary. This highlights the importance of careful sample pretreatment and robust data acquisition procedures. Although these are often the starting point of most metabolomic analyses, they directly affected all downstream processes. Simply put, if you put garbage in you will get garbage out.

# 9. Are there other areas of metabolomics or environmental health that you're excited to explore in the future?

I'm excited to continue exploring the research I presented at CanMetCan in Montreal this year! In that work I analyzed over 5,000 urinary samples to identify biomarkers associated with tobacco smoke exposures and healthy diets. A panel of seven nicotine metabolites was used as robust indicators of recent tobacco exposures. We determined that the fastest metabolizers of nicotine had the highest risk for tobacco smoke related harms. Interestingly these individuals also had distinct unhealthy dietary patterns. An untargeted analysis beyond nicotine and its metabolites is still ongoing to identify prognostic biomarkers in urine associated with incident clinical events in this diverse population.



Giratallah, H. K. et. al. Nicotine Metabolite Ratio: Comparison of the Three Urinary Versions to the Plasma Version and Nicotine Clearance in Three Clinical Studies. Drug and Alcohol Dependence 2021, 223, 108708. Strasser, A. A. et. al. Nicotine Metabolite Ratio Predicts Smoking Topography and Carcinogen Biomarker Level. Cancer Epidemiology, Biomarkers & Prevention 2011, 20 (2), 234–238.

### **Spotlight Article**

\*\*\*Sponsored Content\*\*\*



NIST Metabolomics and Microbiome Reference Materials Now Available!

### Confidence in Data Quality

The National Institute of Standards and Technology (NIST) has launched two new reference material (RM) suites for the metabolomics communities to facilitate high quality measurements, promote reproducibility and reliability of results, and encourage data harmonization and comparability.

#### RM 8231 - Frozen Human Plasma Suite for Metabolomics

RM 8231 was created as a suite of three phenotypically distinct human plasma. Pooled Plasma 1, Diabetic Plasma: designed to represent a Type 2 diabetic plasma material with glucose >126 mg/dL and low/normal triglyceride (<150 mg/dL). Pooled Plasma 2, Hypertriglyceridemic Plasma: designed as a hypertriglyceridemic plasma material with glucose <100 mg/dL and triacylglycerols >300 mg/dL. Pooled Plasma 3, African-American Plasma: created as a young (ages 20-25 years of age), African American plasma material. A unit of RM 8231 consists of two vials each of the three phenotypes.

#### RM 8048 – Human Fecal Material

RM8048 was designed to assist scientists in improving the reproducibility of their data and advancing diagnostics and clinical tools that focus on the gut microbiome. The RM 8048 unit includes four vials from vegetarian cohorts and four vials from omnivores. This material has identified over 150 metabolites and more than 150 genetic signatures.

Requesting community input!

RGTM 10212 – Fecal Calibrant Solution

NIST is developing a fecal metabolite calibrant solution as a research grade test material (RGTM) designed specifically to evaluate the performance and precision of microbiome metabolomics measurements. This solution contains 70 compounds at biologically relevant concentrations, representing a diverse range of chemical classes found within the gut microbiome including short-chain fatty acids (SCFAs), amino acids, phenols, and pyrimidines. We are offering **a unit free of charge** for community evaluation that will aid in assessing suitability for microbiome metabolomics and the data will provide NIST important feedback in the evolution of the RGTM to a reference material.

Materials can be acquired at the **NIST Storefront!** 

Confidence in your data! Confidence in published results! Confidence in deposited data!

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### **MetaboReads**

### Plant metabolism, stress adaptation, and productivity

These studies connect specialized metabolites, hormone signaling, and mechanosensation to agronomic performance. They show how rotation chemistries, wound-responsive pathways, and genome structure set metabolic capacity. The citrus model illustrates how organ-resolved metabolism can anticipate stress outcomes and quality traits. Plant improvement is moving toward metabolite-aware breeding and cropping system design.

Parallel evolution of salinity tolerance in Arabidopsis thaliana accessions from Cape Verde Islands

Martinez Rivas and colleagues in Science Advances found that Arabidopsis thaliana accessions from the Cape Verde Islands accumulate a glucuronyl-mannose metabolite that confers salinity tolerance. They mapped this trait to an alpha-glycosidase family 38 gene, GH38cv, and showed that plants with Cape Verde alleles exhibit better germination, longer roots, improved water status, and higher fitness under salt stress without growth penalties in standard conditions. Deleterious GH38cv mutations arose independently on two islands, indicating parallel evolution. The work points to a tractable path for breeding salt-resilient crops using metabolite-informed genetics.

