MetaboNews

This month in metabolomics

December, 2025
Vol 15, Issue 12

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

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|MC:SUBJECT|

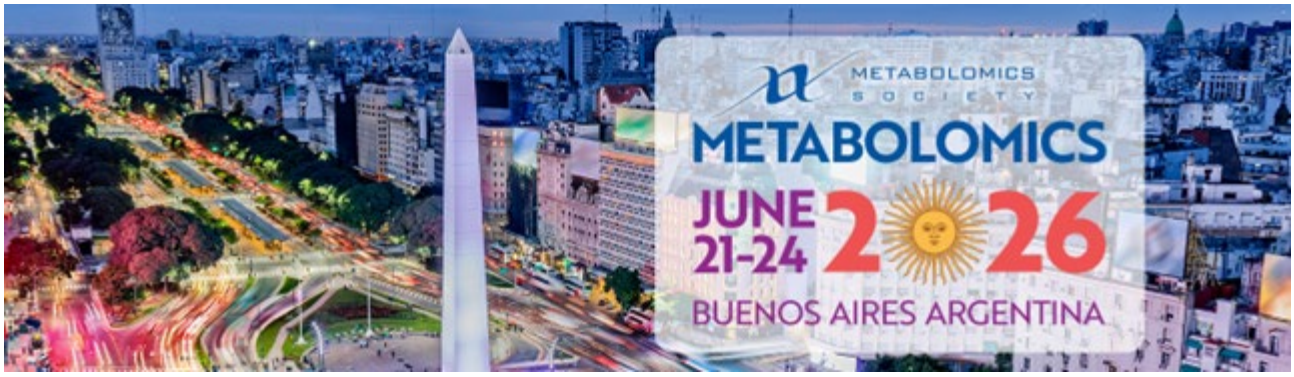
Metabolomics Society News

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

International Affiliates' Corner



See you in Buenos Aires!
We are delighted to invite you to the 22nd International Conference of the Metabolomics Society, Metabolomics 2026. Buenos Aires, Argentina is excited to welcome you! This is the first time the conference will be held in South America.

Save the date for June 21-24, 2026.
All conference activities will take place at the Buenos Aires Convention Center (CEC).

Buenos Aires is known for its vibrant cultural scene with rich food experiences, urban art displays, and lively dance performances. BA is the largest city in and capital city of Argentina, ready to welcome the metabolomics community to engage in science and

technology. Come for the educational content, stay to dance tango!

Check the website often for updates: www.metabolomics2026.org
Follow along on LinkedIn for updates about the Society and the conference.

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 workshop application online before January 30, 2026.

Calling all Sponsors!
The **Sponsorship Brochure** is available!

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, including a few new opportunities to position your brand and product at the forefront of the scientific community. Spots are limited and available on a first-paid, first-served basis, do not delay!

Members Corner

Early-career Members Network (EMN)

EMN Webinars 2025

December Webinar
The EMN committee extends its gratitude to **Dr. Marcos Y. Yoshinaga** from Universidade Cruzeiro do Sul, Brazil and founder of PinguisLab for the December webinar entitled "*Bridging Research and Industry with Precision Lipidomics*". The webinar recording will be available on the MetSoc website: https://metabolomicssociety.org/resources/multimedia/emn-webinars-2025/.

Keep an eye on your inbox for future email blasts and make sure to follow us on social media: Twitter [metabolomicscentre.us21.list-manage.com] and LinkedIn [metabolomicscentre.us21.list-manage.com]!

We strive to ensure geographical diversity in our webinars and would like to invite researchers, especially those from Africa and Asia, to participate in our webinars. If you are interested, or want to recommend someone from your network, please reach out to info.emn@metabolomicssociety.org.

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MetaboInterview

This MetaboInterview series highlights up-and-comers in the field of Canadian metabolomics, and award winners at the 2025 Canadian Metabolomics Conference

Ana Stanciu

Ana's research with the Britz Group started when she did a senior undergrad thesis research project. From there, she continued with an 8-month co-op in which she worked on multiple metabolomic themed projects that focused on nutrition and preventative health. Once she started her Master's, her first project involved a cross-platform metabolomic analysis of repeat serum samples from critically ill patients with severe burn injury in the hopes of finding a biomarker that could predict serious outcomes, such as sepsis or death. Once this project is complete, she will pivot towards developing methods for assessing nutritional status using liquid-chromatography mass spectrometry (LC-MS) and capillary electrophoresis-mass spectrometry (CE-MS) potentially making these assays widely available to the general public in order to promote healthy living and highlight the

importance of nutrition and lifestyle for chronic disease prevention.

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

My journey with metabolomics started by chance when I came across Dr. Britz-McKibbin's research. What started as a co-op opportunity during my undergraduate degree developed into my role today as a graduate student. What I found most interesting about metabolomics research was the thousands of analytes waiting to be detected and quantified. It seems that the biological interpretations and applications in metabolomics research are endless. Metabolomics research also helps bridge laboratory and experimental work directly to clinical applications for improved patient care, which I find quite satisfying.

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

I’m in the final stages of my first research project that aims to identify biochemical signatures for early detection of sepsis risk in burn patients in a critical care setting. Although challenging at times, this project has been very fulfilling since it’s my first completely independent research project as part of a unique collaboration with colleagues from Hamilton General Hospital. From sample preparation, data acquisition, data processing, and statistical analysis to clinical interpretation, I can fully appreciate the entire metabolomics workflow. Since September, I have been mentoring a fourth-year undergraduate thesis student as we are working towards developing a rapid LC-MS assay for the determination of phosphatidylethanol species in dried blood spots to assess changes in alcohol consumption. This work is being completed in collaboration with colleagues from Public Health Ontario as they are interested in correlating the results of this assay with participant self-reports of alcohol consumption as part of a future trial examining behavioral modifications using alcohol labeling. In the future, I plan to begin the development of a comprehensive LC-MS assay for the measurement of fat-soluble vitamins in blood to pursue more nutritional focused metabolomics research. Proper nutrition and healthy living are things that I value, providing me plenty of motivation for my research projects/goals.

