MetaboNews

This month in metabolomics

September, 2024
Vol 14, Issue 9

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

In This Issue

Metabolomics Society News

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

General Enquiries

info@metabolomicssociety.org

Members' Corner

Board of Directors

Dear Society Members,

This will be my last message as the President of the Metabolomics Society.

I'll start by saying that it's been a privilege over the last 2 years to have been a very small cog in the society's wheel, and to thank our members for putting their faith in the Officers and Board of Director's during this term. The last two years have been a lot of fun.

I have many to thank and I know I'll miss some people off, so unlike the Academy Awards, I'll try and be brief. Our society relies on its Officers and Fabien Jourdan as Secretary and Candice Ulmer Holland as Treasurer have been simply brilliant. Their dedication, professionalism and eye for details has been perfect. I'm also very grateful to the whole board of directors and EMN for their valuable input into society business over the last couple of years. The hard work of all these metabolomers has kept the society as

the premier global organization devoted to the development of metabolism-based research.

I won't highlight the board members individually, but I would like to highlight Natasa Giallourou for her leadership, organisation skills, and motivation in her role as chair of the conference committee. She along with Prof. Phillip Britz-McKibbin and Dr Dajana Vuckovic in Niagara Falls, and Prof. Eiichiro Fukusaki and Dr Sastia Prama Putri in Osaka, delivered two fantastic conferences. I enjoyed every moment of these meetings – well except for the bit where I had to wear a tie and jacket!

I also have to give a special thank you to Jessica Lasky-Su, who, as the last president has been a font of knowledge and has helped me appreciate the complexities of the role and kept me on the straight and narrow! Jessica, when I took on this role you helped me keep my foot out of my mouth on several occasions and for that, I'm highly grateful!

Lastly, Leslie and her team have been absolutely amazing. Some have said to me during our annual conferences how do I appear to be so calm and relaxed. Well, this is only because of the magic that Leslie and her SnapIT team are doing behind the scenes. Thanks ever so much to you all, and to Brianna for taking such excellent notes during our monthly board meetings.

The baton has now been passed on. Warwick Dunn from the University of Liverpool shall be our next President, with elections currently ongoing to choose our Secretary. Our society is very privileged to have Rick at the helm. Congratulations Rick!

I'll finish by stating as detailed on our website: Our Metabolomics Society is dedicated to promoting the growth, use and understanding of metabolomics in the life sciences. We are an independent, non-profit organization, governed by a Board of Directors composed of dedicated members of the metabolomics community but ultimately responsive to its members. Please consider getting involved – it is after all Our Society.

This society was formed in 2004. I fondly remember Rima Kaddurah-Daouk lead its foundation along with George Harrigan, Bruce Kristal, Lloyd Sumner, Masaru Tomita and myself. It's been amazing to watch the growth of the society, I certainly feel that we have been successful in promoting the growth, use and understanding of our craft. Next year will be our 20th anniversary and we shall lots of nice things to reflect on.

I will, as ever, look forward to seeing you at future metabolomics meetings – the society-led ones and others. I'll be the one in the mufti and Hawaiian shirt – it'll be nice to be back to my normal phenotype – or should that be metabotype!

All the very best.

Roy Goodacre, University of Liverpool, UK

President, Metabolomics Society

The Global Metabolomics by Chemical Isotope Labeling LC-MS service provides semi-quantitive, untargeted metabolic profiling by using chemical isotope labeling combined with liquid chromatography and mass spectrometry. This advanced technique allows for precise and high-resolution analysis of a wide range of metabolites in biological samples.

By delivering detailed insights into metabolic pathways and biochemical changes, this service supports research in metabolic disease, drug discovery, and systems biology, helping researchers and clinicians understand complex metabolic networks and identify

potential biomarkers.

To learn more check out: https://metabolomicscentre.ca/service/global-metabolomics-by-chemical-isotope-labeling-lc-ms/

Early-Career Members Network (EMN)

EMN Election Results
This year, the EMN call received numerous applications from MetSoc early career members. After a careful evaluation process and newly added interview rounds, we are happy to announce 5 new EMN members have been elected! We want to extend a warm welcome to **Marina Tonetti Botana** (Victoria University of Wellington, New Zealand), **Loic Mervant** (The Francis Crick Institute, UK), **Jayden Lee Roberts** (Murdoch University - Australian National Phenome Centre, Australia), **Ambrin Farizah Babu** (University of Eastern Finland, and Afekta Technologies Ltd. Finland), and **Thomas Dussarrat** (Bielefeld University, Department of Chemical Ecology, Germany).

We also would like to thank our outgoing EMN members for the two wonderful years they have served on the EMN committee: **Millena Barros Santos** (Bordeaux Metabolome-MetaboHUB, INRAE Bordeaux Nouvelle-Aquitaine), **Domenica Berrardi** (Yale University, USA), **Daniel Muthitu** (Cape Heart Institute, University of Cape Town, South Africa), **Marvin Nathanael Iman** (Osaka University, Japan), and **Anza Ramabulana** (University of Johannesburg, South Africa)!

EMN Webinars
The EMN would once again like to thank **Dr. Alan Pilon** for his enriching and compelling presentation entitled "**Deciphering Mass Fragmentation Pathways Through LC-MS Molecular Networking**". He constructively explained and shared tips on how molecular networking can help identify and annotate molecules with similar structures. The webinar recording will be soon available on the MetSoc's website. Don't miss out on the next EMN webinar session in October and keep track of our social media platforms for updates!

International Affiliates' Corner

Nordic Metabolomics Society
Visit www.nordicmetsoc.org

The Nordic Metabolomics Society is together with the Metabolomics Platform at SciLifeLab hosting a one-day seminar: “Microsampling- New Avenues for Metabolomics in Precision Health” on October 11th from 10:00 to 16:00.

