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MetaboNews

This month in metabolomics

AUGUST, 2023
Vol 13, Issue 8

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

METABOLOMICS SOCIETY

TMIC
The Metabolomics Innovation Centre

In This Issue

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Metabolomics Society News

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

General Enquiries

info@metabolomicssociety.org

Members' Corner

Board of Directors

Dear Society Members,

During the summer months (at least for those of us who live in the Northern Hemisphere), many of the Board of Directors have been taking vacations. As a consequence, our next BoD committee meeting will be held in mid-September and thus we have very little society business to report on.

Some of the committees and task groups have been meeting and we look forward as a board to hearing what progress has been made over the summer when we meet online

next month.

Please Vote! We invite all current members of the Society to participate in the annual election to select a new Director for the Board. The election poll is open through **September 15**, and there is (1) open spot on the BOD this year. Please take a moment to review the candidates and their bios: https://metabolomicssociety.org/board-committees/2023-bod-election/

As mentioned in Niagara Falls, Candice Ulmer Holland, Society Treasurer, was not able to join us in person. Nevertheless, the Board are delighted to learn that Candice had her baby son, Aiden on Friday, July 28th. We know how precious this time is when two become three and we wish her family all the very best for the future.

A reminder that if you would like to hear some of our speakers from our annual meeting, Metabolomics 2023, these have been added to the OnAIR platform. Registered conference attendees have been provided with unique login details.

Finally, I hope that those of you who have taken a vacation this summer, had a nice time and are feeling recharged. For those taking your vacations when it's winter in the Northern Hemisphere winter (Southern summer), I also hope you enjoy your time. I shall personally be quite jealous, especially as temperatures hit 40 ˚C this weekend in The Canaries where I am currently on vacation!

All the very best.

Roy Goodacre, University of Liverpool, UK

President, Metabolomics Society

International Affiliates' Corner

Metabolomics Association of North America (MANA)

Visit: https://metabolomicsna.org

5th Annual MANA Conference

The **Plenary Speakers** and list of **Instructional and Interest Group Workshops** has been announced for the 5th Annual MANA Conference, to be held October 23-27, 2023 at the University of Missouri. See below for speaker and workshop details. Don't miss your opportunity to hear these dynamic speakers describe their exciting work! The conference program also includes corporate breakfasts, speakers selected from abstract submissions, poster presenters, and social events. Topics cover the broadness of the metabolomics field, broadly spanning computational advances, plant/environment applications, and clinical/translational applications.

Register for the meeting **here.** While the oral abstract submission deadline has passed, you can still submit your abstract for consideration as a poster presentation up until August 31. **Submit abstracts here.**

Plenary Speakers

- Prof. Andrew Patterson (Penn State University) - **"Bile Acids: The Conversation Starters in the Complex Host-Microbiome Dialogue"**

- Prof. Dajana Vuckovic (Concordia University) - Title TBA
- Prof. Lauren Petrick (Icahn School of Medicine at Mount Sinai) - "**Leveraging Untargeted Metabolomics for Discovery in Cancer Epidemiology**"
- Prof. Arthur Edison (University of Georgia) - "**Unique Strengths of NMR Metabolomics: In Vivo Metabolism and Functional Metabolomics**"

Instructional and Interest Group Workshops

- **MANA Interest Groups: What They Are and How to Get Involved** - Ewy Mathé, Arpana Vaniya
- **The NP-MRD: An NMR Database for Metabolomics and Natural Product Discovery** - David Wishart, Lloyd Sumner, Roger Linington, John Cort
- **Farm to (data)Table: How has your data been Processed?** - Daniel Hitchcock, Yue Wu, Ewy Mathé
- **Opportunities and Challenges in Developing a Web-accessible, Community-sourced Database of Reproducible Metabolomics Methods in Compliance with FAIR Principles: An ABRF Initiative** - Ryan Sheldon, Maryam Goudarzi
- **Multi-omics Analysis and Interpretation** - Isin Tuna Sakallioglu, Stephanie Bishop
- **Challenges and Considerations for Processing Untargeted High-dimensional Mass Spectrometry Data** - Sean Colby
- **Quality Management for Metabolomics Laboratories: A Path to Enable Precision Medicine** - David Wishart, Sindhu Nair, Stephen Barnes, Annie Evans, Katherine Black, Jennifer Kirwan, Rima Kaddurah-Daouk, mQACC, MANA Precision Medicine Interest Group, Metabolomics Society Precision Medicine Task Group
- **The View of the Microbiome Through the Lens of Metabolomics: Data Analysis and Integration Strategies** - Denny Lan, Rob Quinn, Maryam Goudarzi, Chris Zhu
- **The Art of Industry Collaboration: Empowering Early Career Scientists in Establishing Corporate Member Relationships** - Arpana Vaniya, Nicole Prince
- **Lipidomics Minimal Reporting Checklist for Metabolomics** - Kim Ekroos, Tom Metz, Gerhard Liebisch, Ruth Welti
- **Hands-on Processing of Mass Spectrometry-based Metabolomics and Exposomics Big Data Using ADAP-BIG and Compound Identification and Annotation Using ADAP-KDB** - Aleksandr Smirnov and Xiuxia Du
- **SQUAD Metabolomics, the New Standard in Discovery Metabolomics Analyses** - Susan Bird, Eric Tague, Bashar Amer, and Rahul Deshpande
- **COMETS Analytics: An Open-source Analytic Tool for Single Cohort and Meta-analyses of Multiple Cohorts in Metabolomic-based Epidemiological**

Studies - Jessica Lasky-Su, Ewy Mathe, Nicole Prince and Marinella Temprosa

5th Annual MANA Fall Symposium

The 5th Annual MANA Fall Symposium - entitled **Expanding the Exposome: The Power of Mass Spectrometry** - will be held online **September 8, 2023 from 9am - 2pm PT**. This event is hosted and organized by the UC Davis West Coast Metabolomics Center and is free to attend. Speakers include Dr. Dana Barr (Emory University), Dr. Jonathan Martin (Stockholm University), Dr. Lauren Petrick (Mount Sinai Health System), Dr. Antony Williams (U.S. EPA), Dr. Krystal Godri Pollitt (Yale), and Dr. Dinesh Barupal (Mount Sinai Health System). Register **here**, and see the flyer for more details.