3. What excites you most about the potential of metabolomics in your research?

Metabolomics can be applied to so many different patient populations and study types, meaning its applications are quite diverse. I have definitely developed a deeper appreciation of severe burn injuries and what such patients experience given my current research. I'm excited to continue applying metabolomics to better understand unique phenotypic differences in this patient population since burn injuries have historically been quite underappreciated. I also enjoy coming up with different comparisons to make with data exploration and hypothesis generation. For example, in one comparison, I decided to use data from samples collected just prior to sepsis diagnosis to see if there were viable metabolic signatures that could potentially serve as prognostic biomarkers.

4. Can you describe the metabolomics methodologies you use, particularly the application of capillary electrophoresis-mass spectrometry (CE-MS), and why they are suited to your projects?

Our lab group is recognized for developing capillary electrophoresis-mass spectrometry (CE-MS) for biomarker discovery that is well suited for characterization of the ionic metabolome. My study specifically implemented multisegment injection-capillary electrophoresis-mass spectrometry (MSI-CE-MS), a multiplexed microseparation platform for high-throughput analysis. MSI-CE-MS can analyze up to 13 samples within a single analytical run as compared to conventional single-injection methods, which greatly increases sample throughput while reducing operating costs with stringent quality control. Despite this throughput benefit, MSI-CE-MS can suffer from poor concentration sensitivity that can limit metabolome coverage for detection of low abundance metabolites. For my untargeted analysis, we used our on-line preconcentration CE-MS configuration to expand overall metabolome coverage. Other benefits of CE that often get overlooked are its low sample volume requirements as required for analysis of volume-limited samples. CE is also a "greener" analytical platform compared to other alternatives like LC, since it does not require use of large volumes of organic solvents for elution.

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

One of the main challenges in metabolomics is reliable molecular feature annotation given

the large number of redundant and spurious signals when using mass spectrometry. As I was working on my untargeted analysis for my first project, it was overwhelming to establish which signals were metabolically relevant versus features which were redundant like adducts, fragments, or isotopic peaks. I have approached some of my other challenges using basic CE theory. Using this theory, proper metabolite identification is achieved since electrophoretic mobility is dependent on fundamental physicochemical properties of an ion, such as hydrodynamic radius and effective charge. I can also use structural information to make predictions about how these metabolites migrate and can exclude isobaric candidates if they are electrically neutral, since these species are not amenable to CE separations. Of course, we always confirm the identity of metabolites by MS/MS and their co-migration with spike experiments to unambiguously identify molecular features of clinical significance.

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6. What general advice would you give early-career researchers about selecting appropriate metabolomics platforms and methods for clinical applications?

It’s hard to give advice to early-career researchers in the early stages of my own academic career! For clinical researchers, especially those doing biomarker discovery, I would say it is important that having putative biomarkers confirmed using different analytical platforms helps validate findings and proves the robustness of your results. For example, creatinine is an indicator of impaired kidney function and one of the predictors of sepsis onset, is measured regularly in the clinical laboratory by Jaffe reaction; however, we can also measure it using CE-MS in our lab. By reporting biomarkers that can be measured by multiple platforms, I believe this would ensure easier translation to the clinic. Metabolomics platforms and methods should also be highly sensitive and have a relatively quick analysis time.

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7. Beyond your specific study, how do you see metabolomics evolving in terms of technology and methodology in the next five years?

I definitely expect machine learning and artificial intelligence to dramatically influence the field over the coming years. I think it will be particularly useful when it comes to peak picking, identification, and combining/interpreting multi-omic data. This will massively decrease data pre-processing time while ensuring robust data is generated and reported. Using machine learning for multi-omics studies could provide a more holistic perspective on biological processes and metabolic pathways.

8. How do metabolomics approaches you've utilized complement other omics technologies?

Metabolomics complements other -omics technologies by capturing the exact physiological state or phenotype of, in my case, a burn patient. My analysis shows unique serum metabolomic profiles in burn patients, a high-risk patient population. It's more challenging to capture these dynamic changes using genomics, transcriptomics, or proteomics, whereas metabolomics combines the upstream –omics disciplines and can assess, for example, changes in biochemical pathways regulated by certain gene variants or therapeutic interventions which can ultimately impact the clinical outcomes for individual patients.

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9. In your experience, what are the biggest methodological gaps or limitations currently facing metabolomics research?

Personally, I would love to see more advancements for data pre-processing. Data acquisition can be quick and easily automated! Data pre-processing, especially for multiplexed CE-MS based metabolomic data sets, can be cumbersome! One of the main challenges with CE analysis is large shifts in migration time due to changes in the electroosmotic flow over batches of runs which limit the ability to use conventional metabolomics software and peak picking integration. Our lab is developing a software called PeakMeister to overcome this challenge to allow for rapid and standardized MSI-CE-MS data pre-processing. I have gained experience using other software tools like MZmine to process LC-MS based lipidomic data which works well to automatically integrate peaks, but even this software tool requires manual confirmation that each peak is picked successfully.

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10. What role does collaboration play in your metabolomics research?

Collaborative efforts are what makes metabolomics research the most impactful. I'm very lucky to be a part of an interesting project that arose when Dr. Marc Jeschke, who is a critical care physician from Hamilton Health Sciences, reached out to collaborate with our group to perform metabolomic and lipidomic analysis of serum samples from burn patients. Although these collaborations are very rewarding, at times it can be challenging to balance the needs and expectations of our collaborators. Our research group strives to provide high quality data that satisfies stringent quality control measures to dive deep into the data

and validate our findings prior to data sharing. But these collaborative contributions help to bring in different perspectives and clinical expertise critical for translational science. In my case, working with Dr. Jeschke, a renowned burn surgeon, has been valuable given what he is able to bring to the project. We are also beginning a collaboration with public health research scientists to develop a method for phosphatidylethanol species in dried blood spots for robust determination of recent alcohol exposure. This is needed to better validate the utility of labeling strategies to reduce overall alcohol consumption patterns since ethanol is a group 1 carcinogen. It's always exciting when our work is translatable to the real-world, studies, which is only possible thanks to our collaborators' expertise.

