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MetaboNews

This month in metabolomics

October, 2024 Vol 14, Issue 10

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





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Metabolomics Society News



METABOLOMICS SOCIETY EARLY- CAREER MEMBERS NETWORK The Metabolomics Society is an independent, non-profit organization dedicated to promoting the growth, use, and understanding of metabolomics in the life sciences.

General Enquiries info@metabolomicssociety.org

Conference Corner

The Metabolomics Society along with the Scientific Organizing Committee are delighted to extend this invitation to you to attend **Metabolomics 2025**, the 21st Annual Conference of the Metabolomics Society, in Prague, Czech Republic. The conference will be held June 22-26, 2025 at the Prague Congress Centre.

Metabolomics 2025 Prague Congress Centre June 22 - 26 www.metabolomics2025.org

The website will be continually updated, check back often for updates.



Follow @MetabolomicsSoc on X to stay current and meet new peers before the event!

Open Call for Workshop Proposals

The conference workshops provide a terrific venue to discuss a wide range of important topics and practical aspects of metabolomics and may include hands-on learning

opportunities.

You can submit your <u>workshop application</u> online. The deadline for workshop proposals is **December 19.**

Calling all Sponsors!

The <u>Sponsorship Brochure</u> is available for Metabolomics 2025.

As we approach the conference, we look forward to partnering with your organization to continue the success of bringing together all the major international organizations involved in human, plant, microbial, animal, and environmental metabolomics.

We have a variety of packages available to position your brand and product at the forefront of the scientific community. Opportunities are limited and available on a first-come first-served basis!

Your support is extremely important to the success of the meeting, helping to keep registration costs down, which allows more of our younger scientists to attend. We look forward to partnering with you for Metabolomics 2025!

Members' Corner

Board of Directors

Dear Metabolomics Society members and metabolomics friends,

I am a month into the new role and am hugely impressed with my fellow Directors and their desire and passion to drive the society and community forward. All Directors of the board volunteer their significant time contributions and receive no reimbursement for their time and efforts.

The society operates through a set of committees who are chaired by a Director. During the following months I will highlight some of these roles. I am going to start with the conference committee who have the primary objective to schedule, plan and operate an annual conference. Trust me, all of us who arrive on day one for the workshops have no idea the effort and commitment provided by many for up to two years before the actual conference. The conference committee has been chaired by Natasa Giallourou for five years. Her time in the role has been interesting and diverse and includes the online conferences held in 2020 and 2021 and the very successful first post-Covid conference in 2022 - what Natasa does not know about conferences is not worth knowing. Natasa is

in her final year as chair, will be greatly missed from autumn 2025 and I want to provide my sincere thanks for all her work and drive to make the annual conference as successful, diverse and enjoyable as they can be.

We are lucky to have the company SnapIT involved in the operation of the society including many aspects of conference organisation and operation. Leslie and her team work extremely hard behind the scenes, and I send my personal thanks for her support during the transition over the last few months. Planning for Metabolomics 2025 started in 2023 with discussions on venues and budgets being developed by SnapIT with decisions made on the location and venue 12-18 months before the conference starts.

I am sure many in the metabolomics community will be looking forward to travelling to Prague for the great science and networking (and the great architecture, food and alcohol). The conference co-chairs are Tomáš Pluskal (also a Society Director) and David Friedecký; they have constructed a Scientific Organising Committee, developed session themes and chosen plenary and keynote speakers. Our goal as a society is to be balanced and to highlight research across the world – we always look for a balance of male and female speakers from across the globe. Seeing the list this week has me excited about next year already. Place the conference in your calendar now – June 22nd – 26th 2025. Further information about the conference and future announcements will be available on the <u>conference website</u>.

As is usual, workshops will be operated on the Sunday afternoon and Monday morning and anyone can apply to hold a workshop – please submit your applications <u>here</u>.

The society is always appreciative of financial support for the conference which allows us to host world-class science, in high-quality environments with financially appropriate registration fees for all attendees. Please consider supporting the conference – more information is available <u>here</u>.

This may be my last message before the December festivities start. I hope all enjoy their winter or summer breaks, have time to relax, rejuvenate and spend time with family and friends.

All the very best,

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



Are you involved in the metabolomics, genomics, transcriptomics, or proteomics?