## Soil microbial legacy mediated by buckwheat flavonoids enhances cabbage resistance to clubroot disease

Wu and colleagues in Microbiome showed that buckwheat–cabbage rotation reduces cabbage clubroot severity by 67 to 97 percent across three years through a microbiome-dependent mechanism. Buckwheat root flavonoids, notably 6,7,4'-trihydroxyisoflavone and 7,3',4'-trihydroxyflavone, recruited beneficial bacteria (Microbacterium, Stenotrophomonas, Ralstonia) that colonized subsequent cabbage roots. A defined SynCom plus these flavonoids enhanced disease suppression and primed jasmonate-linked defenses. The results outline a metabolite-guided rotation strategy that decouples disease severity from pathogen load.

## Single-cell and spatial multiomics identifies heterogeneous xylem development driven by mechanical stress in Populus.

Hsieh and colleagues in Developmental Cell showed that fibers in normal and tension wood of Populus are the same cell type and lineage, with mechanical stress altering developmental speed and cell-type ratios rather than identity. Single-cell RNA-seq across normal, tension, and opposite xylem, combined with spatial transcriptomics and metabolomics, mapped this heterogeneity. Phosphoproteomics identified conserved mechanosensing programs between stems and roots across angiosperms. Candidate regulators of tension wood formation emerged that could be leveraged to optimize biomass and bioenergy yield.

### Unveiling organ-specific metabolism of Citrus clementina

Passi and colleagues in Proceedings of the National Academy of Sciences of the United States of America found that the iCitrus2616 organ-resolved metabolic model predicts Citrus clementina responses to environmental and nutritional conditions with high accuracy. Simulations linked lower carbon-to-nitrogen ratios to higher growth and showed fourfold increases in starch and hemicellulose under mixotrophy, consistent with enhanced cell-wall rigidity and drought tolerance. The model predicted nutrient-dependent increases in specialized metabolites such as flavonoids. Integrating seasonal, tissue-specific transcriptomes from Huanglongbing infection revealed metabolic reallocations that explain observed stress phenotypes.

### Host-microbiome interactions in health and disease

These studies place microbial metabolism at the center of host physiology across organ systems. Microbiome-linked acetate governs ruminant energy balance, while oral commensals modulate lung metabolites. In production animals, hidden reservoirs of resistance genes raise clear surveillance and mitigation priorities. Functional readouts, not just taxonomic surveys, will be essential for intervention design.

<u>Subclinical disease elevates zoonotic risks of antibiotic resistance and virulence factor genes through gut microbial network in dairy cow production system.</u>

Wang and colleagues in Journal of Hazardous Materials found that subclinically diseased dairy cows harbor gastrointestinal microbiomes enriched for antibiotic resistance and virulence genes

compared with healthy controls. Mobile genetic element analyses and MetaCompare2 profiling indicated higher potential human-health risk from these communities. Specific determinants, including FosM1, associated with bile acid pathways and ketosis pathophysiology. The data support an ARG–VFG–CAZyme co-occurrence network that links animal metabolic disease with One Health risk.

<u>Disruption of hindgut microbiome homeostasis promotes postpartum energy metabolism</u> <u>disorders in dairy ruminants by inhibiting acetate-mediated hepatic AMPK-PPARA axis</u>

Wang and colleagues in Microbiome showed that postpartum energy-metabolism disorders in dairy cows correlate with gut-microbiome shifts that regulate acetate levels and hepatic signaling. A random-forest model based on microbiota predicted disease (AUC 0.74), and multiomics highlighted taxa influencing acetate that associate with PPAR and PI3K/AKT pathways and with circulating  $\beta$ -hydroxybutyrate. In hepatocytes, sodium acetate reduced lipid deposition and  $\beta$ -hydroxybutyrate production via the AMPK–PPARA axis. These findings position acetate-mediated gut–liver signaling as a protective node against metabolic dysfunction.