The hybrid seminar will take place at Karolinska Institutet and it will also be possible to attend the seminar online. Please see the program and register for free here: **https://www.scilifelab.se/event/microsampling-new-avenues-for-metabolomics-in-precision-health/**

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

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

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

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

Home | Metabolomics Circle APA 2024

The Alchemium building - the magic of chemistry of tomorrow - is located on campus A of the Lodz University of Technology.

Upcoming Lecture

The Polish Proteomics Society and the Polish Society of Metabolomics invite you to a lecture titled "Missing data imputation as the potential source of bias in metabolomic data analysis". Michał Burdukiewicz from the Laboratory of Bioinformatics and Multi-omics Analysis at the Medical University of Bialystok & Vilnius University will give the lecture.

The online event will be held on Thursday, April 11th, 2024, at 4 pm CET via the ZOOM platform.
https://zoom.us/j/95105741233?pwd=JbMQyAfiYSGelvWdcR1JLb2LVub6ki.1
Meeting ID: 951 0574 1233
Passcode: 354080

Please feel free to circulate the information among any colleagues who may be interested.
We are looking forward to your participation.

Scottish Metabolomics Society
Visit http://www.scottishmetabolomics.net/

The Scottish Metabolomics Network will host its annual symposium on the 22nd and 23rd of October 2024 within the Institute of Aquaculture at the University of Stirling. There will be a range of talks and posters on all aspects of metabolomics and local and international metabolomics researchers are encouraged to visit Stirling and experience its rich medieval history and stunning scenery. On the Monday before the event (21st) there will also be a hands-on chemometrics training workshop aim at developing stats skills for ECRs.

The conference will include plenary sessions from Professor Paul Fraser from Royal Holloway University of London and Dr Thierry Schmidlin from the University of Mainz.

Details available on the Scottish Metabolomics Network website!

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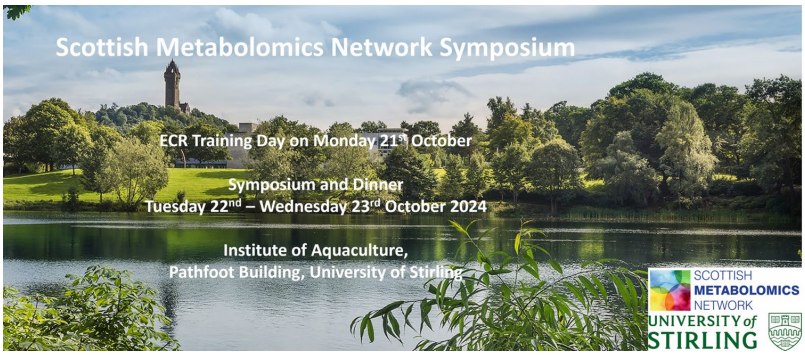

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MetaboInterview

Shuang Zhao

Dr. Shuang Zhao

Vice President, Nova Medical Testing Inc.

Node Manager, The Metabolomics Innovation Centre (TMIC)

Biography

Dr. Shuang Zhao is the Vice President of Nova Medical Testing Inc. (NovaMT), based in Canada. He earned his Ph.D. in Analytical Chemistry from the University of Alberta, specializing in LC-MS-based metabolomics. Since joining NovaMT in 2018, Dr. Zhao has played a pivotal role in overseeing operations and leading the development and commercialization of innovative technologies, including the innovative HP-CIL Metabolomics Platform and in-depth Global Lipidomics Platform.

In addition to his role at NovaMT, Dr. Zhao is a node manager at The Metabolomics Innovation Centre (TMIC), where he contributes to groundbreaking research in clinical, biomedical, and agricultural metabolomics. His expertise and leadership continue to drive NovaMT’s mission of advancing medical diagnostics through cutting-edge technology for large-scale small molecule analysis.

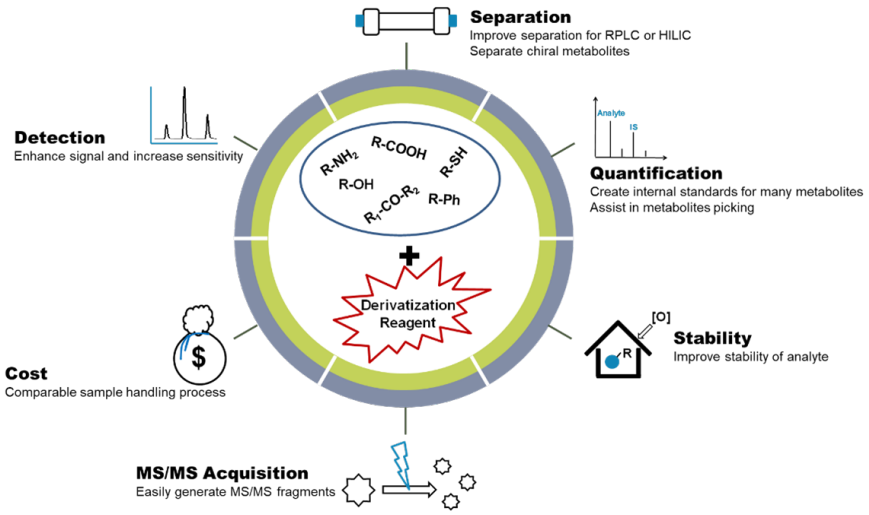
When did you first learn about Metabolomics and How did you get involved?

I was first introduced to the concept of metabolomics during my Master's program at Tsinghua University in 2012, where I focused on pharmacology and pharmacokinetics. Through using LC-MS to analyze drug metabolism, I learned about the significant potential of metabolomics. It's a powerful emerging tool that can elucidate how drugs affect the body and how the body responds. This realization sparked my interest in the field, which I saw as having revolutionary implications for various types of scientific research.