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Spotlight Article

TMIC 2025: A Year of Meaningful Progress and Collaboration

A look though this year's highlights at The Metabolomics Innovation Centre. From advancing technologies in metabolomics to building strong connections with our partners and the community our year was filled with many milestone. Take a look through TMIC's 2025 down below:

Canadian Metabolomics Conference 2025

TMIC hosted the 6th annual Canadian Metabolomics Conference on April 24-25th in Montreal, Canada. This year's conference featured topics in the applications of metabolomics, with sessions on Clinical Metabolomics, Computational Metabolomics and Machine Learning, Metabolomics of Nutrition and Health, and Public Health and Population Metabolomics.

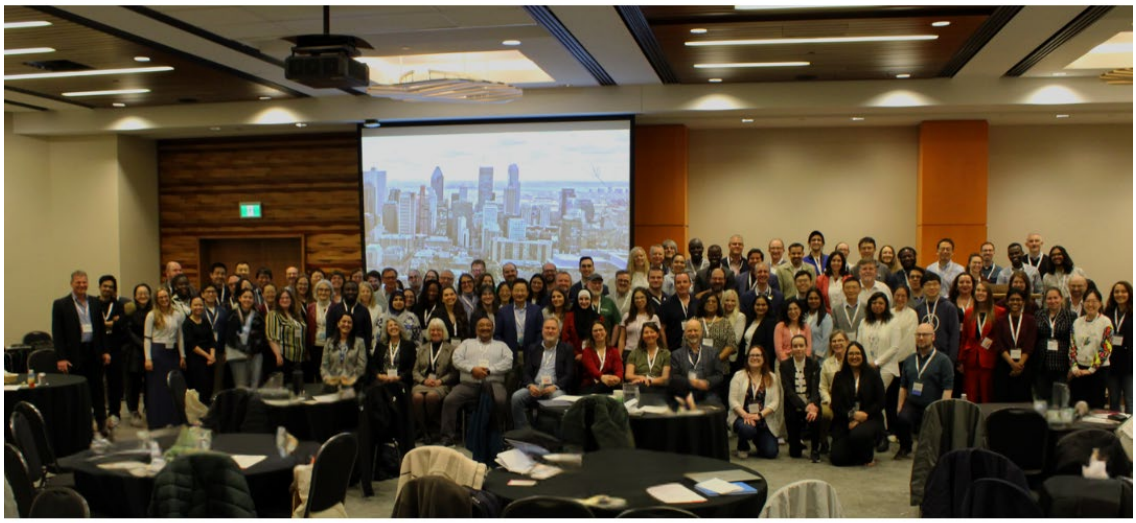
The conference featured plenary presentations from Dr. Erin Baker, Dr. Gary Suzidak, and Dr. Mary-Ellen Harper, as well as, oral and poster presentations, and lightning talks from participants.

Thank you again to all the attendees for your participation and engagement, and to our event sponsors, without whom we wouldn't be able to deliver on our commitment to an accessible annual metabolomics conference in Canada. We look forward to welcoming you all at CanMetCon 2026 in Toronto!

TMIC

6th Annual Canadian Metabolomics Conference 2025
April 24-25, 2024 - New Residence Hall, McGill, Canada

McGill University



Agilent BRUKER ZefSci LINEARIS ThermoFisher SCIENTIFIC Waters SCIEX
cmbio LGC trc metabolites GenomeQuébec MS ACL Genome Alberta MRM Proteomics

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Awards & Recognitions

1. Dr. David Wishart won the Gerard Herzberg Gold Medal Award
2. Dr. Tao Huan, TMIC Node Leader, awarded the 2025 President's Award by Metabolomics Society
3. Dr. David Wishart, TMIC Node Leader, was awarded the 2025 ASTech Award in the AI/ML & Quantum category

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Technology Advancements for Metabolomics Services

With continued support from Genome Canada and Genome Alberta, in partnership with the Canada Foundation for Innovation (CFI), TMIC successfully launched new service offerings in 2025, including SHARP and TMIC GIGA further expanding access to advanced genomics and metabolomics technologies.

1. Originally introduced in **2024** for cell samples, the **Small-Scale Highly Accurate and Reproducible Platform Metabolomics (SHARP)** was fully launched in 2025, expanding its capabilities to include blood-based samples such as plasma and serum. This enhanced service empowers researchers working with minimal sample

volumes by delivering high-sensitivity metabolome profiling using advanced liquid chromatography–mass spectrometry (LC-MS). By leveraging TMIC's signature Chemical Isotope Labeling (CIL) LC-MS technology, SHARP improves metabolite detection and enables confident compound identification, bridging the gap between analytical power and limited sample availability.

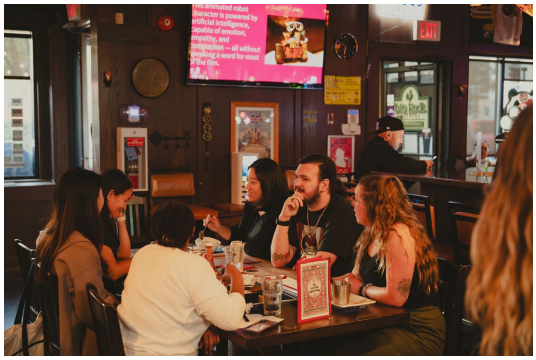
2. Expanded in 2025, the **TMIC GIGA Assay** delivers comprehensive, targeted metabolomic analysis across an extensive range of biological matrices, including plasma, serum, urine, tissue, milk, CSF, cell media and cells. This enhanced service enables the identification and absolute quantification of up to 1,780 metabolites, encompassing clinical biomarkers, exposomic compounds, and microbial metabolites across 38 chemical classes, along with 900+ metabolite sums and ratios.