TMIC Node Leader <u>Dr. Jianguo (Jeff) Xia</u> focuses his work on developing cutting-edge computational frameworks. These frameworks incorporate cloud computing, machine learning, and visual analytics, aiming to streamline and enhance the analysis of complex biological data.

Undergraduates, graduate students, postdoctoral fellows, researchers, and PIs interested in opportunities surrounding omics data analysis are encouraged to join the upcoming winter session offered through <u>Xia Lab Analytics</u>.

Early-Career Members Network (EMN)

EMN Webinars 2024-2025

October Webinar

The EMN committee extends its sincere gratitude to **Prof. Dr. Mingxun Wang** from the University of California, Riverside, USA, and his senior PhD candidate **Reza Shanheh**, for the insightful webinar on 28th October 2024 entitled "*Illuminating Metabolomic Dark Matter - Reshaping How to Mine and Reuse Big Mass Spectrometry Data*". The webinar recording is now available on the MetSoc website:

https://metabolomicssociety.org/resources/multimedia/emn-webinars-2024/.

November Webinar

The next EMN webinar will occur on Thursday, 28th November 2024, 16:00 UTC (17:00 CET) featuring **Dr. Álvaro Fernández-Ochoa** from the Bioactive Ingredients AGR-274 research group, Analytical Chemistry Department, Faculty of Science, University of Granada, Spain. The EMN committee is delighted to invite you for the talk about "*Untargeted Metabolomics Approaches in Nutritional Intervention Studies: Uncovering Insights into Bioactive Compounds*", focusing on food metabolomics. Registration is available via the following Zoom link:

https://zoom.us/webinar/register/WN_NSMLTDKLR6ayA-CAX2K1bQ.

December Webinar

The last webinar of the year will be hosted on Wednesday, 11th December 2024, 16:00 UTC (17:00 CET) and we are happy to host **Dr. Daniel Petras**, assistant professor from the University of California, Riverside and the University of Tuebingen and **Dr. Paolo Stincone**, a postdoctoral researcher from the University of Tuebingen who will deliver a joint webinar titled: "A Functional Metabolomics Toolbox for Uncovering Small Molecule Dynamics in Microbial Communities". Registration is available via the following Zoom link: <u>https://zoom.us/webinar/register/WN_nQ20WcHxQPeSHDBIASMR-Q</u>.

Keep an eye on your inbox for email blast and make sure to follow us on social <u>Twitter</u> and <u>LinkedIn</u>! This year, we would like to invite the researchers especially from South America, Africa and Asia to participate in our webinars. If you are interested, or want to recommend someone from your network, please reach out to <u>info.emn@metabolomicssociety.org</u>.

International Affiliates' Corner

Latin American Metabolic Profiling Society (LAMPS)

Visit https://jwist.github.io/lamps/

On October 2nd the Latin American Metabolic Profiling Society (LAMPS) and the Metabolomics Society were introduced by Dr. Ian Castro Gamboa and Dr. María Eugenia Monge to the members of Portal Metabolomica Brasil during a virtual meeting attended by more than 25 Brazilian researchers.

Later that month, between October 29th and November 1st, the V LAMPS Meeting was held in Montevideo, and brought together a robust network of metabolomics researchers, sponsors, and thought leaders with the aim of fostering innovation and collaboration across the region. The meeting featured 12 short talks, four sponsor presentations, 5 workshops, 5 keynotes, 8 plenary lectures, and two poster sessions with nearly 60 contributions covering key areas of metabolomics research that ranged from technological innovations to practical applications. In addition to 8 full travel grants and 6 accommodation grants, awards for the best short talks and best posters showcased the work of young researchers, emphasizing creativity, innovation, and impactful scientific contributions.

The meeting was enriched by distinguished participants, whose expertise and insights guided attendees through the evolving landscape of metabolomics, including Facundo Fernández, Dajana Vuckovic, Julia Kuligowski, María Eugenia Monge, Tuulia Hyötyläinen, Matej Orešič, José Luis Izquierdo-García, Gonzalo Hernández Dossi, Tomáš Pluskal, Tito Damiani, Norberto Peporine Lopes, Alan Pilon, Cecilia Queijo, Leo Cheng, Art Edison, Pablo Hoijemberg, Oscar Millet, Ewy Mathé and Roy Goodacre. Their talks and workshops addressed a range of critical topics, shedding light on new methodologies, emerging challenges, and the latest findings in the field.