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

The most exciting aspect of my work in metabolomics is the opportunity to develop innovative solutions that address challenges in the field and assist others in their research. Metabolomics is a dynamic and evolving field, filled with both challenges and uncertainties, especially from an analytical perspective. The process of developing new technologies is always thrilling and inspiring. Even more rewarding is the ability to commercialize these technologies, making them accessible to the broader society, which I find truly fascinating.

For instance, in conventional LC-MS-based metabolomics, achieving high coverage while quantitatively measuring the metabolome has been a long-standing challenge. Collaborating with my Ph.D. supervisor, Dr. Liang Li, we developed an innovative approach known as differential chemical isotope labeling LC-MS. This technique incorporates chemical derivatization into routine LC-MS analysis, significantly enhancing several aspects of metabolomics performance, including metabolome coverage, quantification accuracy and precision, and workflow robustness. The potential impact of these advancements on both research and practical applications is truly inspiring.

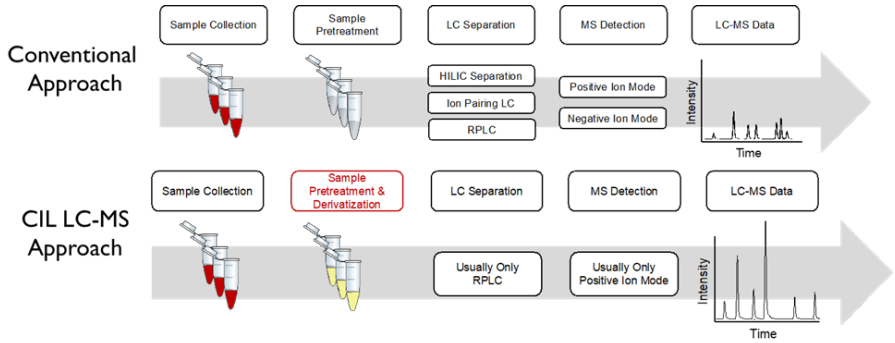


Shuang Zhao and Liang Li, 2020, “Chemical Derivatization in LC-MS-Based Metabolomics Study”, Trends in Analytical Chemistry (TrAC), 131, 115988.

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

We are focused on developing advanced technologies and ensuring their commercialization to benefit the broader scientific community. A key initiative has been the development and commercialization of the Chemical Isotope Labeling LC-MS technique for metabolomics. We have packaged this technology into a comprehensive solution that includes kits, methods, software, and databases, making it accessible to

laboratories around the world and significantly enhancing their research capabilities.



Shuang Zhao and Liang Li, 2021, “Chemical Derivatization for Polar Metabolome Analysis”, in Rawi Ramautar (eds) Advanced Mass Spectrometry-based Analytical Separation Techniques for Probing the Polar Metabolome, The Royal Society of Chemistry, Cambridge, UK, pp27-40.

In addition, we have developed a complete platform for in-depth global lipidomics analysis, offering unique advantages and world-leading performance in lipid analysis. By integrating these two approaches, we achieve exceptionally high coverage for large-scale small molecule analysis.

We also leverage these platforms in our own facility to support researchers from various scientific fields by analyzing their samples, thereby extending the impact of our work and contributing to advancements across multiple disciplines.

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

Our work in metabolomics has already yielded several innovative, comprehensive solutions, such as the HP-CIL Metabolomics Platform and the In-depth Global Lipidomics Platform. These systems are widely used in various research studies, making significant contributions to areas like disease biomarker discovery—including early diagnosis biomarkers for neurodegenerative diseases funded by the Brain Canada program—and drug development through collaborations with global pharmaceutical entities like AbbVie and Gilead. Additionally, our platforms have applications in agriculture and food sectors, in partnership with Agriculture Canada. The unique and leading features of our platforms have achieved remarkable success both academically and practically. Looking ahead, as we continue to develop and commercialize more advanced techniques, we aim to remain at the forefront of innovative small molecule analysis.

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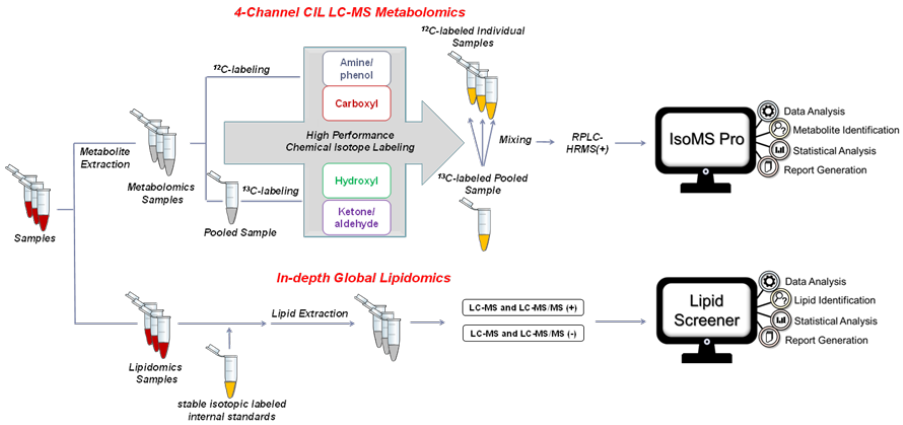

What is happening in your country in terms of metabolomics?

I am from China and currently work in Canada. In both countries, we are witnessing a significant surge in metabolomics research, each with its unique strengths. In Canada, we benefit from a well-organized structure and a long history of innovation. For instance, the Human Metabolome Database (HMDB) and MetaboAnalyst are two of the most widely used, freely available tools in the field, both developed here. Numerous researchers utilize these tools to bolster their studies. Meanwhile, in China, although metabolomics development began later than in North America or Europe, there is a dramatically increasing trend and a strong capability for development, particularly in large-scale, population-based studies.