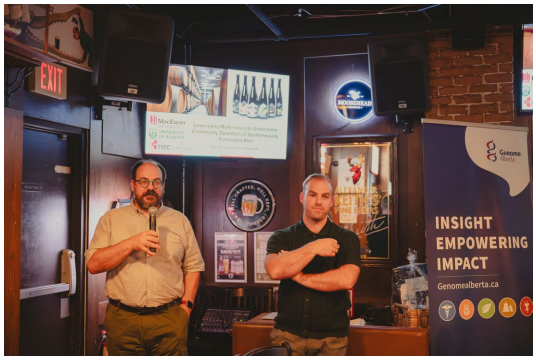
Double Helix & Friends Trivia Night

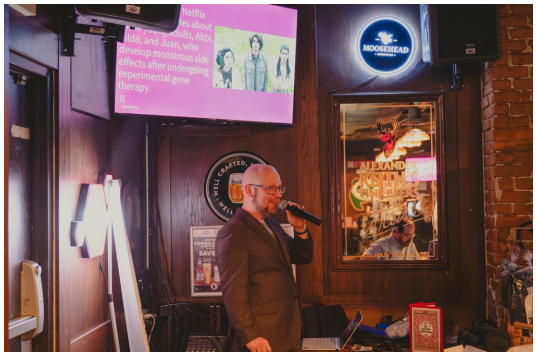
This year TMIC partnered with Genome Alberta to host a trivia night during the Life Science Week organized by Applied Pharmaceutical Innovation (API).

The night featured DNA-themed music rounds to science-meets-pop-culture questions and a special beer-omics talk by Dr. James Harynuk and Dr. Benjamin Bourrie.

Thank you to all the participants and congratulations to the winning teams!

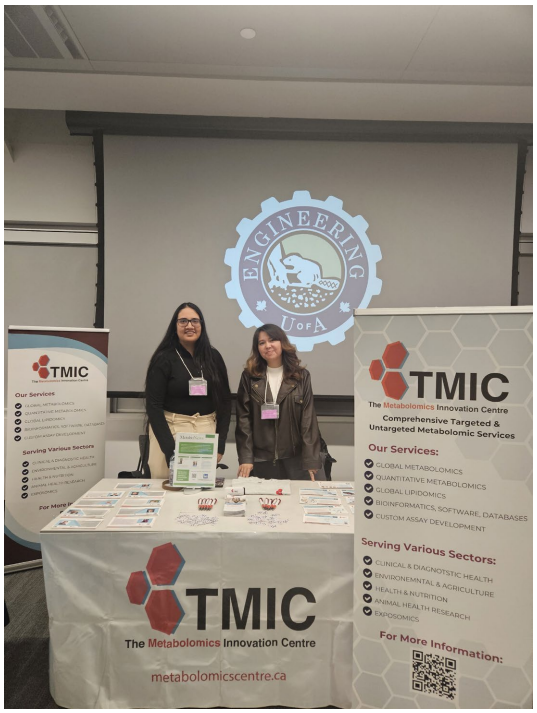


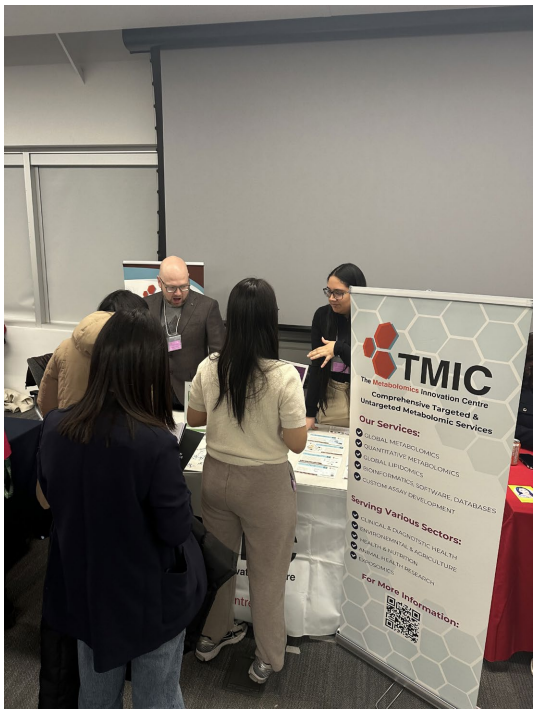




Conferences

Advancing metabolomics research and broadening its visibility continued to be a key priority for TMIC in 2025. TMIC Nodes highlighted their latest work at major national and international conferences, including MANA, ASMS 2025, WISER, and MetSoc 2025.





2025 Top 5 Publications

1. Metabolites are not genes — avoiding the misuse of pathway analysis in metabolomics
2. Effects of lyophilised faecal filtrate compared with lyophilised donor stool on *Clostridioides difficile* recurrence: a multicentre, randomised, double-blinded, non-inferiority trial
3. Cardiometabolic benefits of a non-industrialized-type diet are linked to gut microbiome modulation
4. MarkerDB 2.0: a comprehensive molecular biomarker database for 2025

5. Comprehensive, Quantitative Analysis of SRM 1950: the NIST Human Plasma Reference Material

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Happy Holidays and Best Wishes for the New Year!

It has been a busy year here at TMIC, as we look back on another year of collaboration, innovation and progress in this field, the discoveries made by our scientific team, and some of the recognition we have been honoured to receive. It really is a privilege to coordinate and work with some of the top talent in this field, and contribute to Canada's international leadership as the field continues to grow and develop. Looking forward to a productive 2026!