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MetaboInterview

Justin J.J. van der Hooft

Assistant Professor
Van der Hooft Computational Metabolomics Group
Bioinformatics Group
Wageningen University and Research
Netherlands
https://vdhooftcompmet.github.io.

Biography

Justin J.J. van der Hooft is an Assistant Professor in Computational Metabolomics in the Bioinformatics Group at Wageningen University, NL, and an author of over 90 peer-reviewed articles in the metabolomics field. Justin is very fascinated by the ingenuity of nature in creating marvellous chemical structures and their diverse roles in ecosystems that include inter-kingdom communication and this a main driver of his research. He obtained his MSc (2007) in Molecular Sciences (Wageningen University, NL) and his PhD (2012) at the Biochemistry and Bioscience groups in Wageningen (Wageningen University & Research, NL). After a postdoctoral period in Glasgow, UK, studying both analytical and computational aspects of metabolite structure annotation, he returned to Wageningen in 2017 to work on linking metabolome and genome mining workflows. Since he started his own group in 2020, his team has continued to develop computational metabolomics methodologies to decompose the mass spectral data of complex metabolite mixtures into structure and substructure information. By linking genome and metabolome mining, his team studies plant, food, and microbiome-associated metabolites to find novel bioactive metabolites and infer their source and function. Since 2022, he is also affiliated with the University of Johannesburg, SA, as a visiting professor. Got interested? Find out more and meet the team here: https://vdhooftcompmet.github.io.

How did you get involved in metabolomics?

My first encounter with what we would now call metabolomics and especially the metabolite annotation and identification aspects of the field was during my MSc in Molecular Sciences (Wageningen University, the Netherlands). During my MSc, I have been to Copenhagen, Denmark, for my research internship. There, I used the two metabolomics powerhouse methods of mass spectrometry (MS) and nuclear magnetic resonance spectroscopy (NMR) to elucidate specialized metabolites from South African medicinal plant extracts. These can contain beneficial molecules, but also harmful ones, especially when ingested in too much quantities. For example, I characterized cardenolides that pose a threat to grazing cattle when the dose gets at such levels that the molecules start to influence the heart rhythm. During my project, using a combination of MS fragmentation analyses and NMR studies of semi-purified molecules, I could elucidate several glycosylated cardenolides. Ironically, to do so, I had to remove flavonoids from the plant extracts - a group of molecules that I extensively studied during my Ph.D. project in Wageningen that formed a part of the Netherlands Metabolomics Center. All in all, my metabolomics experience in Denmark further triggered my fascination for the intriguing chemistry that nature produces, and the role small molecules play in ecosystems.

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

There are several aspects of my work that I feel are exciting and motivating me to pursue my career in metabolomics:

It is really inspiring to witness the inventive use of tools developed with my group and how these shine new light on the chemical space around us. For example, by now, MolNetEnhancer has been used by many groups around the globe and it is great to see all the nice figures of organized and annotated metabolomics profiles as part of biochemical studies. It is rewarding for our team to see that both academia as well as industry use computational metabolomics workflows to get a grip on their metabolomics data. It is also nice to see how vibrant the metabolomics field is nowadays with many bioprospecting projects that involve a metabolomics phenotyping component.

In our group's work, I regard the use of text mining-inspired machine learning approaches as one of the exciting aspects as we demystify the complex spectral data by pattern mining by treating it as its own language. Manually, you would browse the mass spectral files and compare mass peaks to find relevant peak patterns that can guide structure annotation. From my own experience during my Ph.D. project, I know this can take substantial time, even for one metabolomics profile. Therefore, during my Postdoc time in Glasgow, we pioneered text topic modelling on metabolomics data and indeed were able to guide the pattern discovery resulting in MS2LDA unsupervised substructure

discovery. However, afterward, my human expertise (and that of the metabolomics community) was still needed for the biochemical interpretation... Since then, we continued to develop databases and machine learning algorithms to ease the structural annotation of metabolomics profiles: MotifDB, Spec2Vec, MS2DeepScore, and, most recently, MS2Query for analogue search.

Finally, the rise of Artificial Intelligence (AI) in the field of metabolomics is exciting. Following up on the machine learning work that we have pioneered in the structure annotation of metabolomics profiles, the role of AI in the field of metabolomics could also substantially increase once sufficient well-curated reference datasets are available. This is akin to how three-dimensional protein structure prediction has been revolutionized by deep learning (i.e., AlphaFold) once sufficient reference structures were collected in the Protein Structure Database. Compared to protein structure prediction, metabolomics has the challenge that the data are much more heterogeneous: i.e., different mass spectrometers, adducts, and fragmentation types result in different mass spectra for the same molecule. In other words, one molecule can have many representations in metabolomics, and this poses challenges on how to effectively combine these representations and compare them between various molecules. Currently, we are witnessing the first examples of how AI can help in several aspects of the metabolomics workflow: data preprocessing (think of noise removal), data processing (think of peak picking), data organization (think of logical groupings based on mass spectral features), and data annotation with structure and functions (think of source organism and bioactivity), and finally complete data pipelines that output possible relevant mass features to further study. With the current development of various explorative AI-based tools, the metabolomics community is hopefully in good shape to pick up on it once sufficient reference data is in place.