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

The greatest strength of metabolomics lies in its comprehensive "omics" approach, which allows for the simultaneous detection and quantification of thousands of metabolites from a single sample. This capability marks a significant evolution from the past when only a few compounds could be quantified. Today’s advanced technologies enable us to identify and quantify thousands of metabolites at once, greatly enhancing our ability to support other fields. For instance, this robust analytical capacity facilitates the development of pan-panel biomarkers, which could revolutionize disease diagnosis and health monitoring.

What do you see as the greatest barriers for metabolomics?

One of the greatest challenges in metabolomics is efficiently extracting and interpreting meaningful biological information from the vast and complex data generated. Metabolomics often involves handling large datasets, and managing this data effectively is critical. Another key barrier is how to integrate data from different techniques or across multiple research centres. Successfully linking and harmonizing these diverse datasets is

one of the most complex tasks we face in advancing the field.

What improvements, technological or otherwise, need to take place for metabolomics to really take off?

To truly propel metabolomics forward, we need to further develop tools that can interpret data and directly provide biologically relevant information to end-users such as clinicians and researchers. More importantly, these tools need to be designed with user-friendliness in mind, ensuring that even those without a deep background in metabolomics can easily utilize them. Making sophisticated analyses accessible and practical for everyday use will be a key advancement for the field.

What advice would you give to new researchers and students wishing to enter the field?

Metabolomics is a vibrant, rapidly evolving interdisciplinary field. For those interested in entering this area, I highly recommend immersing yourself in a wide range of subjects and techniques. It's crucial to develop a diverse skill set that spans analytical chemistry to bioinformatics, and techniques from NMR to LC-MS. Equally important is gaining proficiency in both untargeted and targeted approaches, and extending your expertise from multiomics (e.g., metabolomics, lipidomics, glycomics). This broad knowledge base will equip you well to contribute effectively in this dynamic scientific landscape.

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

As an emerging field, metabolomics offers extensive opportunities for collaboration across the entire scientific community. The nature of the work invites diverse expertise and encourages cross-disciplinary partnerships. This collaborative environment not only enriches the field but also accelerates the development of innovative solutions that can address complex biological questions. Engaging with a wide range of scientists and disciplines is key to advancing our understanding and application of metabolomics.

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MetaboReads

This month, our search query returned just under 600 papers published in metabolomics for the month. The articles we're showcasing in this edition cover a wide range of topics, including agricultural metabolomics, cancer, and cardiovascular health. Metabolomics continues to show its promise as a critical multidisciplinary research tool. Based on some feedback from last month, I have slightly re-structured how articles in this section are presented, including listing each first author's full name and using the more technically correct 'and colleagues' instead of 'et al' - please keep the feedback coming!

As the 2024-2025 academic year gets underway, the team here at MetaboNews wishes you all a smooth start, reasonably restrained teaching load, and best of luck analyzing and writing up all the data we're sure you generated over the summer!

Plant Metabolomics in Environmental Stress and Crop Improvement

Plant metabolomics is a powerful tool for understanding how plants respond to environmental stresses such as heavy metals, UV radiation, and pathogen attacks. Recent studies have utilized metabolomic profiling to identify key metabolites and genetic regulators involved in stress responses. These findings not only enhance our understanding of plant biology but also offer potential strategies for crop improvement, phytoremediation, and sustainable agriculture.

Co-expression analyses reveal key Cd stress response-related metabolites and transcriptional regulators in Kentucky bluegrass

Yong Wang and colleagues in Chemosphere investigated the mechanisms underlying cadmium (Cd) accumulation and tolerance in Kentucky bluegrass (Poa pratensis). By examining variances in the transcriptome and metabolome of a Cd-tolerant variety (Midnight) and a Cd-sensitive variety (Rugby II), they pinpointed crucial regulatory genes and metabolites associated with Cd response. The study identified that metabolites in the shikimate-phenylpropanoid pathway (phenolic acids, phenylpropanoids, and polyketides) were highly induced by Cd treatment and more abundant in the Cd-tolerant variety. Exogenous application of L-phenylalanine enhanced Cd uptake and alleviated Cd stress, suggesting potential strategies for phytoremediation of Cd-contaminated soils.

Dissecting the genetic basis of UV-B responsive metabolites in rice

Feng Zhang and colleagues in Genome Biology performed comprehensive metabolic profiling of leaves from 160 diverse rice accessions under UV-B and normal light conditions using a widely targeted metabolomics approach. Their results revealed substantial differences in metabolite accumulation between the two major rice subspecies, indica and japonica, especially after UV-B

treatment. They identified key metabolites and genes involved in amino acid and flavonoid pathways that contribute to UV-B tolerance. Functional validation showed that manipulating specific genes, such as OsMYB44 and OsUVR8, can enhance UV-B resistance, offering new avenues for crop improvement.

Metabolome-driven microbiome assembly determining the health of ginger crop (Zingiber officinale L. Roscoe) against rhizome rot

Wenbo Wang and colleagues in Microbiome conducted a thorough examination of the biodiversity of soilborne and endophytic microbiota in healthy and diseased ginger plants, highlighting the impact of bacterial and fungal microbes on plant health. Using metabarcoding and untargeted metabolomics analysis, they identified specific microbial species and metabolites that correlate with plant health. Dominant genera, such as Sphingomonas and Bacillus, were associated with healthy plants, while pathogens like Pectobacterium were linked to disease. Their research enhances understanding of plant-microbe interactions and could inform strategies to protect crops from diseases.