Sponsor talks provided attendees with insights into cutting-edge technological advancements and practical solutions for metabolomics research, reinforcing the synergy between academia and industry. We thank all speakers, sponsors, the local Organizing Committee, the Scientific Committee and the Young LAMPS Network members for making this edition such a great event. As LAMPS grows, it remains dedicated to promoting inclusivity, fostering collaborations, and driving advancements in metabolic profiling across the region and beyond, and envisions the renewal of the Board of Trustees. The VI LAMPS meeting, scheduled for 2026, will be held in São Paulo, Brazil.

Thailand Metabolomics Society (TMS)

Visit https://thailand-metabolomics.org/

Metabolomics Data Processing and Analysis Workshop Using Metabox 2.0 at

Siriraj Hospital, Thailand

On November 6th, 2024, from 8:30 am to 4:00 pm, the Siriraj Center of Research Excellence in Metabolomics and Systems Biology (SiCORE-MSB) and the Siriraj Center of Research Excellence (SiCORE-M) jointly hosted an onsite workshop. It was held in the computer training room (Room 620) on the 6th Floor of the Srisavarindira Building at the Faculty of Medicine, Siriraj Hospital, Mahidol University.

The workshop featured by Dr. Kwanjeera Wanichthanarak and Dr. Sakda Khoomrung, from SiCORE-MSB (<u>https://metsysbio.com/</u>), who provided a comprehensive overview of the Metabox 2.0 program. Participants engaged in hands-on sessions focused on data processing, statistical analysis, and data interpretation, gaining practical skills in metabolomics data analysis under the expert guidance of the presenters. See more details of Metabox2.0 publication:

https://academic.oup.com/gigascience/article/doi/10.1093/gigascience/giae005/7629842 ?login=false



Upcoming event: Hands-on Metabolomics Workshop on "Evaluating the quality of animal products using phenomics technology" at Khon Kaen University

The animal product industry in Thailand, including milk, chicken, and eggs, is facing new challenges related to quality demands, product safety, and compliance with international standards. Phenomics technology, which involves studying and analyzing the observable characteristics of living organisms resulting from the interaction between genetics and

the environment using advanced tools and technologies, is being adopted as a key approach to improve the quality of animal products. This technology emphasizes precision and efficiency in quality analysis, directly enhancing consumer confidence and the competitiveness of products in the global market.

Khon Kaen University National Phenome Institute will be organizing the Hands-on Metabolomics Workshop on "Evaluating the quality of animal products using phenomics technology" at Khon Kaen University Science Park, Thailand during 28th – 31st January 2025. For more information, please visit <u>https://nationalphenomeinstitute.kku.ac.th</u>

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Spotlight Article

Solnul - MSP Starch Products Inc.

Biography

MSP Starch Products Inc. is the developer of <u>Solnul</u>®, an upcycled, patented resistant starch ingredient used by formulators of dietary supplements and functional food and beverages. Solnul® is labeled as 'Resistant Potato Starch,' a prebiotic dietary fiber, and is Upcycled Certified[™], FODMAP Friendly, Gluten-Free, Glyphosate Residue Free, and Non-GMO Project Verified.

Resistant starch prebiotics are thought to have tremendous impacts because they were historically an important dietary fibre that is no longer present at meaningful levels in the diet. To fully appreciate the benefits associated with low dose resistant starch supplementation, the company expanded its research 'Beyond-the-Gut' to include serum metabolomics.

The Technology

Targeted metabolomics is an approach in metabolomics research that quantifies and examines a select set of known metabolites within a sample. Unlike untargeted metabolomics, which seeks to profile all detectable metabolites, targeted metabolomics zeroes in on a predefined group, typically chosen for their significance in a specific biological pathway, disease, or phenotype. This method enables researchers to address particular metabolic questions with heightened sensitivity and precision.

For this study, the team at MSP Starch Products Inc. were interested in a systematic review of the effects Solnul® on human health. Specifically, in order to discover their product's impacts on intestinal barrier integrity, mitochondrial function, collagen decomposition, serum histamine and free fatty acid levels, a marker of insulin sensitivity, the Goodlett Node at The Metabolomics Innovation Centre was approached to examine their trial data using the Fatty Acids Analysis, Amino Acid Metabolism Assay, Bile Acids Analysis, and others.