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

At the moment, I work on the following initiatives in Wageningen:

Establishing a team with computational metabolomics core expertise: here, we are focusing on organizing mass spectral data, prioritizing relevant signals, and facilitating structural and functional annotations of specialized metabolites in natural mixtures (see Figure 1 for the graphic with some recent examples of tools for these categories). It is noteworthy that we are also aiming to aid and guide the researcher in making informed decisions based on the analyzed data, for example through visualization in a dashboard.

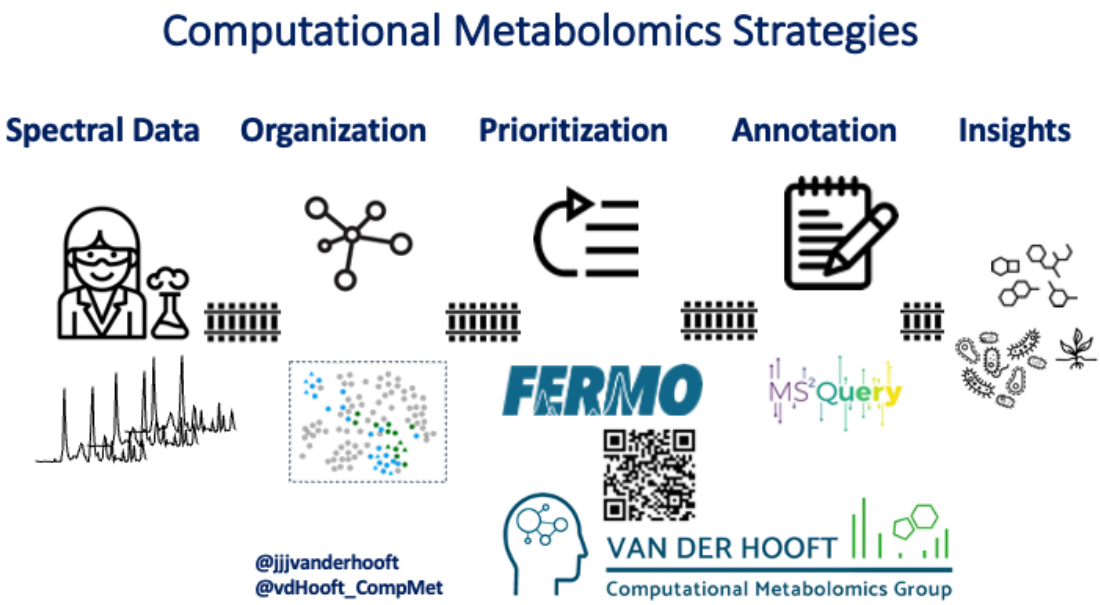


Figure 1: An overview of the various computational metabolomics activities that the Van der Hooft Computational Metabolomics Group is working on to get from mass spectral data to biochemical insights. Below the key activities organization, priotirization, and annotation, several examples of recently developed tools are highlighted.

Connecting methodical advances with natural product applications: whilst metabolite annotation remains a grand challenge in many metabolomics disciplines, it is especially so in natural products research as the specialized metabolites are relatively large. This leaves many possibilities in terms of elemental formulas, and subsequently atomic configurations, for measured mass signals. Our team is connecting to other groups within (and outside) the institute to facilitate the implementation and application of recently developed or updated computational metabolomics tools.

Combining computational metabolomics workflows with other omics disciplines to get to integrative omics mining framework for accelerated natural products discovery: as is generally known, the metabolomics workhorses MS and NMR can only bring us so far in elucidating the structure, function, and origin of metabolites. Additional omics technologies, in particular computational genomics workflows such as genome mining for biosynthetic gene clusters, have proven to provide complementary information about complex metabolite mixtures. Together with collaborators both within the Netherlands as well as outside, my team is working on facilitating such integrative omics approaches that combine genome mining and metabolome mining workflows. For example, the creation of a modular and expendable python framework is ongoing with the Netherlands eScience Center and collaborators. Of course, we welcome everyone who is enthusiastic to contribute to make it a truly community-managed and community-driven framework.

What is happening in Netherlands in terms of metabolomics?

Since the start of the Netherlands Metabolomics Center (NMC) in 2008, there are several growing metabolomics centers across the country. For several years, the NMC has been representing BeNeLux (Belgium, Netherlands, Luxemburg), and we see increasing involvement from various institutes and groups. As of 2019, the YoungNMC connects early-career researchers across the BeNeLux. Due to Covid-19, the committee could not organize in-person meetings; however, this will change soon... The Covid period also brought something nice: the bimonthly NMC online seminar series will continue to run to connect scientists around a specific theme such as plant metabolomics or fluxomics-related applications.

With strong metabolomics centers at universities and medical centers across the country as well as the active involvement of several companies, expect that metabolomics will remain to be a vibrant field in the Netherlands for the foreseeable future! This is also boosted by large initiatives such as X-omics (cross(!)-omics) of which metabolomics is one of the pillar techniques.

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

With the typical increase in samples measured within one metabolomics experiment, and the increased coverage and thus the complexity of the data, structural annotation at the level of chemical compound class or substructure will become increasingly important to aid in prioritization, i.e.: is the metabolite of the compound class we are interested in? Is the metabolite novel or merely a structural analogue of a well-known bioactive? The work I have been doing so far on MS2LDA unsupervised substructure discovery and MolNetEnhancer that combines the previous with molecular networking is facilitating the navigation of larger-scale metabolomics datasets. Researchers use these tools worldwide, oftentimes in combination with GNPS molecular networking, to explore and annotate their datasets.