- The Metabolomics Innovation Centre (TMIC)

MetaboReads

Immunometabolic inflammation and barrier biology in complex disease

Across inflammatory skin, pancreatic, and airway disease models, these studies converge on a recurring logic: immune pathways are not merely accompanied by metabolic change, they are organized by it. NLR-family inflammasome signaling, type 2 airway inflammation, and IL-17-driven programs are repeatedly linked to shifts in purine, lipid, and amino acid metabolism that can be read out in tissue and plasma. A notable strength is the use of integrated designs that connect molecular targets to multi-omics signatures and, in the case of pancreatitis, to causal microbiota transfer. The field is now positioned to test whether metabolite-defined axes, such as eicosanoid and purine modules, can provide earlier diagnosis and more actionable target selection than cytokines alone.

Exploring therapeutic mechanism of Fuzhenghefuzhiyang Formula in psoriasis: inflammation and metabolism regulation.

Tang and colleagues in FRONTIERS IN IMMUNOLOGY showed that the topical herbal formula Fuzhenghefuzhiyang (FZHFZY) ameliorated erythema, scaling, and epidermal thickening in a psoriasis-like mouse model while reshaping lesion immune and metabolic states. Network pharmacology pointed to pathways spanning inflammation, proliferation, pyroptosis, and metabolism, providing an a priori target map for multi-omics validation. Transcriptomic profiling of lesional skin highlighted modulation of NOD-like receptor and IL-17 signaling, and RT-PCR corroborated downregulation of IL-17 and NLRP3 transcripts. Lesion metabolomics identified 169 differential metabolites, with FZHFZY regulating carbohydrate and purine catabolism and broad

amino acid metabolism, alongside ether lipid metabolism. Cross-omics integration implicated purine and ether lipid metabolism as coupled to key nodes within the NLR signaling network, suggesting an immunometabolic mechanism for clinical benefit.

Astragalin attenuates caerulein-induced acute pancreatitis by targeting the NLRP3 signaling pathway and gut microbiota.

Jia and colleagues in BIORESOURCES AND BIOPROCESSING found that astragalin protected pancreatic acinar cells and reduced tissue injury, apoptosis, and systemic inflammation in a caerulein-induced acute pancreatitis mouse model. By combining network pharmacology with RNA sequencing, the authors prioritized NLRP3 signaling as a central pathway, then supported target engagement with molecular docking and western blot validation. Metagenomics and metabolomics extended the mechanism upstream, showing that astragalin restored microbial diversity, shifted community composition, and rewired metabolite profiles linked to amino acid and tryptophan-related pathways. A correlation network highlighted specific taxa (including Lachnoclostridium, Roseburia, and Anaerobutyricum) connected to a set of 22 metabolites and NLRP3-related genes, providing a tractable microbial-metabolic module. Fecal microbiota transplantation transferred protection, strengthening the case that astragalin's efficacy is mediated in part through microbiota-dependent immunometabolic regulation.

Multiomics and Machine Learning Reveal Distinct Immune-Metabolic Signatures and Diagnostic Biomarkers for Asthma Inflammatory Endotypes.

Liu and colleagues in ACS OMEGA showed that eosinophilic and neutrophilic asthma endotypes can be separated by distinct immune-metabolic programs captured through integrated sputum proteomics and metabolomics. Network analysis and immune deconvolution linked eosinophilic disease to Th2-associated signaling with dysregulated histidine and purine metabolism, whereas neutrophilic asthma was characterized by oxidative stress, hypoxia-associated signaling, and perturbed arginine metabolism. The authors used multiple machine-learning strategies to define diagnostic panels, reporting strong discrimination of asthma versus controls with a seven-protein model and accurate endotype stratification with two overlapping biomarkers. Pathway-level differences, including ROS metabolism and cytokine production in eosinophilic disease and NF-kappa B and hypoxia responses in neutrophilic disease, offer mechanistic hypotheses that align with therapeutic heterogeneity. The work illustrates how multi-omics feature selection can translate airway biology into noninvasive diagnostic models that are plausibly actionable in precision care.

Metabolomics reveals pro-inflammatory effects of 12R-HETE and ALOX12B in maternal allergic asthma.

Wang and colleagues in COMMUNICATIONS BIOLOGY found that house dust mite exposure during pregnancy drives a metabolite-linked amplification of type 2 airway inflammation in both dams and offspring. Untargeted HILIC-MS profiling identified broad metabolic differences across groups, and targeted analysis singled out 12R-HETE as consistently elevated in plasma and lung tissue in the allergic asthma model. The authors linked this signature to increased expression of ALOX12B in bronchial epithelium by immunohistochemistry, positioning a defined enzymatic

source for the eicosanoid signal. In bronchial epithelial cells, ALOX12B overexpression increased inflammatory mediators including IL-33 and IL-6, whereas knockdown reduced these responses, supporting a causal role for the pathway. Together, the data nominate 12R-HETE and ALOX12B as candidate biomarkers and intervention targets for pregnancy-associated allergic asthma, a setting in which early detection remains clinically constrained.

Microbiome-derived metabolites and metabolic resilience

These papers reinforce a shift from associational microbiome studies toward mechanistic, metabolite-centered models of metabolic disease. Interventions as different as a tamarind-derived polysaccharide, a defined microbial biogenic amine, and a short-chain fatty acid converge on a shared readout: changes in insulin signaling and lipid handling that can be indexed by targeted metabolite pathways and, in the strongest cases, by fecal transfer experiments. Notably, the tyramine study links microbial metabolite exposure to intestinal barrier dysfunction, aligning gut permeability with hepatic lipid accumulation through PPAR-regulated processes. At the same time, the butyrate work highlights that even simplified in vitro systems can map transcriptional nodes in insulin signaling that are plausibly responsive to microbial metabolites. The next conceptual step will be to integrate these mechanistic signals into scalable biomarkers that retain causal interpretability in heterogeneous human populations.

Tamarind Seed-Derived Xyloglucan Attenuates Insulin Resistance in Mice through Gut Microbiota.