The Discovery

Analysis revealed several interesting discoveries. Most notable was that Solnul® consumption improved multiple factors associated with intestinal barrier function, including improvements in carnitine ratios, reductions in acetylated polyamines, and reductions in various amino acids previously associated with 'leaky gut'. This provided an explanation for the most perplexing finding, which was a reduction in serum histamine levels: Given that most of the histamine is found in the intestines, coming from food and commensal gut bacteria, the findings suggested that improved intestinal barrier function likely keep histamine in the gut, preventing it's translocation to the blood. Additionally, the analysis revealed significant decreases in collagen breakdown products, and in the levels of free fatty acids, a marker of insulin sensitivity.

Metabolomics analysis has been instrumental in mapping both the host's response and changes in signaling molecules originating from gut bacteria. This dual insight is vital for understanding the complex communication between gut microbiota and host physiology.

The Future

MSP Starch Products Inc. sees tremendous potential for metabolomics in nutrition research, with recent findings opening avenues to explore new health applications of prebiotics. The company is now evaluating these possibilities based on clinical trial feasibility and potential commercial impact.

"We feel that we are only scratching the surface when it comes to metabolomic applications in the nutritional health space. Findings from the metabolomics analysis of our serum samples have opened several unexpected avenues to address aspects of health that have not been previously connected to prebiotics.." – MSP Starch Products Inc.



MetaboReads

This month's papers really showcase the power of metabolomics in peering into 'black boxes' of everything from tumour microenvironments to plant chemosynthesis. We here at MetaboNews continue to be excited at the growth and maturation of our discipline foundational methodological advances continue to expand what we're even able to look at, and that expansion is, in turn, driving what research questions we can ask. It continues to be a very exciting time.

- The MetaboNews Team

Gut Microbiota, Exposomics, and Metabolomics

The intricate relationship between environmental pollutants, gut microbiota, and host metabolism is a focal point in understanding health and disease. The featured studies explore how drugs and environmental toxins influence gut microbial communities and host metabolism, affecting disease progression and therapeutic outcomes. These studies emphasize the pivotal role of the gut microbiome and metabolomics in assessing environmental impacts and developing potential interventions.

Emergence of community behaviors in the gut microbiota upon drug treatment.

Garcia-Santamarina and colleagues in Cell investigated how pharmaceuticals affect gut bacteria within complex communities. By comparing the effects of 30 drugs on a 32-species synthetic community versus each species in isolation, they discovered that communal behaviors emerged in 26% of cases. Cross-protection, where drug-sensitive species were protected within the community, was six times more frequent than cross-sensitization. Metabolomic profiling showed that both drug biotransformation and bioaccumulation contribute to communal protection, offering insights into microbial interactions upon drug exposure.

Flumethrin exposure perturbs gut microbiota structure and intestinal metabolism in honeybees (Apis mellifera)

Liu and colleagues in the Journal of Hazardous Materials examined the impact of flumethrin on the gut microbiota and metabolism of adult honeybees. Exposing bees to flumethrin resulted in reduced survival rates and decreased activities of antioxidative enzymes (superoxide dismutase and catalase) and detoxification enzymes (glutathione S-transferase). Gut microbiota diversity diminished, and untargeted metabolomics revealed alterations in metabolic pathways, particularly increased metabolism of phenylalanine, tyrosine, and tryptophan derivatives. These findings underscore the need for cautious pesticide use to protect honeybee health and their gut microbiota.

<u>A comparative study on the toxic effects of lead pollution and nanoplastic-lead mixed</u> pollution on red drum and their detoxification strategies.

Sun and colleagues in the Journal of Hazardous Materials compared the toxic effects of lead pollution and nanoplastic-lead mixed pollution on red drum fish. They found that nanoplastics significantly enhance lead accumulation in muscle tissues, leading to more severe toxic effects. Histological analyses revealed liver lipid droplets and gill epithelial lifting as primary lesions. The study revealed different detoxification strategies employed by the fish under each type of pollution, providing valuable insights for environmental pollution monitoring and management.

Systemic inflammatory response to daily exposure to microcystin-LR and the underlying gut microbial mechanisms

Zhao and colleagues in the Journal of Hazardous Materials explored chronic exposure to microcystin-LR (MC-LR) in mice to understand its systemic effects. Long-term exposure led to intestinal microbial dysbiosis, colitis-like changes, and systemic chronic inflammation marked by elevated serum levels of inflammatory cytokines. Multi-omics analyses suggested that specific gut bacteria, such as Muribaculaceae, promote a systemic infection-inflammatory response, while Lachnospiraceae may have protective roles. Fecal microbiota transplantation confirmed the causal role of microbiota alterations in MC-LR-induced inflammation.