Most metabolomics studies involve typical questions like which samples or spectral features are relevant for my experiment? To answer these questions, we are dependent on the combined use of the processed and annotated spectral data, metadata containing groupings and sample information, as well as bioactivity (phenotype) information. To ease the integration of these heterogeneous data, my team is building FERMO that automates a large part of this integration, adds annotations, and computes various metrics that can be used for prioritizing features following the elimination principle. After running the tool, the results appear in a dashboard to facilitate inspection, check out the FERMO dashboard example page to see how that looks!

Another initiative that resulted from my collaboration with the Netherlands eScience Center is the Python package matchms. We recognized that where several R packages for metabolomics data analyses existed and were successfully used and implemented in workflows, not many Python-based packages were available to the community. During the development of MS2LDA and later on Spec2Vec we recognized the need for a modular and well-tested basis for a Python framework, and with the help of eScienceCenter validation funding, the matchms package was realized. The matchms package primarily focuses on reading in the mass spectral library and experimental data and allows us to compare (match) these spectra against and across each other using a variety of mass spectral similarity scores. Currently, existing extensions allow for networking analyses. Furthermore, many recent tools, i.e., Spec2Vec, MS2DeepScore, and MS2Query were built on top of matchms (see Figure 2 for an overview of Python-based tools for metabolite annotation). I hope that matchms and its extensions will be further adopted by the research community both in academia and industry.

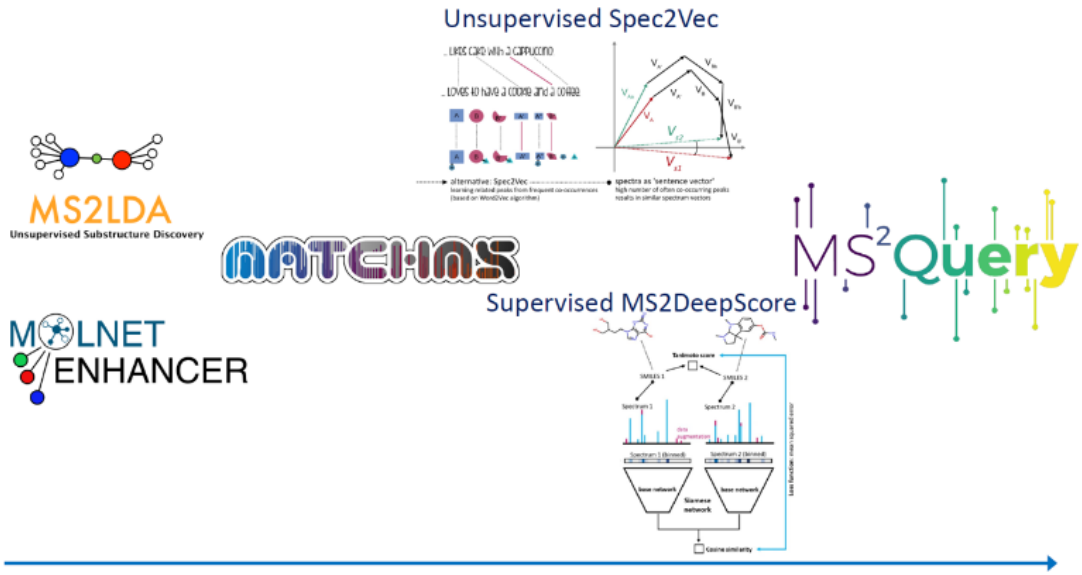


Figure 2: An overview of Python-based tools for metabolite annotation. MS2LDA and MolNetEnhancer are earlier examples developed before the matchms framework was coined. Afterwards, several tools such as the highlighted Spec2Vec, MS2DeepScore, and MS2Query, were built on top of matchms.

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

Although I am probably quite biased, I see metabolomics as a fantastic multidisciplinary field that can let us both appreciate the chemical space on Earth as well as screen for harmful components. We see explorative data analysis approaches emerging to generate novel hypotheses as well as targeted often quantitative approaches to do large-

scale sensitive screenings. I foresee that we will remain to be amazed by the creative chemistry of nature and we will keep filling in molecular details about pathways in model organisms. Fueled by the technical advances of the instrumentation, increasingly complex yet information-rich datasets are generated. This has sparked the field of computational metabolomics in which my team is active. It is great to see how the metabolomics community is generally very collaborative with many workshops and summer schools that are being organized to teach early-career scientists. This is important given the spur of computational metabolomics tools that are being proposed these days.

What do you see as the greatest barriers for metabolomics?

Apart from the grand challenge of metabolite annotation and identification, there are several new challenges that the metabolomics field will face in my view. First of all, the community has enabled the use of many metabolomics profiles and spectra, however, the accompanying metadata is not always fully correct. As we increasingly rely on computational workflows, manual verification of results becomes increasingly difficult. Thus, the quality of metadata, i.e., all different kinds of sample information relevant for data analysis, is one of the barriers to overcome to more accurate tools for annotation. This is true for both reference mass and NMR spectra as well as the raw and preprocessed experimental data. Only when the metadata is recorded in a comparable manner, larger-scale analyses will enable novel insights by discovering previously unseen patterns. The ReDU project is an example that has started to address this challenge by allowing researchers to add a controlled vocabulary to metabolomics data deposited in GNPS-MassIVE.

Another emerging challenge is to connect things at scale: several repository scale tools have been proposed such as MASST, however, their effective use as part of complete metabolomics workflows is still hampered by a lack of tools and visual aids to appreciate the emerging patterns in this connected data. Recently, knowledge graphs have been proposed as a solution, for example, to link annotated metabolites to diseases, and I look forward to seeing how they will affect the metabolomics field.