Dual nematode infection in Brassica nigra affects shoot metabolome and aphid survival in distinct contrast to single-species infection

Jessil Ann Pajar and colleagues in Journal of Experimental Botany assessed how single (root-knot nematode Meloidogyne spp. and root-lesion nematode Pratylenchus penetrans) and concurrent nematode infections affect the shoot metabolome of Brassica nigra and subsequent aphid performance. They found that dual nematode infections led to distinct changes in the plant's leaf and phloem metabolic profiles compared to single-species infections. Notably, the dual infection influenced the levels of indole glucosinolates and hydroxycinnamic acids, which are linked to plant defense mechanisms. Aphid survival was reduced on plants with dual infections, suggesting that the metabolic changes adversely affected herbivore performance.

Gut Microbiota, Metabolomics, and Disease

The gut microbiome plays a critical role in human health, influencing metabolic processes, immune responses, and disease progression. Recent research has focused on how modulation of the gut microbiome and its metabolites can alleviate conditions such as asthma, cerebrovascular diseases, liver injury, and metabolic disorders. These studies highlight potential therapeutic targets and biomarkers for disease management through gut microbiome regulation.

Hydrogen-rich water alleviates asthma airway inflammation by modulating tryptophan metabolism and activating aryl hydrocarbon receptor via gut microbiota regulation

Li Li and colleagues in Free Radical Biology and Medicine investigated the potential therapeutic impact of hydrogen-rich water (HRW) on the gut-lung axis in asthma. Using 16S rRNA and serum metabolomics, they examined changes in gut microbiota and serum metabolites in asthmatic mice after HRW intervention. HRW influenced the gut microbiota by increasing the abundance of beneficial bacteria such as Ligilactobacillus and Bifidobacterium, enhancing levels of indole-3-acetic acid (IAA), a microbially derived serum metabolite. Both in vivo and in vitro experiments showed that HRW's protective effects against airway inflammation may be linked to the gut microbiota, with IAA potentially playing a role in reducing asthmatic airway

inflammation through the aryl hydrocarbon receptor (AhR) signaling pathway.

Multi-omics analysis of gut-brain axis reveals novel microbial and neurotransmitter signatures in patients with arteriosclerotic cerebral small vessel disease

Jiayuan Huang and colleagues in Pharmacological Research explored the role of gut microbiota in the pathogenesis of arteriosclerotic cerebral small vessel disease (aCSVD). By comparing the gut microbiome and metabolome between aCSVD patients and healthy controls, they found a marked reduction in beneficial bacterial species such as Faecalibacterium prausnitzii and Roseburia intestinalis, alongside an increase in taxa from Bacteroides and Proteobacteria. Integrated metagenomic and metabolomic analyses revealed alterations in microbial metabolic pathways, including lipopolysaccharide (LPS) biosynthesis and phenylalanine-tyrosine metabolism. These changes may influence the symptoms and progression of aCSVD via pro-inflammatory effects and modulation of systemic neurotransmitters, implying that gut microbiota characteristics could serve as indicators for early detection and potential therapeutic targets.

Fucoidan ameliorates alcohol-induced liver injury in mice through Parabacteroides distasonis-mediated regulation of the gut-liver axis

Lu Wang and colleagues in International Journal of Biological Macromolecules demonstrated that fucoidan extracted from Scytosiphon lomentaria alleviates alcohol-induced liver injury in mice. The beneficial effects are closely associated with the gut bacterium Parabacteroides distasonis. Further mice experiments showed that P. distasonis reduced liver injury and inflammation by suppressing the NF-κB/MAPK pathways and activating the Nrf2 pathway. The underlying mechanism involves modulation of the gut microbiota, particularly an increase in microbiota diversity and beneficial bacteria, and a reduction in Proteobacteria. Targeted metabolomics indicated that P. distasonis ameliorated alcohol-induced dysbiosis of microbial metabolites, primarily affecting amino acid metabolism. Additionally, P. distasonis improved bile acid profiles, affecting the expression levels of bile acid-associated genes in the liver and ileum. This study suggests that fucoidan can benefit alcohol-induced liver injury via P. distasonis-mediated regulation of the gut-liver axis.

Thyroid hormone receptor-beta agonist HSK31679 alleviates MASLD by modulating gut microbial sphingolipids

Yu-Hang Zhang and colleagues in Journal of Hepatology found that the efficacy of the thyroid hormone receptor-beta (THR-β) agonist HSK31679 in treating metabolic dysfunction-associated steatohepatitis (MASLD) is influenced by the gut microbiota. Specifically, they identified that gut microbial glucosylceramide synthase (GCS) affects sphingolipid metabolism. In germ-free mice and a randomized, double-blind multiple-dose cohort study, they observed that microbial GCS modulates the therapeutic response to HSK31679. For participants with high fecal GCS activity, HSK31679 induced a shift towards an immunosuppressive niche, characterized by decreased CD8α+ dendritic cells and MINCLE+ macrophages. Their findings suggest that microbial GCS may serve as a prognostic biomarker and therapeutic target in MASLD treatment.

Salmonella re-engineers the intestinal environment to break colonization resistance in the presence of a compositionally intact microbiota

Andrew WL Rogers and colleagues in Cell Host & Microbe revealed that Salmonella enterica serovar Typhimurium can disrupt colonization resistance without changing the gut microbiota composition. Using metabolite profiling and genetic analysis, they showed that the initial rise in luminal pathogen abundance was powered by a combination of aerobic respiration and mixed acid fermentation of simple sugars, such as glucose, leading to their depletion from the metabolome. This depletion coincided with a reduction in cecal concentrations of acetate and butyrate and an increase in epithelial oxygenation. The study concludes that changes in the host environment, induced by Salmonella, can weaken colonization resistance even in the absence of overt compositional changes in the gut microbiota.