Benzo(a)anthracene Targeting SLC1A5 to Synergistically Enhance PAH Mixture Toxicity.

Wang and colleagues in Environmental Science & Technology explored the synergistic toxicity of polycyclic aromatic hydrocarbon (PAH) mixtures, focusing on benzo(a)anthracene (BaA). They discovered that BaA enhances oxidative damage by targeting the glutamine transporter SLC1A5, leading to glutamine depletion and impaired glutathione synthesis. Through metabolomics and chemical proteomics, they elucidated the mechanism by which BaA amplifies the toxicity of PAH mixtures, highlighting the importance of considering mixture effects in environmental toxicity assessments.

Dose rate dependent genotoxic and metabolic effects predict onset of impaired development and mortality in Atlantic salmon (S. salar) embryos exposed to chronic gamma radiation

Maremonti and colleagues in Science of the Total Environment investigated the effects of chronic gamma radiation on Atlantic salmon embryos. Exposure led to dose-dependent increases in DNA damage, developmental impairments, and mortality rates. Metabolomic profiling showed shifts in pathways related to oxidative stress and DNA repair at higher dose rates. The study provides crucial information on the long-term ecological impacts of radionuclide contamination in aquatic environments.

Metabolomics in Metabolic and Neurological Diseases

Metabolomics continues to play a vital role in understanding metabolic and neurological

diseases. This month's studies shed light on the associations between plasma metabolites and type 2 diabetes progression, the role of lysine metabolism in cold acclimation, and metabolic profiles in neurological conditions. These findings enhance our understanding of metabolic regulation and could inform the development of novel diagnostic and therapeutic approaches.

Role of human plasma metabolites in prediabetes and type 2 diabetes from the IMI-DIRECT study.

Sharma and colleagues in Diabetologia analyzed plasma metabolites from 3,000 individuals to identify associations with prediabetes and type 2 diabetes. They found that branched-chain amino acids, lipids, and other metabolites were significantly different when comparing glycemic status groups. Mendelian randomization suggested causal roles of specific phosphatidylcholines and n-3 fatty acids in diabetes development. Their work highlights metabolites that could serve as biomarkers for disease progression and potential therapeutic targets.

<u>Cold exposure accelerates lysine catabolism to promote cold acclimation via remodeling</u> <u>hepatic histone crotonylation</u>

Xue and colleagues in Environment International studied the effects of cold exposure on lysine metabolism and cold acclimation in humans and mice. They found that continuous cold exposure decreased plasma lysine levels and that lysine supplementation improved thermogenesis and cold tolerance. Lysine influenced hepatic histone crotonylation, promoting the expression of genes involved in metabolism. The study identifies lysine as a critical amino acid for remodeling hepatic histone crotonylation that facilitates cold acclimation.

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

Otto and colleagues in the Journal of Neuroinflammation performed Nuclear Magnetic Resonance spectroscopy to analyze metabolites in cerebrospinal fluid (CSF) and serum samples from patients with Parkinson's disease, other neurodegenerative diseases, cerebral ischemia, multiple sclerosis, and controls. They detected 99 metabolites and found that metabolome profiles could distinguish between conditions such as multiple sclerosis and neurodegenerative diseases. The study emphasizes the value of metabolomics in identifying biomarkers and understanding neurological disease mechanisms.

Palmatine protects against atherosclerosis by gut microbiota and phenylalanine metabolism

Wang and colleagues in Pharmacological Research investigated the anti-atherosclerotic effects of palmatine (PAL) via gut microbiota modulation. In ApoE^{-/-} mice, PAL treatment reduced plaque formation and inflammation within arteries. Metabolomics and microbiota analyses showed that PAL decreased the abundance of Desulfovibrio piger and serum hippuric acid levels, linked to phenylalanine metabolism. Their findings suggest that PAL exerts protective effects against atherosclerosis by modulating the gut microbiota and associated metabolic pathways.

Omics Data Integration and Multi-omics Approaches

The integration of omics data is pivotal for comprehensive biological insights. The featured studies focus on developing resources and approaches to facilitate data integration in kidney transplantation research and eosinophilic esophagitis, highlighting the importance of multi-omics analyses and advanced computational methods in tackling complex diseases.