Finally, effective comparative and benchmarking analyses for metabolomics workflows are still hampered by the lack of common ground when it comes to testing and training new algorithms and tools and reporting the results. Most tools use (slightly) different spectral datasets cleaned in (slightly) different ways, sometimes also consisting of properatory data, making it very complex to judge the performance of tools across different papers. I believe that there is a role for editors, reviewers, and most importantly

authors to enable fair (FAIR) comparison by providing all test and training data and settings used for training and testing.

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

This question implies that metabolomics did not take off (yet). In my view, it already did! If there is one thing that could give metabolomics an enormous boost, than it would be opening up all annotated mass and NMR spectra as well as profiles to the scientific community. This will both assist in the structural and functional annotation of metabolomics profiles as well as the training and testing of the next-generation models that will underpin the entire metabolomics analysis workflow. I am well aware that one of the challenging aspects of applying computational metabolomics workflows is the choice of parameter and threshold settings that impact the final outcome of the metabolomics experiment. I expect that the increased availability of completely or partially characterized metabolite features will help researchers to make informed decisions on what works best for their data and experiment as they can confirm their choices with annotated spectra. Of course, this implies that experiment-specific settings may be found that describe the data "locally" in the best way. Thus, it will be even more important to share these settings and it is encouraging that tools like MZmine 3 now facilitate the easy sharing and implementation of data processing and analysis settings, at the same time avoiding long written descriptions in papers.

Another aspect that could help in the above challenge that - as a metabolomics community - we can still further improve on is the availability of tutorials and workshops to train and educate future metabolomics scientists. It is great to see that many conferences nowadays include workshops in which concepts and tools are being explained. Furthermore, several summer school initiatives are successfully running, for example on untargeted (clinical) metabolomics. As a community, we could do more efforts in making relevant materials available, and I am doing my FAIR share there as well. Further, I believe that to enthuse scientists to start using metabolomics, it is important to put effort in taking newcomers up into the community. During my talks, I do my best to explain core concepts to connect to newcomers in the field. During Metabolomics2023 in Niagara Falls, CA, it was nice to get feedback that a novice to the metabolomics field was captivated by my ability to convey complex concepts through visual presentations using well-designed slides. I will continue to do my best to do so!

Dr. Justin van der Hooft was delivering a keynote presentation "Breaking Bonds & Barriers: Computational Metabolomics Strategies to Organize, Prioritize, and Annotate Metabolites in Mass Spectrometry Profiles" at Metabolomics 2023 Conference, Niagara Falls.

The audience thanks Dr. Justin van der Hooft after his keynote presentation during Metabolomics 2023.

How does the future look in terms of funding for metabolomics?

The phenotyping power of metabolomics has become increasingly popular due to recent improvements in both analytical equipment as well as data handling and analysis. Thus, larger consortia now oftentimes contain a metabolomics component when it involves understanding biological systems using omics approaches. Currently pressing challenges like biodiversity loss and finding natural alternatives for synthetic harmful chemicals require full characterization of complex metabolite mixtures to map the current chemical space and understand the metabolic capacities and interactions of plants and microbes. Hence, on the application side, I think the future of metabolomics is bright. Nevertheless, it is still difficult to obtain funding for the tools and resources that underpin these applications: to support the development of new add-ons, maintenance, and performance improvements. Of course, this is not metabolomics specific, but true for science in general. Therefore, I highly applaud recent initiatives within the Dutch scientific funding landscape towards Open Science and Sustainability grants that will greatly impact currently developed tools in the longer term.

What role can metabolomics standards play?

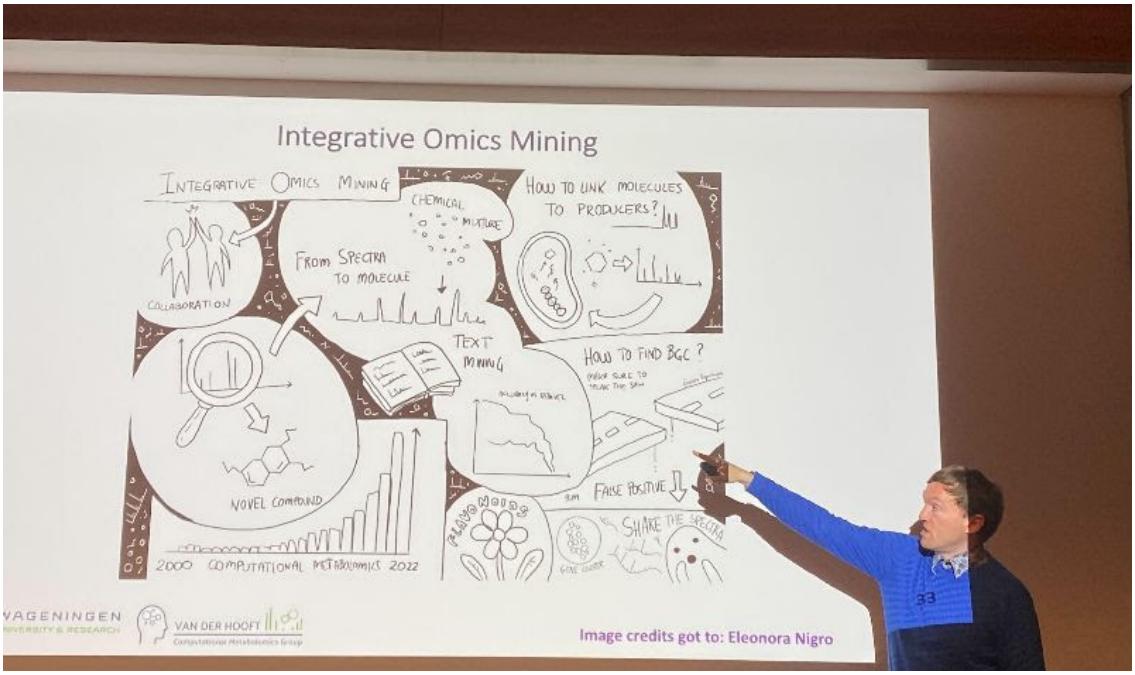
Metabolomics standards are very important to make analyses comparable and accountable. Ideally, all studies adhere to the most recent standards (using ontologies where defined and controlled vocabulary where available) and they are updated if newer definitions emerge. This also relates to the concept of "living data" that the GNPS platform hosted in San Diego, USA, coined, where certain analyses are rerun using updated reference libraries and improved tools to hopefully gain additional insights into the dataset. In this case, the rerunning can be done automatically, however, further analysis to check for additional insights still needs to be done with human expertise of both the biochemistry involved and the generated spectral data. In contrast, the metadata is quite challenging to update automatically as the adoption of new standards and ontologies is to a large extent relying on human expertise, and this raises the question of how long we are responsible to make metabolomics data and tools available in an active manner. In other words, how long should we care for our software and data to remain compatible with current standards (i.e., generic supportive software packages, metadata ontologies) and how can we fund these activities? We can see some nice initiatives such as the GNPS platform that by integrating computational metabolomics tools and data visualization dashboards make metabolomics workflows accessible to and