Cancer Metabolomics and Therapeutics

Metabolic reprogramming is a hallmark of cancer, and understanding these metabolic alterations can lead to the development of novel therapeutic strategies. Recent studies have explored how specific metabolites and metabolic pathways contribute to cancer progression, immune evasion, and therapy resistance. Targeting these metabolic vulnerabilities holds promise for improving cancer treatment outcomes.

Nervonic acid triggered ovarian inflammation by inducing mitochondrial oxidative stress to activate NLRP3/IL-1β pathway

Xiangzhou Zeng and colleagues in Journal of Advanced Research discovered that elevated levels of nervonic acid (NA), a fatty acid, trigger ovarian inflammation by inducing mitochondrial oxidative stress and activating the NLRP3 inflammasome and IL-1β pathway. Utilizing metabolomics and transcriptomics, they compared fatty acid compositions in sows with high and low reproductive performance and found that those with low embryo survival rates had abnormal accumulation of NA. In vitro and in vivo experiments showed that NA induces mitochondrial oxidative stress by inhibiting respiratory chain proteins, leading to ovarian dysfunction. The study suggests that NA is a typical metabolite of metabolic syndrome that influences ovarian function and provides insights into potential therapeutic strategies targeting mitochondrial ROS production.

MYC induces oncogenic stress through RNA decay and ribonucleotide catabolism in breast cancer

Jitendra K. Meena and colleagues in Cancer Discovery showed that the oncogene MYC increases RNA degradation and downstream ribonucleotide catabolism, resulting in the accumulation of cytotoxic RNA catabolites and reactive oxygen species in breast cancer cells. Combining genetics and metabolomics, they found that MYC-induced RNA decay leads to oncogenic stress. Purine salvage acts as a compensatory pathway, and inhibitors of this pathway impaired tumor progression. Their findings suggest that therapeutics targeting ribonucleotide catabolism provide a tractable approach to treating MYC-driven cancers.

TBC1 domain-containing proteins are frequently involved in triple-negative breast cancers in connection with the induction of a glycolytic phenotype

Mariadomenica Lupi and colleagues in Cell Death & Disease investigated the role of TBC1 domain-containing proteins (TBC1Ds) in the regulation of cancer metabolism. They found that

several genes encoding TBC1Ds are overexpressed in triple-negative breast cancers (TNBC) compared to other subtypes and predict poor prognosis. Orthogonal transcriptomics and metabolomics analysis revealed that the expression of prognostic TBC1Ds correlates with elevated glycolytic metabolism in breast cancer cell lines. In-depth investigations of TBC1D31, TBC1D22B, and TBC1D7 showed that their elevated expression causes a glycolytic phenotype in TNBC cells. Specifically, TBC1D7 acts independently of its known participation in the TSC1/TSC2 complex. The study suggests that TBC1Ds connect disease aggressiveness with metabolic alterations in TNBC and could serve as prognostic biomarkers and therapeutic targets.

Mitochondrial reprogramming by activating OXPHOS via glutamine metabolism in African American patients with bladder cancer

Karthik RK Reddy and colleagues in JCI Insight revealed that African American (AA) patients with bladder cancer exhibit elevated mitochondrial oxidative phosphorylation (OXPHOS) due to complex I activation. Through comprehensive RNA-Seq, proteomics, and metabolomics analysis, they found that this metabolic phenotype is characterized by activation of complex I and glutamine-mediated metabolic rewiring. Mechanistic studies demonstrated that knockdown of NDUFB8, a component of complex I, reduced basal respiration, ATP production, and proliferation in AA bladder cancer cells. Preclinical studies showed that targeting complex I and glutamine metabolism decreased tumor growth, highlighting metabolic reprogramming as a contributor to racial disparities in bladder cancer outcomes and suggesting potential therapeutic interventions.

BCKDK modification enhances the anticancer efficacy of CAR-T cells by reprogramming branched-chain amino acid metabolism

Quanjun Yang and colleagues in Molecular Therapy engineered chimeric antigen receptor (CAR) T cells to overexpress branched-chain α-ketoacid dehydrogenase kinase (BCKDK), reprogramming branched-chain amino acid (BCAA) metabolism to enhance anticancer efficacy. They found that BCKDK overexpression in CAR-T cells significantly improved cancer cell lysis, while BCKDK knockout resulted in inferior lysis potential. In vivo experiments showed that BCKDK-overexpressing CAR-T cell treatment prolonged the survival of mice bearing NALM6-GL cancer cells, with an increased proportion of CAR-T cells in the peripheral circulation. The study concludes that BCKDK-engineered CAR-T cells exert a distinct phenotype for superior anticancer efficiency, potentially improving CAR-T cell therapies for advanced cancers.

Cardiovascular Metabolomics

Cardiovascular diseases remain a leading cause of morbidity and mortality worldwide. Metabolomics offers insights into the metabolic alterations associated with these diseases, aiding in the identification of biomarkers and therapeutic targets. Recent studies have focused on the metabolic heterogeneity of cells involved in atherosclerosis and heart disease, and the role of specific metabolites and enzymes in disease progression.

SPTLC3 is essential for complex I activity and contributes to ischemic cardiomyopathy

Anna Kovilakath and colleagues in Circulation reported that SPTLC3, a subunit of serine

palmitoyltransferase involved in sphingolipid metabolism, is induced in both human and mouse models of ischemic cardiomyopathy. This induction leads to the production of atypical sphingolipids bearing 16-carbon sphingoid bases, resulting in changes in cell sphingolipid composition. Cardiomyocyte-specific depletion of SPTLC3 in mice attenuated oxidative stress, fibrosis, and hypertrophy in chronic ischemia, improving cardiac function and survival. Mechanistically, SPTLC3 alters the membrane environment and subunit composition of mitochondrial complex I, decreasing its activity. Their findings suggest a novel role for SPTLC3 in electron transport chain function and contribution to ischemic injury, offering a potential therapeutic target.