#### Microbial contribution to metabolic niche formation varies across the respiratory tract

Wong and colleagues in Cell Host & Microbe found that the functional activities of airway microbiota vary along the respiratory tract and associate with immunomodulatory metabolites. Oral commensals such as Prevotella, Streptococcus, and Veillonella were more active in lower airways and correlated with metabolites including methionine and glutamate. Mouse inoculation with these taxa reproduced regional metabolite changes, and isotope labeling traced specific products to Prevotella melaninogenica. The work reveals how microbial metabolism shapes lung niches and potentially host responses.

### **Environmental toxicology and metabolic resilience**

Across taxa, lipid remodeling and vitamin-linked metabolites recur as stress integrators and protectants. The cnidarian work aligns with reptile and nematode studies by elevating subtle metabolic endpoints over crude toxicity readouts. These approaches sharpen risk assessment and suggest low-risk, metabolite-based mitigation strategies for environmental exposures.

Gut microbiota mitigate the reproductive toxicity of silver nanoparticles through thiamine-derived metabolites.

Gong and colleagues in Nature Communications showed that colonizing nematodes with Pseudomonas mendocina rescues reproductive toxicity caused by silver nanoparticles. Transcript profiling indicated suppression of initiating and key adverse-outcome events. Metabolomics identified two thiamine-derived metabolites, 4-methyl-5-thiazoleethanol and thiamine monophosphate, as mediators of protection. The findings nominate microbiota manipulation and vitamin-derived metabolites as organism-level detoxification strategies.

<u>Tris(2-chloroethyl) phosphate alters gut microbiota and hepatic metabolism in freshwater turtles at environmentally relevant concentrations.</u>

Liu and colleagues in Journal of Hazardous Materials found that tris(2-chloroethyl) phosphate exposures alter gut microbiota composition and hepatic metabolism in Mauremys reevesii turtles without overt toxicity. Low doses enriched Akkermansia with increased feeding, whereas high doses favored Odoribacter, Bilophila, and Laribacter and reduced intake. Hepatic metabolomics highlighted 67 differential metabolites, with glycerophospholipid disruption as a primary signature. Correlation patterns support a gut–liver axis in reptilian responses to flame retardants.

Metabolic responses of sea anemone and jellyfish to temperature and UV bleaching: Insights into stress adaptation using LCMS-based metabolomics, molecular networking and chemometrics.

Farag and colleagues in Journal of Advanced Research showed that heat and UV stress in photosymbiotic cnidarians produce organism- and stress-specific metabolomic signatures. Newly reported compounds, including cyclic tetraglutamate, campestriene, and ceramide aminoethyl phosphonate, were detected. Phospholipids, steroids, and ceramides predominated as markers, with anemone LPC species and echinoclasterol sulfate tracking stress and jellyfish GlcCer and peptides separating UV from heat responses; LPE 20:4 marked stress in both. GNPS molecular networking and chemometrics provided high-resolution classification of bleaching-related states.

### Metabolic reprogramming and therapeutic targets in human disease

Nucleotide and lipid pathways emerge as control points for survival, fibrosis, and tissue integrity. Convergent evidence supports pairing metabolic inhibitors with apoptosis or immune modulators. Several agents are clinically plausible, including statins and antisense oligonucleotides, which could speed translation if biomarker-guided patient selection is developed in parallel.

De novo pyrimidine biosynthesis inhibition synergizes with BCL-XL targeting in pancreatic cancer

Zhang and colleagues in Nature Communications showed that inhibiting de novo pyrimidine synthesis via DHODH reshapes apoptotic control in pancreatic ductal adenocarcinoma and creates a dependency on BCL-XL. Screens and multi-omics pinpointed BCL2L1 as a rational partner target, and combining the DHODH inhibitor brequinar with the BCL-XL degrader DT2216 induced synergistic apoptosis. Patient-derived organoids and mouse models confirmed efficacy. The study defines adaptive escape routes to DHODH blockade and supplies a combination strategy for pancreatic ductal adenocarcinoma.

Mevalonate pathway promotes liver cancer by suppressing ferroptosis through CoQ10 production and selenocysteine-tRNA modification.

Chen and colleagues in Journal of Hepatology found that the mevalonate pathway shields hepatocellular carcinoma from ferroptosis by supplying CoQ10 and enabling selenoprotein translation through selenocysteine-tRNA modification. Pharmacologic inhibition of MVD with 6-FMEV or upstream blockade with atorvastatin lowered IPP and CoQ10, impaired selenoprotein

synthesis, and triggered ferroptotic death. Genetic disruption of TRSP or TRIT1 reproduced ferroptosis and enhanced therapy responses. Pathway inhibitors synergized with tyrosine kinase inhibitors or anti-PD-1, including in steatotic HCC models.