reproducible for the metabolomics community. In the end, it will likely remain a balance between time investment and returns and available technology - especially after a study was published and researchers need to choose between starting new adventures or further documenting previous work. The easier we can make these processes, possibly with the help of AI to auto-fill text fields, the more likely the balance will shift toward maintenance with FAIR care...

Perhaps an alternative question to this one could be: "What is the role of Open Science for metabolomics?" I think it is clear also from previous answers that I believe that this will be essential for community efforts and initiatives to improve current tools and create new ones. Furthermore, connecting existing workflows is also best done in collaboration and best supported through Open Science.

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

Metabolomics has been, is, and will remain to be a multidisciplinary discipline... thus, connect, collaborate, and coproduce the next equipment, tools, and computational metabolomics strategies to better understand metabolism and the chemical space surrounding us!



Justin's group is also working on integrative omics mining tools and approaches where genome mining approaches for biosynthetic gene clusters in sequenced genomes of organisms are linked to metabolome mining approaches to accelerate natural product discovery research. Here, Justin is showing an overview during the Applied Meta-Omics Summer School keynote lecture in Zürich, Switzerland.

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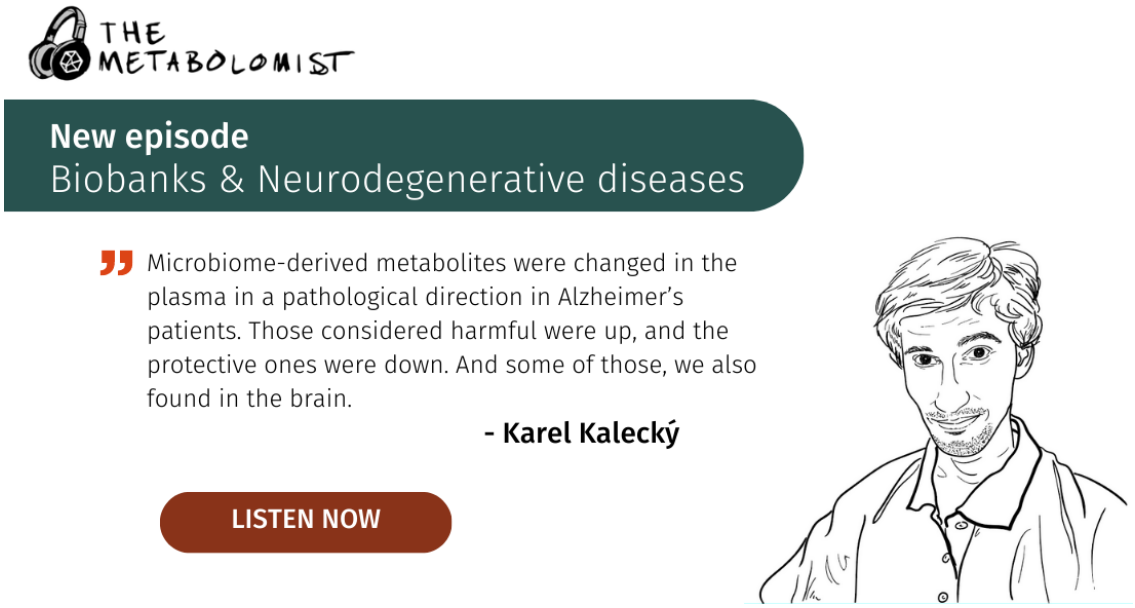
The Metabolomist Podcast



Recent Publications

Reviews:

- Cancer metabolites: promising biomarkers for cancer liquid biopsy (Open access)
- Emerging pre-clinical safety assessments for potential probiotic strains: a review
- Recent advances in mass spectrometry-based computational metabolomics
- Unlocking the secrets of the microbiome: exploring the dynamic microbial interplay with humans through metabolomics and their manipulation for synthetic biology applications (Open access)
- Urinary exosomal metabolites: Overlooked clue for predicting cardiovascular risk

Articles:

- Brand-Specific Toxicity of Tire Tread Particles Helps Identify the Determinants of Toxicity
- Chlorothalonil induces obesity in mice by regulating host gut microbiota and bile acids metabolism via FXR pathways