Yang and colleagues in JOURNAL OF AGRICULTURAL AND FOOD CHEMISTRY showed that a tamarind seed xyloglucan improved glucose tolerance and liver function in high-fat diet mice, while reducing inflammation and oxidative stress. By pairing 16S profiling with metabolomics, the authors linked benefit to shifts in carnitine and tryptophan metabolism and to selective enrichment of Bifidobacterium. A key mechanistic test came from fecal microbiota transplantation, which transferred the metabolic improvements to recipient mice. Antibiotic depletion abolished the effect, indicating that the polysaccharide acts through a microbiota-dependent pathway rather than direct host pharmacology. The study supports the view that food-grade polysaccharides can function as microbiome modulators with measurable downstream metabolic signatures.

Gut microbial tyramine facilitates intestinal damage and metabolic dysfunction-associated steatotic liver disease development.

Wei and colleagues in BMC MEDICINE found that gut microbial tyramine promotes intestinal barrier disruption and accelerates metabolic dysfunction-associated steatotic liver disease (MASLD) in pediatric-relevant contexts. Using Enterococcus faecium B6 and tyramine supplementation in mice, the authors showed increased intestinal permeability alongside a hepatic phenotype marked by lipid accumulation. Integrated liver transcriptomics and proteomics implicated PPAR signaling, and targeted validation suggested tyramine increases lipid synthesis and uptake while suppressing beta-oxidation. Targeted metabolomics in a hospital-based pediatric cohort identified higher fecal tyramine in MASLD cases, and a larger school-based

sample linked high serum tyramine to elevated disease risk. The work provides a coherent mechanistic chain from a specific microbial metabolite to barrier injury and hepatic lipid handling, with supportive human association across study designs.

Butyrate-Mediated Upregulation of Insulin Pathway Gene Expression Suggests Potential Antidiabetic Effects.

Shapira and colleagues in DRUG DEVELOPMENT RESEARCH showed that sodium butyrate exposure increased transcription of selected insulin pathway genes in human lymphoblastoid cell lines from healthy donors. Using targeted RT-PCR after 48 hours of treatment, the authors observed upregulation of MT2A, RRAGD, IGF1R, OXTR, and INSR, while other preselected insulin-related genes were unchanged. The design is intentionally reductionist, prioritizing a direct host-cell readout that complements the extensive in vivo literature from rodent models. Although the work is preliminary and does not establish physiological benefit, it nominates specific transcriptional nodes through which butyrate could modulate insulin responsiveness. The study motivates follow-on experiments that connect gene expression changes to protein-level signaling and metabolomic endpoints in disease-relevant tissues.

Metabolic reprogramming in cancer and therapy-related toxicity

Cancer metabolism remains most informative when it is interpreted in context, and these studies explicitly place metabolic state within microenvironmental signaling, therapy response, and cell fate transitions. Purine metabolism emerges as a recurrent axis, appearing both as a driver of tumor-immune interactions and as a transcriptionally anchored module with prognostic value. At the same time, lipid-associated metabolites at diagnosis forecast chemotherapy hepatotoxicity in pediatric leukemia, underscoring that pre-treatment metabolic phenotypes can condition adverse outcomes. Finally, the senescence study frames polyamine dynamics as a timed checkpoint that integrates oncogenic signaling with irreversible growth arrest. Together, the section illustrates the value of metabolomics when coupled to perturbation experiments and clinically anchored endpoints.

Metabolomic and transcriptomic profiling of HNSCC identifies AMIGO2 as a therapeutic target modulating tumor microenvironment.

Liu and colleagues in NPJ PRECISION ONCOLOGY showed that head and neck squamous cell carcinoma progression is accompanied by spatially resolved metabolic heterogeneity, with prominent enrichment of purine metabolism during malignant transformation. By integrating spatial metabolomics and transcriptomics with single-cell and bulk data, the authors derived a ligand-receptor-based signature linked to NT5E that stratified prognosis and immunotherapy responsiveness. Low-signature tumors exhibited greater immune infiltration and improved response to immunotherapy, suggesting that the purine-associated signaling state reflects an immunologically permissive microenvironment. Functional validation identified AMIGO2 as a core regulator of tumor-associated purine metabolism, with AMIGO2 downregulation suppressing invasion and myofibroblast differentiation while increasing immune effector infiltration. Combining AMIGO2 targeting with anti-PD-1 therapy enhanced efficacy, positioning purine-modulating nodes as rational combinatorial targets in immuno-oncology.

An analysis of diagnostic metabolomic profiles associated with hepatotoxicity during childhood ALL induction therapy.

Mason and colleagues in BLOOD ADVANCES found that specific phosphatidylcholine-related metabolites present at ALL diagnosis are associated with subsequent hepatotoxicity during induction chemotherapy. In a discovery and replication design spanning 314 pediatric patients, untargeted profiling measured 519 metabolites and linked pre-treatment metabolite levels to grade 3 or higher transaminitis and to conjugated hyperbilirubinemia. Two glycerophosphocholine species replicated as predictors of transaminitis, with effect estimates persisting after adjustment for demographic and treatment intensity covariates. A broader metabolite set was associated with conjugated hyperbilirubinemia in the discovery cohort, with 1,2-dipalmitoyl-GPC showing the strongest association. These results suggest that lipid dysregulation may predispose to chemotherapy-related liver injury and support risk stratification efforts that begin at diagnosis rather than after toxicity emerges.

Putrescine functions as a metabolic checkpoint in replication stress-induced senescence.

Vasilogiannakopoulou and colleagues in CELLULAR AND MOLECULAR LIFE SCIENCES showed that intracellular putrescine dynamics act as a timed metabolic checkpoint governing replication stress-induced senescence. In a CDC6-induction model in human bronchial epithelial cells, targeted metabolomics revealed an early rise in putrescine followed by a sharp decline coincident with senescence onset. Putrescine supplementation attenuated senescence, while ODC1 knockdown accelerated senescence and increased TP53 accumulation, supporting functional necessity of the polyamine axis. Mechanistically, ERK and GSK3 beta signaling regulated MYC stability, linking early-phase MYC-driven polyamine biosynthesis to later MYC degradation and commitment to senescence. Reanalysis of single-cell data from COVID pneumonia patients showed elevated CDC6 with reduced MYC and ODC1 in senescence-marked alveolar epithelial cells, suggesting disease-relevant deployment of the same circuit in vivo.