<u>Decreased LONP1 expression exacerbates MASH-induced liver fibrosis via elevated orotic acid levels.</u>

Xu and colleagues in Journal of Hepatology showed that loss of hepatic LONP1 elevates DHODH abundance and orotic acid, which aggravates fibrosis in metabolic-dysfunction-associated steatohepatitis. Restoring LONP1 or inhibiting DHODH reduced orotic acid and attenuated fibrosis in mice. Mechanistically, LONP1 selectively degrades DHODH in an ATP-dependent manner, limiting ATF3-driven stellate-cell activation. Patient samples linked low LONP1 to high plasma orotic acid and higher fibrosis scores.

c-Myc promotes metabolic reprogramming in pulmonary hypertension via the stimulation of glutaminolysis and the reductive tricarboxylic acid cycle.

Yegambaram and colleagues in Redox Biology found that c-Myc upregulation drives glutaminolysis, reductive TCA flux, and glycolysis in pulmonary arterial endothelial cells from experimental pulmonary hypertension. This metabolic program increased proliferation, reactive oxygen species, and apoptosis resistance while suppressing nitric oxide. The c-Myc inhibitor 10058-F4 and HIF-1α targeting reversed the hyperproliferative phenotype and normalized fluxes. The results implicate glutamine metabolism as a tractable target in vascular remodeling.

Hypertriglyceridemia as a Key Contributor to Abdominal Aortic Aneurysm Development and Rupture: Insights From Genetic and Experimental Models.

Liu and colleagues in Circulation showed that hypertriglyceridemia causally contributes to abdominal aortic aneurysm development and rupture. Mendelian randomization analyses aligned with mouse models in which Lpl or Apoa5 deficiency or human APOC3 overexpression accelerated aneurysm formation, dissection, and lethality. Elevated triglycerides and palmitate impaired lysyl oxidase maturation, reducing enzyme activity critical for vascular integrity; local lysyl oxidase repletion abrogated the effect. An Angptl3-targeting antisense oligonucleotide lowered triglycerides and attenuated aneurysm progression.

### Clinical metabolomics for diagnosis and staging

Blood and keratinized-tissue assays are approaching clinical readiness for ophthalmology and neurology. The Alzheimer's result hints at a metabolic dimension that is orthogonal to amyloid status. Next steps include inter-lab standardization, longitudinal validation, and integration with imaging and genetics to refine decision thresholds.

Serum metabolite biomarkers for the early diagnosis and monitoring of age-related macular degeneration.

Li and colleagues in Journal of Advanced Research showed that a serum panel of hypoxanthine, 2-furoylglycine, and 1-hexadecyl-2-azelaoyl-sn-glycero-3-phosphocholine

accurately distinguishes age-related macular degeneration from controls and other eye diseases. Random-forest models achieved perfect discrimination in discovery and an AUC of 0.962 with 0.88 accuracy in external validation. The three metabolites also stratified disease severity with excellent performance in both phases. Analyte stability across freeze—thaw cycles supports practical deployment.

<u>Fingernail-based metabolomics reveals a stepwise decline in dodecanoic acid associated with Alzheimer's disease progression.</u>

Zhang and colleagues in Journal of Advanced Research found that fingernail metabolomics reveals a stepwise decline in dodecanoic acid across Clinical Dementia Rating categories from normal to advanced Alzheimer's disease. The association remained after adjusting for demographics, lifestyle, and sleep and correlated with cognitive scores. Within each severity group, levels were independent of amyloid PET status, suggesting a complementary disease axis. A multi-feature classifier achieved AUCs of 0.71 to 0.87 for tri-class discrimination, with dodecanoic acid the top contributor.

# Methods and systems-level advances in metabolomics and metal biology

These contributions expand metabolomics from descriptive catalogs to predictive, manipulable systems. Quantitative platforms that retain breadth, spatial methods that localize features, and elemental physiology maps together elevate target discovery and assay robustness. Methodological convergence across labs will be key to reproducibility and clinical adoption.