- Cholesterol modulates the physiological response to nanoparticles by changing the composition of protein corona
- Detection of common adulterants in olive oils by bench top 60 MHz 1H NMR with partial least squares regression
- Does mask wearing affect skin health? An untargeted skin metabolomics study (Open access)
- Early sex-dependent differences in metabolic profiles of overweight and adiposity in young children: a cross-sectional analysis (Open access)
- Enhanced correlation-based linking of biosynthetic gene clusters to their metabolic products through chemical class matching (Open access)
- Increased genital mucosal cytokines in Canadian women associate with higher antigen-presenting cells, inflammatory metabolites, epithelial barrier disruption, and the depletion of L. crispatus (Open access)
- Inflammation and the pathological progression of Alzheimer's disease are associated with low circulating choline levels (Open access)
- Metabolomics and Machine Learning Identify Metabolic Differences and Potential Biomarkers for Frequent versus Infrequent Gout Flares (Open access)
- Relationships between sensory properties and metabolomic profiles of different apple cultivars (Open access)
- Study on taste quality formation and leaf conducting tissue changes in six types of tea during their manufacturing processes (Open access)
- Targeted metabolomic analysis in Parkinson's disease brain frontal cortex and putamen with relation to cognitive impairment (Open access)
- The integrated metabolomics and sensory analyses unravel the peculiarities of mountain grassland-based cheese production: The case of Parmigiano Reggiano PDO
- TopNEXt: Automatic DDA Exclusion Framework for Multi-Sample Mass Spectrometry Experiments (Open access)

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Metabolomics Events

The 8th Lipidomics Forum of iLS

August 27 - 30, 2023

Venue: Vienna, Austria.

Learn More Here

A Conference of the International Lipidomics Society and Partners. You will get a chance to learn about the latest lipidomics research from your presentations, posters, and of course from the keynote speakers Frances Platt, Giovanni D'Angelo, Maria Fedorova, Valerie O'Donnell, Peter Meikle, Christoph Thiele, Zoltan Takats, Julijana Ivanisevic, and Andrej Shevchenko. The abstract book is now available. Regular registration is open until **August 30, 2023.**

Bits & Bites # 05: Identification of unknown compounds in untargeted metabolomics using freely available software

September 7, 2023

Venue: Online

Learn More Here

This 5th course is taught by Dr. Arpana Vaniya from UC Davis, and participants required to have basic knowledge of computer skills and no coding experience is needed. The tuition for #5 is $350 and it takes approximately 8 hours.

Short description of the course: Compound identification is known as the bottleneck in metabolomics. However, there are many approaches one may consider while tackling this challenge (i.e. mass spectral library search, in silico fragmentation tools, or database searching). This short course will provide an overview of the current status of compound ID in metabolomics, participants will learn how to use freely available in silico fragmentation tools MS-FINDER and SIRIUS+CSI: FingerID, web-based tools such as MetFrag and CFM-ID and learn how to use MassBank of North America in NIST MS Search.

Early Career Members (ECM) Virtual Job Fair

September 7, 2023

Venue: Online

Learn More Here

Are you seeking new lab members or exploring new career opportunities? If so, consider attending the Metabolomics Society of North America (MANA) ECM Virtual Job Fair! This event is for employers, recruiters, and job seekers alike, providing a platform to connect with potential candidates or employers from diverse sectors such as academia, industry, or government/ nonprofit organizations. Through the virtual Zoom setup, organizers facilitate effortless interactions between employers and prospective candidates, helping you make valuable connections for your career or organization.

5th Annual MANA Fall Symposium "Expanding the Exposome: The Power of Mass Spectrometry"

September 8, 2023

Venue: Online

Register Here

5th MANA Fall Symposium "Expanding the Exposome: The Power of Mass Spectrometry" is hosted and organized by the UC Davis West Coast Metabolomics Center on September , 2023, from 9 am - 2 pm PT. The list of distinguished speakers:

Dr. Dana Barr, Emory University
Dr. Jonathan Martin, Stockholm University
Dr. Lauren Petrick, Mount Sinai Health System
Dr. Antony Williams, EPA, Center of Computational Toxicology and Exposure
Dr. Krystal Godri Pollitt, Yale
Dr. Dinesh Barupal, Mount Sinai Health System

MANA sponsors will also join and present their recent updates. Seize this unique opportunity to engage with leading scholars and expand your understanding of mass spectrometry's role in exposome studies. Registration is free, and for more details click here.

2023 World Critical Care & Anesthesiology Conference

September 8-9, 2023

Venue: Hybrid, Singapore

Learn More Here

The 5th 2023 WCAC will serve as a platform for discussions on current trends, emerging technologies, advancements, challenges and research in the field of critical care and various surgical procedures. This conference aims to bring together a diverse group of professionals including Intensivist Doctors, Professors, Pulmonologists, Anesthesiologists, Nursing officers, Scientists, and Researchers.

2023 World Pediatrics Conference

September 8-9, 2023

Venue: Hybrid, Singapore

Learn More Here

2023 World Pediatrics Conference (WPC) will focus on the latest advancements and innovations in different fields of Pediatrics research. The theme of the conference is "Scientific advancement and exploration in Pediatrics and Neonatology." where professionals from around the world exchange their views on a wide range of topics related to childcare and pediatric diseases globally.