Molecular landscape of kidney allograft tissues data integration portal (NephroDIP): a curated database to improve integration of high-throughput kidney transplant datasets

Boshart and colleagues in Frontiers in Immunology developed NephroDIP, a curated database compiling open-access high-throughput omics datasets from human kidney transplant studies. By integrating data from 134 studies detailing 260 comparisons and 83,262 molecules, the portal enables researchers to identify common gene, protein, and microRNA networks disrupted in patients with chronic antibody-mediated rejection. NephroDIP facilitates data visualization and aims to advance understanding and improve outcomes in kidney transplantation.

Advances in omics data for eosinophilic esophagitis: moving towards multi-omics analyses

Matsuyama and colleagues in the Journal of Gastroenterology reviewed recent omics research in eosinophilic esophagitis (EoE), a chronic allergic inflammatory disease. They discussed how genomic, epigenetic, transcriptomic, proteomic, and metabolomic studies have provided insights into EoE pathogenesis. The review emphasized challenges in integrating diverse omics data due to complexity and the need for advanced computational methods. They highlighted the potential of machine learning and multi-omics integration in revealing new aspects of EoE pathogenesis, improving diagnostics, and enhancing treatment effectiveness.

Metabolomics Methodologies and Applications

Advancements in metabolomic methodologies are crucial for expanding our capacity to analyze complex biological systems. The studies highlighted introduce novel techniques and applications in archaeometabolomics, plant-soil interactions, quantitative LC-MS metabolomics, and taste compound identification, enhancing our ability to investigate past human behaviors, plant physiology, and food science.

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

Badillo-Sanchez and colleagues in Science Advances utilized untargeted metabolomics to analyze cortical bone samples from 323 archaeological individuals. They identified 45 discriminating molecular features that differed between tobacco users and non-users, demonstrating that tobacco consumption leaves a detectable metabolic record in human bone. This study pioneers the application of archaeometabolomics to uncover past human behaviors and could inform future research in bioarchaeology.

A Comprehensive LC–MS Metabolomics Assay for Quantitative Analysis of Serum and Plasma

Zhang and colleagues in Metabolites developed a comprehensive liquid chromatography– tandem mass spectrometry (LC–MS/MS) assay called MEGA that quantitatively measures over 700 metabolites in human serum or plasma. Utilizing chemical derivatization, reverse-phase LC–MS/MS, and direct flow injection MS in both positive and negative ionization modes, they achieved absolute quantification of 721 metabolites across 20 classes, including many clinical biomarkers. The assay demonstrated detection limits ranging from 1.4 nM to 10 mM, recovery rates between 80% and 120%, and quantitative precision within 20%. Validated in a large dietary intervention study, the MEGA assay promises to make comprehensive quantitative metabolomics more affordable, accessible, and applicable to large-scale clinical studies

Differential Exudation Creates Biogeochemically Distinct Microenvironments during Rhizosphere Evolution.

Garcia Arredondo and colleagues in Environmental Science & Technology combined in situ microsensors with high-resolution mass spectrometry to measure exudation and associated biogeochemical dynamics along single growing plant roots (Avena sativa). They found significant variations in metabolite concentrations, microbial growth, redox potential, and pH dynamics among bulk soil, root tip, and mature root zones. The study illustrates how different exudates released along growing roots create functionally distinct soil microenvironments that evolve over time.

Key umami taste contributors in Longjing green tea uncovered by integrated means of sensory quantitative descriptive analysis, metabolomics, quantification analysis and taste addition experiments.

Shan and colleagues in Food Chemistry investigated the compounds contributing to the umami taste of Longjing green tea. Using sensory analysis and LC-MS-based metabolomics on 36 tea infusions, they identified 17 candidate umami-enhancing substances, including amino acids like glutamic acid and aspartic acid, as well as galloylglucose derivatives. Quantification and taste addition experiments confirmed their roles in enhancing the umami taste. This study provides a novel perspective on the taste-modifying compounds in tea, potentially guiding quality improvement efforts.

Analysis of In Vivo Plant Volatiles Using Active Sampling and TD-GC×GC-TOFMS

Schmidt and colleagues in Metabolites presented a novel in vivo active sampling method for analyzing plant volatile organic compounds (VOCs) using thermal desorption tubes and comprehensive two-dimensional gas chromatography coupled to time-of-flight mass spectrometry (TD-GC×GC-TOFMS). This technique offers broader compound coverage and larger peak areas compared to traditional methods like solid-phase microextraction. By successfully applying it to various plant species, the method demonstrates versatility and reliability for plant VOC analysis, aiding research in plant physiology and ecology.