Zinc-α2-glycoprotein modulates blood pressure by regulating renal lipid metabolism reprogramming-mediated urinary Na^+ excretion in hypertension

Xiaoxin Zhou and colleagues in Cardiovascular Research found that Zinc-α2-glycoprotein (ZAG) regulates blood pressure by modulating renal lipid metabolism and urinary sodium excretion. In a cross-sectional study, serum ZAG levels were significantly decreased in hypertensive participants and associated with morning urine Na^+ excretion. Azgp1 knockout mice exhibited increased blood pressure and impaired urinary Na^+ excretion, which were restored by AAV9-mediated renal tubule Azgp1 rescue. The deficiency of Azgp1 increased malonyl-CoA-mediated inhibition of carnitine palmitoyltransferase 1 (CPT1) activity, leading to renal lipid metabolism reprogramming and increased Na^+/H^+-exchanger activity. The study suggests that targeting Azgp1 may provide a potential kidney-targeted therapy in the prevention and treatment of hypertension.

Food Metabolomics and Taste Perception

The flavor and taste profiles of foods and beverages are determined by complex mixtures of metabolites. Metabolomics enables the detailed analysis of these compounds, helping to understand how processing, storage, and ingredient interactions affect sensory properties. Recent studies have provided new insights into the key components responsible for aftertaste and flavor intensity in tea and other products.

A new insight into the key matrix components for aftertaste in Ampelopsis grossedentata (vine tea) infusion: From the intensity and duration of taste profiles using non-targeted metabolomics and molecular simulation

Le Chen and colleagues in Food Chemistry investigated the prolonged aftertaste of Ampelopsis grossedentata infusion (AGTI), identifying key metabolites contributing to its unique flavor profile. Using non-targeted metabolomics and molecular simulations, they found that aftertaste-A and richness were the characteristic aftertastes of AGTI. Metabolites such as 5-KETE and theobromine were identified as differential components. Specific compounds like p-coumaroyl quinic acid and xanthine contributed more to aftertaste-A and richness, respectively. Molecular docking showed stable bonding between these characteristic metabolites and their receptors, offering novel insights into the interaction mechanism of aftertaste in tea infusion.

Dynamic changes of key metabolites in Longjing green tea during processing revealed by widely targeted metabolomic profiling and sensory experiments

Lin Zeng and colleagues in Food Chemistry utilized widely targeted metabolomics and chemometrics to comprehensively analyze the formation of taste compounds in Longjing green tea. They identified 580 non-volatile metabolites using ultra-performance liquid chromatography-electrospray ionization-tandem mass spectrometry. The study investigated alterations in three metabolic pathways during processing, finding that the fixation process reduced phosphatidic acid levels and resulted in the formation of lyso-phosphatidylcholine and lyso-phosphatidylethanolamine. Additionally, cultivar differences were noted, with Baiye No.1 having high levels of L-glutamic acid and L-glutamine, and Longjing 43 showing elevated levels of flavones. Correlation analysis and sensory verification indicated that specific amino acid concentrations influenced the tea's umami taste. These findings advance understanding of Longjing green tea quality improvement and cultivar development.

Methodological Advances in Metabolomics

Advances in metabolomics methodologies enhance our ability to detect, quantify, and interpret metabolic changes at high resolution, including at the single-cell level. Innovations in sample collection, preservation, and analytical techniques are crucial for expanding metabolomics applications in clinical and environmental settings.

Single-Cell Time-Resolved Metabolomics and Lipidomics Reveal Apoptotic and Ferroptotic Heterogeneity during Foam Cell Formation

Yiwen Wang and colleagues in Analytical Chemistry developed time-resolved, single-cell metabolomics and lipidomics approaches to explore the heterogeneity of macrophages during foam cell formation, a crucial process in atherosclerosis. Their dynamic analyses revealed a dual regulatory axis involving inflammation and ferroptosis. Single-cell metabolomics and lipidomics delineated a continuum of macrophage states with varied susceptibilities to apoptosis and ferroptosis. Single-cell transcriptomic profiling confirmed these divergent fates, providing insights into the complex molecular interactions that dictate these cell states. This research enhances understanding of plaque formation and stability, potentially informing therapeutic strategies.

GC×GC-TOFMS Analysis of Fecal Metabolome Stabilized Using an At-Home Stool Collection Device

Ryland Geibelhaus and colleagues in Applied Biosciences investigated the challenges of preserving stool sample integrity for fecal metabolomics, particularly for at-home collection and ambient storage. The authors evaluated a commercially available stool collection device containing a stabilization reagent designed to maintain the metabolite profile during storage at room temperature. Using comprehensive two-dimensional gas chromatography time-of-flight mass spectrometry (GC×GC-TOFMS) and chemometric analysis, they compared stool samples processed immediately after collection with those stored in the device for seven days. The results showed that the device with the stabilization reagent effectively minimized metabolite profile changes, making it a viable option for at-home sample collection and transport without requiring complex equipment or immediate processing.