9th Swiss Metabolomics Society Annual Meeting

September 15, 2023

Venue: Zurich, Switzerland

Learn More Here

This year's science day will be hosted by Nicola Zamboni in the historic main building of the Eidgenössisch Technische Hochschule Zürich (ETHZ). The theme for this meeting is "Frontiers in Metabolomics", focusing on the latest advancements in analytics, small molecule structure elucidation, omics integration & application, cheminformatics, and computational mass spectrometry. The event has confirmed two distinguished plenary speakers: Emma Schymanski and Matej Orešič, who will be joining the gathering in Switzerland. The deadline for the poster submission deadline is extended to **August 31, 2023.** For more details click here.

Bits & Bites # 06: Mass Spectrometry for Metabolomics

October 5, 2023

Venue: Online

Learn More Here

This 6th course is taught by Dr. Uri Keshet from UC Davis, and no prior knowledge or software is required. The tuition is $175.

Short description of the course: Mass spectrometry (MS) is an important analytical technique in many metabolomics labs. With a wide range of MS systems available, such as GC-MS, LC-MS, EI, ESI, TOF, QQQ, and Orbitrap, selecting the appropriate instrument to suit specific needs and constraints can be a daunting task. In this short course, the fundamental principles of MS will be explored, encompassing various sample introduction methods, ionization techniques, and mass analyzer options, with a particular focus on their application in metabolomics. Whether for targeted or untargeted applications, participants will gain insights into reading and comprehending MS output data, including EI-MS, ESI-MS, or ESI-MS/MS spectra. The course will also provide valuable guidance on developing high-throughput MS methods, (i.e., short 5-min method) that can be used in metabolomics. By the end of the course, attendees will have acquired a solid understanding of the available MS systems in the market, the challenges associated with their use, the essentials of designing studies using different MS approaches, and the tools required for reading and processing MS data files.

MANA SODAMeet

October 10, 2023

Venue: Online

Learn More Here

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.

5th Annual Metabolomics Society of North America (MANA) Conference

October 23 – 27, 2023

Venue: Columbia, MO, USA

Learn More Here

The 2023 conference will be held October 23-27, 2023 on the campus of the University of Missouri in Columbia, MO. Professor Lloyd Sumner will chair the meeting and is developing an exciting program that will appeal to many interests in metabolomics. This year, MANA is excited to partner with the International Lipidomics Society (ILS), and the 2023 conference will have dedicated sessions for lipidomics, and an evening workshop with the ILS. Check out the conference website for program updates.

- Poster abstract submissions deadline is extended to **August 31, 2023**
- Click here to register

14th European Nutrition Conference (ENC) FENS 2023

November 17 – 25, 2023

Venue: Belgrade, Serbia

Learn More Here

The 14th European Nutrition Conference will be held in Belgrade, the capital city of Serbia. The theme of the conference is “Food, Nutrition, and Health: Translating science into practice”. Around this theme, the conference will deliver a high-quality program, featuring international speakers across plenary sessions and symposia. Other features of the program will be discussions and debates, industry symposia, panel sessions, and networking opportunities including several specifically catering to early career researchers.

- Abstract submission for late posters extended to **September 21st, 2023**
- Regular registration is until **November 10, 2023**

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Metabolomics Jobs

Metabolomics Jobs

If you have a job to post, please email the MetaboNews team at metabolomics.innovation@gmail.com

We may remove a listing after 6 months if we do not receive a confirmation that it is still necessary. However, if you would like us to repost it, please contact us.

Job Title	Employer	Location	Source
Postdoctoral Research Scientist Position in Exposomics	Britz-Mckibbin Lab at McMaster University	Hamilton, ON, Canada	TMIC website
Post-Doctoral Fellow	Department of Medical Microbiology & Immunology, University of Alberta	Edmonton, AB, Canada	University of Alberta Careers
Postdoctoral Researcher in Mass Spectrometry Workflows for Unknown Chemicals	Luxembourg Centre for Systems Biomedicine (LCSB)	Luxembourg	Luxembourg Centre for Systems Biomedicine
Postdoctoral Position for Metabolomics Research in Mitochondrial Disorders	Luxembourg Centre for Systems Biomedicine (LCSB)	Luxembourg	Luxembourg Centre for Systems Biomedicine
Research Specialist - Metabolomics	UMass Chan Medical School	Worcester, MA, USA	Metabolomics Society

Operations Assistant	NovaMT and TMIC Li Node at the University of Alberta	Edmonton, Alberta, Canada	Dr. Liang Li (please contact liang.li@ualberta.ca)
Postdoctoral Research Associate-Sumner Lab	Nutrition Research Institute	Kannapolis, North Carolina, US	The University of North Carolina
Metabolomics Project Coordinator	Human Metabolome Technologies of America	Remote or Boston, MA, USA	Metabolomics Society
Doctoral Candidates	HUMAN – Harmonising and Unifying Blood Metabolomics Analysis Networks	Europe	HUMAN Doctoral Network
Postdoctoral Fellow in Omics	Georgia Institute of Technology	Atlanta, USA	Metabolomics Society
Postdoctoral Research Fellow (LC-MS and Data Science for Metabolomics)	The Li Lab and the Li Node of TMIC, University of Alberta	Edmonton, Alberta, Canada	University of Alberta

MetaboNews Feedback Form

As you noticed, we have changed to a new format starting in April 2023. We hope to provide enough useful content to keep you interested and informed and appreciate your comments and feedback on how we can make this newsletter better. Please fill out this quick survey and let us know your thoughts (your answers will be anonymous). It will only take less than one minute with only two mandatory questions

Fill Out Your Survey Here

We carefully considered all feedback to enhance our newsletter and deliver an improved experience. The issue on the "clipped email" link at the beginning of the newsletter is fixed, now, you are able to navigate to the clipped section and extend the content.

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

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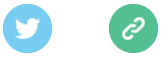

Our mailing address is:
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