Metabolomics in mental health, neurocognition, and life-course exposure

Metabolomics is increasingly being used as an intermediate phenotype that links psychosocial and occupational exposures to downstream clinical outcomes. The two epidemiologic analyses here highlight that the strongest signals are often modest in magnitude but consistent in direction, implicating glucose regulation, lipid handling, amino acid metabolism, and HPA-axis biology. Importantly, both studies explicitly quantify overlap with depression or dementia-related outcomes, moving beyond single-disorder framing toward shared vulnerability pathways. The EPHOR-NIGHT cohort paper complements these findings by describing a harmonized resource designed to connect shift work exposures to multi-system endpoints using sensors and deep biomarker profiling. As these resources mature, the central challenge will be to distinguish biomarkers of exposure from biomarkers of early disease, and to embed metabolomic measures within causal, longitudinal models.

The Metabolomic Signature of Childhood Trauma.

Souama and colleagues in BIOLOGICAL PSYCHIATRY showed that retrospectively assessed childhood trauma is associated with a dose-dependent plasma metabolomic signature in adults followed longitudinally in NESDA. Using untargeted Metabolon profiling at baseline and 6-year follow-up, mixed-effect models identified 18 trauma-associated metabolites after adjustment for sociodemographic, lifestyle, health, and technical covariates. Upregulated metabolites were nominally enriched for fatty acid and branched-chain amino acid pathways, while downregulated metabolites were enriched for corticosteroids, consistent with metabolic and HPA-axis perturbation. Several metabolites were linked to trauma but not to depression, and findings were partially replicated using an alternative trauma measure and an external sample. The results support a biologically embedded trauma signature that could help explain elevated cardiometabolic and psychiatric risk across the life course.

Comorbidity of undiagnosed mood symptoms with dementia risk in multi-regional multi-ethnic adults: evidence from epidemiological findings and plasma metabolites.

Zhang and colleagues in EPIDEMIOLOGY AND PSYCHIATRIC SCIENCES found that comorbid undiagnosed depressive and manic symptoms are associated with markedly increased long-term dementia risk across multi-regional cohorts. In UK Biobank and three Asian studies, the authors related symptom categories to incident dementia and to domain-specific cognitive outcomes, then examined plasma levels of 168 metabolites as potential explanatory intermediates. Symptom comorbidity was associated with higher dementia risk, particularly Alzheimer's disease, and with worse reasoning and numeric memory alongside evidence of metabolic dysfunction. Glucose and total esterified cholesterol explained a measurable portion of the association, with glucose contributing the largest share. The findings place glucose regulation at a plausible intersection of psychiatric symptom burden and neurodegenerative risk, while also underscoring the importance of detecting subclinical mood symptoms in midlife.

Exposome project for health and occupational research night shift cohort (EPHOR-NIGHT): a unique resource to advance research on night shift work and chronic disease.

Harding and colleagues in BMJ OPEN described the EPHOR-NIGHT cohort, a multi-country resource designed to interrogate how night shift work shapes biological pathways linked to chronic disease. The cohort includes 937 workers across Spain, Sweden, Denmark, and the Netherlands, with harmonized collection of questionnaires, ecological momentary assessments, wearable sensor data, and repeated biospecimens. The platform supports layered molecular profiling including metabolomics, transcriptomics, proteomics, methylation, hormone and inflammatory markers, enabling integrated analyses of cardiometabolic, mental health, cognitive, and biological aging outcomes. Early descriptive results indicate poorer sleep duration and quality among permanent night workers and substantial prevalence of anxiety, depression, and metabolic disturbances. With a two-year follow-up completed in June 2025, the cohort is positioned to move beyond exposure description toward pathway-level mediation analyses that can inform occupational prevention strategies.

Metabolomics across agriculture, plant biology, and fermentation ecosystems

Applied metabolomics increasingly functions as an engineering readout in complex biological systems, whether the goal is crop protection, nutritional enhancement, or fermentation control. The interventions surveyed here span chemical ecology in fungi, physical stimulation of seeds, induced pigment rewiring in ornamentals, rhizosphere manipulation via intercropping, and RNA-based pest control. Across these settings, multi-omics integration is used to translate compositional shifts into plausible mechanisms, for example linking phenolic acids to pathogen suppression or mapping microbial succession to esterification activity in Baijiu. A recurring lesson is that high-dimensional measurements are most persuasive when paired to clear perturbations and to tractable intermediate phenotypes such as specific metabolites or enzyme activities. These studies collectively illustrate how metabolomics can bridge discovery and implementation in agriculture and food systems, while also revealing the complexity that accompanies real-world, multi-organism contexts.

Is heptelidic (koningic) acid a microbial hormone that regulates secondary metabolism in the biocontrol fungus Trichoderma virens?.

Bansal and colleagues in CURRENT GENETICS found that loss of heptelidic acid biosynthesis in Trichoderma virens coincides with broad suppression of secondary metabolite production, consistent with a hormone-like regulatory role. Building on genetic deletions in a terpene cyclase (has1) and other cluster-associated genes, the authors compared wild type to a Delta has1 mutant using transcriptomics and metabolite profiling. The mutant showed widespread transcriptional downregulation, including coordinated suppression of gene clusters responsible for gliovirin, viridin, and related metabolites. Metabolomics corroborated this collapse, failing to detect heptelidic acid and multiple major non-volatile metabolites in the Delta has1 strain. The study supports a model in which heptelidic acid participates in feedback control of secondary metabolism, a concept with implications for biocontrol optimization and natural product engineering.

Laser-driven sustainable modulation of growth, metabolomics, bioactive compounds, and physical attributes in broccoli, radish, and kale sprouts.