<u>Drug-resistant Escherichia coli metabolomics via pseudo-targeted SWATH/IDA-MRM: Bridging high coverage and precision.</u>

Jia and colleagues in Journal of Advanced Research showed that a pseudo-targeted SWATH/IDA-MRM workflow unites the coverage of untargeted metabolomics with the quantitative rigor of targeted analysis. Using complementary chromatography and acquisition modes, the platform detected 3,529 features with superior linearity, reproducibility, sensitivity, and dynamic range. Applied to drug-resistant Escherichia coli, it uncovered broad reprogramming across nucleotide, amino acid, energy, lipid, and redox pathways. The method provides a template for mapping resistance-linked metabolic vulnerabilities.

Engineering a novel bifunctional nanoplatform integrating metabolic profiles and tissue imaging for fingerprints characterization of Polygonatum cyrtonema Hua

Li and colleagues in Chemical Engineering Journal found that MXene–GO–Au films enable a bifunctional LDI-MS and MS-imaging platform with high sensitivity, clean background, and salt tolerance for rapid plant metabolomics. Ridge regression with cross-validation achieved up to 100 percent accuracy in differentiating Polygonatum cyrtonema cultivation sources and selected 14 key metabolites. Imaging validated tissue-level localization of discriminants, supporting biological relevance. The platform streamlines quantitative fingerprinting and spatial mapping in medicinal plants.

#### The molecular landscape of cellular metal ion biology

Aulakh and colleagues in Cell Systems showed that cellular networks in yeast are broadly metal responsive, with roughly half the proteome and major signaling pathways, including TOR, changing across gradients of essential metals. Metallomic, proteomic, genetic, and growth profiles revealed interdependencies among metals that shape homeostasis. Many understudied proteins likely function in metal biology, and metalloenzymes occupy central positions in metabolic networks. The resource offers strategies to manipulate metal availability for biotechnology and therapeutic discovery.

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### The Metabolomist Podcast



Are the metabolites the outcome or the exposure? And if they're the exposure; are they measured prior to your outcome?... Being aware of these epidemiological fundamentals is very important when designing a metabolomic study.

- Sandi Azab

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### **Metabolomics Events**

# 7th Annual Metabolomics Society of North America (MANA) Conference

**September 2 - 5, 2025** 

Venue: Banff, Canada

The 7th Annual Conference of the Metabolomics Association of North America (MANA) will be hosted in the heart of the Rocky Mountains. Visit the website for program information, speakers, events, registration, awards, and more.

Check for more details

# Bits & Bites #5: Bayesian Statistics for Metabolomics September 11, 2025

**Venue: Online** 

The short course is taught by Dr. Christopher Brydges. This introductory-level session requires JASP (version will be announced before the course) and assumes only basic knowledge of statistics (for example, you know what a t-test and a correlation are); no coding experience is needed.

#### **Short description of the course:**

Bayesian statistics are a useful method for estimating effect sizes and testing the strength of evidence in favor of one hypothesis over another - things that p-values and traditional statistics can't do. However, they are under-utilized in metabolomics research. This short course will provide a brief refresher on traditional statistics, teach the basic principles behind Bayesian statistics, learn how to conduct basic Bayesian analysis in JASP, and learn how to report the results in the style of a journal article.

Check for more details

# DG5th Annual Metabolomics Society of North America (MANA) Conference

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

**September 11, 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
- Expand collaborative networks with metabolomic experts from multiple domains

Check 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 Jobs**

### **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
Principal Scientist, Metabolomics	Novartis	Cambridge, MA, USA	<u>Novartis</u>
Research Associate II - Metabolomics	Broad Institute of MIT and Harvard	Cambridge, MA, USA	Broad Institute
Research Specialist - Analytical (metabolomics)	University of Melbourne	Melbourne, Victoria, Australia	<u>University of</u> <u>Melbourne</u>
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
Metabolomics Associate Director	Botany and Plant Pathology Department at Purdue University	West Lafayette, IN, USA	Botany and Plant Pathology Department at Purdue University
Post Doctoral Fellow Research - American Elderberry Metabolomics (Dr. Lloyd Sumner's Lab)	University of Missouri- Columbia	Columbia, MO, USA	University of Missouri-Columbia
Assistant Professor, Cell Metabolism	University of Saskatchewan	Saskatoon, SK, Canada	<u>University of</u> <u>Saskatchewan</u>
Manager, Quantitative Metabolite Analysis Center	University of California, San Francisco	San Francisco, CA, USA	UC San Francisco

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