Metabolomics in Cancer Research

Advancements in metabolomics are deepening our understanding of cancer biology, offering new insights into tumor metabolism, progression, and therapeutic resistance. This month's featured studies explore metabolic heterogeneity in colorectal cancer, the influence of the tumor microenvironment and metabolic reprogramming in gastrointestinal cancers, strategies to overcome drug resistance in renal cell carcinoma via metabolic remodeling, and the role of metabolomic pathways in neuroblastoma. Collectively, these works underscore the critical role of metabolomics in identifying novel therapeutic targets and strategies to improve cancer treatment outcomes.

<u>Charting the metabolic biogeography of the colorectum in cancer: challenging the right</u> <u>sided versus left sided classification</u>

Jain and colleagues in Molecular Cancer conducted a comprehensive metabolomic profiling of colorectal cancer (CRC) along seven subsites of the colorectum using liquid chromatographymass spectrometry on 372 patient-matched tumor and normal mucosa tissues. They identified significant metabolic heterogeneity and gradual changes in metabolite abundances from cecum to rectum, including bile acids and amino acids. Their findings challenge the conventional right-sided vs. left-sided CRC classification and reveal distinct metabolites associated with patient survival unique to each subsite. An interactive and publicly accessible CRC metabolome database was developed to facilitate further research.

Emerging Trends in Gastrointestinal Cancer Targeted Therapies: Harnessing Tumor Microenvironment, Immune Factors, and Metabolomics Insights

Rauth and colleagues in Gastroenterology reviewed the influence of the tumor microenvironment on gastrointestinal (GI) cancers and the implications for treatment. They highlighted how components like fibroblasts, extracellular matrices, microbiome, immune cells, and the enteric nervous system modulate tumor cell functions. The review emphasized metabolic reprogramming as a hallmark of tumor cells and discussed how understanding these metabolic alterations could lead to new therapeutic strategies. They also summarized current targeted agents under study for GI cancers, pointing to the potential of metabolomics in developing effective treatments.

Engineered Biomimetic Nanovesicles Synergistically Remodel Folate-Nucleotide and y-Aminobutyric Acid Metabolism to Overcome Sunitinib-Resistant Renal Cell Carcinoma

Lv and colleagues in ACS Nano designed CD276-CD133 dual-targeting biomimetic nanovesicles to overcome sunitinib-resistant clear cell renal cell carcinoma (ccRCC). By targeting the metabolic enzyme MTHFD2 and using manganese dioxide nanoparticles to remodel gamma-aminobutyric acid (GABA) metabolism, they demonstrated that these nanovesicles deactivated the epithelial-mesenchymal transition process and reconstructed the tumor microenvironment. In immune-humanized mouse models, the treatment overcame drug resistance, reduced recurrence, and inhibited metastasis by remodeling cellular metabolism pathways.

Spliceosomal vulnerability of MYCN-amplified neuroblastoma is contingent on PRMT5-

mediated regulation of epitranscriptomic and metabolomic pathways.

Bojko and colleagues in Cancer Letters investigated the therapeutic potential of PRMT5 inhibition in MYCN-amplified neuroblastoma. They found that the selective PRMT5 inhibitor GSK3203591 induced growth inhibition and apoptosis in MYCN-dependent neuroblastoma cells. RNA sequencing revealed deregulated MYCN transcriptional programs and altered mRNA splicing, converging on key metabolic pathways such as glutamine metabolism. In vivo studies confirmed the efficacy of PRMT5 inhibition, highlighting the critical role of epitranscriptomic and metabolomic pathways in the sensitivity of neuroblastoma to this therapeutic strategy.

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Metabolomics Events

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

Venue: Online

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

Short description of the course: Where do you start when a multitude of approaches exist to address the challenge of metabolite identification? There are so many options from mass spectral library searches, *in silico* fragmentation tools, and database searching. We will provide tips on how to explore the landscape of compound identification, leverage *in silco* fragmentation tools, and gain valuable hands-on experience by using real-world challenges.

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

Join the course

Imperial College London Metabolomics training course: Hands-on Data Analysis for Metabolic Profiling December 9-13, 2024

Venue: Online

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

The deadline for registering is November 29, 2024.