Yildiz and colleagues in FOOD CHEMISTRY showed that brief blue-laser seed treatment can enhance the biochemical quality of broccoli, radish, and kale sprouts without chemical inputs. The authors optimized exposure at 450 nm and quantified increases in total phenolics, flavonoids, antioxidant activity, gamma-aminobutyric acid, and phenylalanine ammonia-lyase activity after 120 hours of germination. UHPLC-HRMS metabolomics indicated enrichment of glucosinolate and flavonoid pathways, providing a pathway-level explanation for the improved antioxidant phenotype. Physical analyses including SEM, DSC, and texture testing suggested accompanying changes in surface roughness, thermal stability, and compressibility. The work positions laser priming as a controllable, scalable lever to tune plant specialized metabolism and functional traits in sprouts.

Integrated metabolomic and transcriptomic profiling unveils anthocyanin regulation in chemically induced flower color variation of Impatiens hybrida 'Solarscape'.

Tian and colleagues in BMC PLANT BIOLOGY found that colchicine-induced flower color conversion in Impatiens hybrida 'Solarscape' is underpinned by coordinated remodeling of anthocyanin composition and gene regulation. By integrating metabolomics and transcriptomics across wild-type purple and mutant orange flowers, the authors identified 93 differential metabolites dominated by cyanidin- and pelargonidin-like species. Transcriptome analysis revealed 1888 differentially expressed genes, including canonical biosynthetic enzymes and candidate transcriptional regulators with altered expression in mutant flowers. Co-expression analysis linked specific anthocyanins, such as pelargonidin-3-O-sophoroside and cyanidin derivatives, to multiple genes, indicating a polygenic control architecture. The study provides a molecular framework for breeding ornamental color traits and illustrates how combined omics can resolve pathway control points in plant specialized metabolism.

Mechanism of tobacco-sweet potato intercropping in suppressing Ralstonia solanacearum in flue-cured tobacco.

Yang and colleagues in FRONTIERS IN PLANT SCIENCE showed that tobacco-sweet potato intercropping reduces bacterial wilt incidence and lowers soil Ralstonia solanacearum abundance while reshaping rhizosphere chemistry and microbiota. Comparative profiling between monoculture and intercropping systems linked disease suppression to higher total phenolic acids and to metabolite differences enriched in carbohydrate metabolic pathways. Specific sugars and polyols were positively correlated with pathogen abundance, whereas phenolic acids such as syringic, ferulic, caffeic, and gallic acids were negatively correlated, implicating inhibitory chemical ecology. Metagenomic analysis indicated enrichment of several bacterial taxa in intercropped soils, including Acidobacteriota, Chloroflexota, and Sphingomonas, that were negatively associated with pathogen levels. The work supports a synergistic suppression model in which intercropping reorganizes soil metabolites and beneficial microbes to destabilize pathogen persistence.

LDH-dsRNA nanocarrier-mediated spray-induced silencing of juvenile hormone degradation pathway genes for targeted control of Helicoverpa armigera.

Joshi and colleagues in INTERNATIONAL JOURNAL OF BIOLOGICAL MACROMOLECULES found that a nanoclay LDH-dsRNA formulation can silence juvenile hormone degradation genes in Helicoverpa armigera and delay developmental transitions. The authors targeted three pathway genes with bacterially expressed dsRNAs, achieving more than 50% silencing and producing prolonged larval and pupal stages in bioassays. Combinatorial dsRNA application increased mortality relative to single targets, suggesting functional redundancy within juvenile hormone degradation. Metabolomic profiling showed reduced accumulation of pathway-associated metabolites, supporting pathway specificity rather than nonspecific toxicity. This work advances spray-induced gene silencing as a practical pest management strategy with metabolomics providing a biochemical verification layer.

Multiomics analysis of microbial succession and flavor formation mechanism during the fermentation process of Maotai-flavour Baijiu.

Shi and colleagues in FOOD CHEMISTRY-X showed that the flavor trajectory of Maotai-flavour Baijiu fermentation is shaped by stage-specific microbial succession coupled to metabolite production networks. Metagenomics and metabolomics distinguished stacking fermentation, enriched in organisms such as Weissella, Pichia, and Aspergillus with predicted hydrolytic enzyme activity, from pitting fermentation dominated by anaerobes including Acetilactobacillus and Pichia. Volatile profiling indicated that acids, alcohols, and esters accumulated predominantly during pitting fermentation, aligning with predicted glycosyltransferase and esterification activities. The study links microbial community transitions to defined classes of flavor compounds, offering mechanistic handles for process optimization. By combining community and chemical readouts, the work provides a template for modernizing traditional fermentations while retaining their signature sensory outcomes.

Bioinformatics and Methodology

SigmaCCS2: Collision cross section prediction using molecular topological and geometric information with graph neural network.

Liao and colleagues in CHEMOMETRICS AND INTELLIGENT LABORATORY SYSTEMS showed that CCS values can be predicted accurately by a graph neural network that explicitly encodes both molecular topology and geometry. SigmaCCS2 represents each molecule using dual graphs, with a molecular graph capturing connectivity and a line graph encoding geometric relationships, allowing the model to learn complementary structural signals. Across external test sets, the method achieved competitive performance that was generally superior or comparable to prior state-of-the-art approaches. The authors also reported robustness across instruments and molecular superclasses, a critical requirement for practical deployment in diverse IMS platforms. A public web server is provided, supporting broader adoption and enabling database-scale CCS augmentation for metabolomics and related applications.

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Metabolomics Events

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2nd ASMS Winter Conference

Mass Spectrometry in Microbial Sciences

January 29 - February 1, 2026

Venue: Santa Fe, New Mexico, United States

The conference will showcase leading work in the development (instrumentation, methods, data analysis, etc.) and application (natural products discovery, biotransformation, microbiome research, etc.) of mass spectrometry to microbial systems. Join the conference for a unique opportunity to gather mass spectrometrists and forward-thinking microbiologists.

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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.

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|MC:SUBJECT|

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.

Visit the website for more details

MANA SODAMeet

February 10, 2026

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

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.

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