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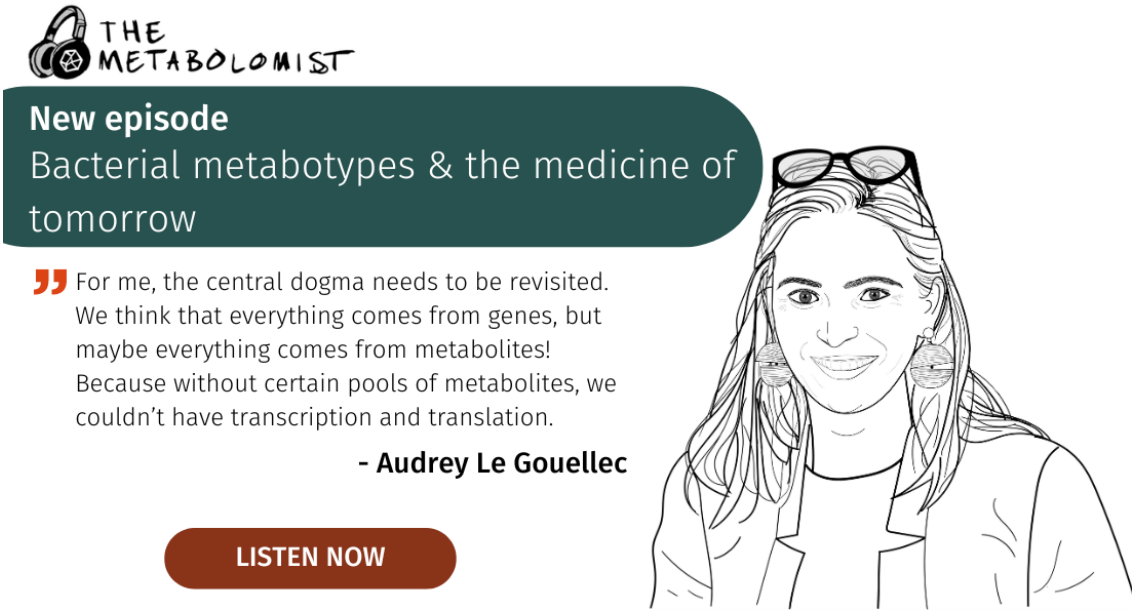
The Metabolomist Podcast



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Metabolomics Events

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

October 3, 2024

Venue: Online

This course is taught by Prof. Jeff Xia, McGill University. The level of the course is introductory,

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

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

Check for more details

Metabolomics in Toxicology course

October 7 – 9, 2024

Venue: School of Biosciences - University of Birmingham, England

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

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

For more information, including registration, click here.

Learn more here

MANA SODAMeet

October 8, 2024

Venue: Online

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

relevant information on these software/data presented.

Join the web seminar

Untargeted Metabolomics LC/MS Data Processing course

October 14 – 16, 2024

Venue: School of Biosciences - University of Birmingham, England

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

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

For more information, including registration, click here.

Learn more here

6th Annual Metabolomics MANA Conference

October 21 – 24th, 2024

Venue: Tampa, Florida

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

For more information, including registration, click here.

Learn more here

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

October 24, 2024

Venue: Online

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

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

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

Check for more details

Bits & Bites # 09: Biochemical interpretation and visualization of metabolomics data *New Course*

November 7, 2024

Venue: Online

This course is taught by Prof. Oliver Fiehn, UC Davis. The level of the course is introductory, requiring no specific software or experience. In this short course, participants will focus on interpreting data, generating hypotheses, integrating biological and metabolomics data, and making the most of freely available online databases. The course provides practical tips on curation, data mapping, and visualization.

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

Check for more details

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

Metabolomics and Human Health

Gordon Research Seminar

Using Small Molecules in Medicine to Decode Biological Complexity

February 1 - 2, 2025

Venue: Ventura, California

The Metabolomics and Human Health GRS provides a unique forum for young doctoral and post-doctoral researchers to present their work, discuss new methods, cutting edge ideas, and pre-published data, as well as to build collaborative relationships with their peers. Experienced mentors and trainee moderators will facilitate active participation in scientific discussion to allow all attendees to be engaged participants rather than spectators.

The seminar will feature approximately 10 talks and 2 poster sessions. All attendees are expected to actively participate in the GRS, either by giving an oral presentation or presenting a poster. Therefore, all applications must include an abstract.

Applications for this meeting must be submitted by **January 4, 2025**. Please apply early, as some meetings become oversubscribed (full) before this deadline.
GRS Speaker Abstract Deadline: Although applications will be accepted until the date noted above, any applicants who wish to be considered for an oral presentation should submit their application by **October 27, 2024**.

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

Check for more details

2025 Metabolomics and Human Health Gordon Research Conference

The Interaction Between Humans, Lifestyles and the Environment Viewed through Metabolism

February 2 - 7, 2025

Venue: Ventura, California

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

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

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

Check for more details

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

Certified reference materials (CRM) values provide a known and standardized reference point against which the results of a metabolomic study can be compared. However, the certification of hundreds of individual metabolites is a cumbersome and time-consuming process. The Standard Reference Material (SRM) 1950, Metabolites in Frozen Human

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

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

Metabolomics Jobs

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
Researcher for development of advanced metabolomics methods	The Metabolomics & Analytics Centre (MAC), Leiden University	Leiden, Netherlands	Leiden University

Postdoc in microbiome metabolomics	Department Biomolecular Health Sciences, Utrecht University	Utrecht, Netherlands	Utrecht University
Lab Scientist in Metabolomics	Thermo Fisher Scientific	Basel, Basel-City, Switzerland	Roche
Application Scientist III	Thermo Fisher Scientific	Vilnius, Lithuania	Thermo Fisher Scientific
12 PhD positions in Xpose doctoral training unit (various topics)	Luxembourg Institute of Health (LIH), University of Luxembourg, Luxembourg Institute of Socio-Economic Research (LISER)	Luxembourg City or Belval, Luxembourg	Xpose, Luxembourg Institute of Health (LIH)
Data Scientist / Senior Data Scientist		Oxford, England	Metabolomics Society
Research Associate	MetaCom, Institute for Plant Biochemistry	Halle, GE, Germany	Leibniz Institute of Plant Biochemistry

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

Fill Out Your Survey Here

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

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