For more information and to register, click here.

Check for more details about the course

MANA SODAMeet

December 10, 2024

Venue: Online

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

relevant information on these software/data presented.

Join the web seminar

GRC: Metabolomics and Human Health - The Interaction Between Humans, Lifestyles and the Environment Viewed through Metabolism February 2 - 7, 2025

Venue: Ventura, California, USA

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

Apply now

6th Annual Canadian Metabolomics Conference (CanMetCon) 2025 April 24 - 25, 2025

Venue: Montreal, QC, Canada

The 6th Canadian Metabolomics Conference (CanMetCon) 2025 will be held at New Residence Hall, McGill University, Montreal, Quebec on April 24th–25th.

This year's conference is themed "Clinical Metabolomics". Our proposed program on day 2 features four broad topics in the applications of metabolomics, focusing on Clinical Metabolomics, Computational Metabolomics and Machine Learning, Metabolomics of Nutrition and Health, and Public Health and Population Metabolomics.

Mark your calendars and stay tuned for more details.

Check for more details

EMBL-EBI Introduction to Metabolomics Analysis Course May 20 - 23, 2025

Venue: Hinxton, United Kingdom

This course will provide an introduction to metabolomics through lectures and hands-on sessions, using publicly available data, software, and tools. Participants will become familiar with standardised workflows as well as with the current state of experimental design, data acquisition (LC-MS, MS imaging), processing, and modelling. In addition, they will learn about community standards and sharing in metabolomics, particularly through the use of EMBL-EBI's MetaboLights repository and Galaxy infrastructure. Participants will learn through hands-on tutorials to use tools available for data analysis and data submission. Additionally, case studies will be discussed to show how to employ the week's learning.

Check for more details

21st Annual Conference of the Metabolomics Society Metabolomics 2025

June 22 - 26, 2025

Venue: Prague, Czech Republic

21st Annual International Metabolomics Conference of the Metabolomics Society will be held on June 22-26, 2024 in Prague, Czech Republic. The conference will follow the same pattern as previous years, with Workshops taking place on Sunday and Monday, and the full conference beginning on Monday afternoon, and running through Thursday afternoon.

Call for workshops are now open - <u>click here</u> for details.

Check for more details

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

Certified reference materials (CRM) values provide a known and standardized reference point against which the results of a metabolomic study can be compared. However, the certification of hundreds of individual metabolites is a cumbersome and time-consuming process. The Standard Reference Material (SRM) 1950, Metabolites in Frozen Human Plasma, is by far the most used reference material by the metabolomics community. NIST SRM 1950 provides certified and/or reference values for select metabolites and lipids such as fatty acids, electrolytes, vitamins, hormones, and amino acids. The metabolomics community would greatly benefit from consensus values and identification of metabolites and lipids in SRM 1950 that are not tied to a single analytical platform or method. This increases the accuracy, reliability, harmonization, and meaningful comparisons of metabolomic studies utilizing the material. Additionally, having more values and information available for SRM 1950 metabolites and lipids would allow researchers to investigate a broader range of analytes in their studies, which in turn could lead to a better understanding of the underlying biology of the metabolic processes. To that end, the Reference and Test Materials Working Group of mQACC is actively collecting information on qualitative identifications and quantitative values of metabolites and lipids in NIST SRM 1950 beyond those listed on the NIST Certificate of Analysis. Any data from instrumental platforms with compound identification (LC-MS, GC-MS, NMR) are welcome to participate. The data was combined in order to produce a publicly available database of community-generated 1) consensus concentration values for quantified metabolites and lipids of critical interest within the community and 2) compounds identified but not quantified in SRM 1950.

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

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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
Chromatography and Mass Spectrometry Technologist	The James Hutton Institute	Dundee, United Kingdom	<u>The James Hutton</u> <u>Institute</u>
Postdoctoral Research Fellow Positions in Exposomics and Environmental Health	Department of Environmental Health at the Harvard T.H. Chan School of Public Health	Boston, MA, United States	Department of Environmental Health at the Harvard T.H. Chan School of Public Health
Post Doctoral Fellow in Clinical Exposomics	Emory University	Atlanta, GA, United States	Emory University
Data Scientist / Senior Data Scientist		Oxford, England	<u>Metabolomics</u> <u>Society</u>

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Fill Out Your Survey Here

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

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