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Metabolomics Society News

Conference Corner

Metabolomics 2022: Valencia, Spain - June 19-23

Dear Colleagues,

Much is happening and there are several updates that we would like to share. First, we are delighted to invite you to **Metabolomics 2022**: the 18th International Conference of the Metabolomics Society!

We welcome you back to an **in-person event to be held in Valencia, Spain**. Save the date for **June 19-23, 2022** – see you at the Valencia Conference Center!

This year's conference will be run by two conference chairs: *Natasa Giallourou* and *Antonio Granell* who will be organizing, together with an International *Scientific Organizing Committee (SOC)*, and the Society's *Conference Committee* headed by *Dan Raftery*. Valencia is one of the most vibrant cities in Europe and a significant hub for science and technology. The meeting will also be co-organized with the *Spanish Society for Metabolomics (SESOMET)* and the *Spanish Network for Metabolomics*. This is the first time that the conference is held in Spain and our first in-person meeting after two years in the virtual space. Please check the website soon ([Metabolomics2022.org](https://www.metabolomics2022.org)) for updates on workshop and abstract submissions as well as conference registration.

We also want to send a reminder for the Special Issue of *Metabolites* dedicated to Metabolomics 2021 Online. We particularly, but not exclusively, welcome papers presented at or resulting from Metabolomics 2021 Online, the second virtual conference of the Metabolomics Society that took place on 22–24, June 2021. The focus of this issue is on topics relevant to metabolomic science. More information about the Special Issue can be found at: https://www.mdpi.com/journal/metabolites/special_issues/Metabolomics_2021.

The deadline has been extended to December 1, 2021.

We are looking forward to seeing you all at Metabolomics 2022!

Jessica Lasky-Su, President, Metabolomics Society

Natasa Giallourou, Co-Chair of Metabolomics 2022

Antonio Granell, Co-Chair of Metabolomics 2022

Dan Raftery, Conference Committee Chair



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

Members Corner

Early-career Members Network (EMN)

New Expert Opinion

Our new Expert Opinion is now out! Dr. Michael Witting has shared his work on *C.elegans* and his career experience providing valuable tips for early-career researchers! Follow [Michael Witting - Metabolomics Society Wiki](#) to find out more.

EMN Webinar Series

The EMN would like to thank once again Professor Tim Ebbels and Ms. Cecilia Wieder for their great presentations on computational metabolomics and metabolomic pathway analysis explaining why they are useful and providing recommendations for the use of over-representation analysis. If you missed our latest webinars, the recordings are now available on [EMN Webinars – 2021 – Metabolomics Society](#).

Stay tuned for announcements sent over email and posted on our social media platforms for the upcoming webinar!

International Affiliates Corner

Metabolomics Association of North America (MANA)

Visit <https://metabolomicsna.org>.

The 3rd Annual MANA Conference was held virtually October 18-21, 2021 and was attended by over 440 participants! It featured 6 plenary speakers, 5 instructional workshops, 10 corporate member events, 36 oral presentations, 7 interactive forums, and 2 poster sessions. In addition, a number of awards were made, including:

- **MANA Early Career Award**
 - *Dr. Robert Quinn*, Michigan State University
- **Mark P. Styczynski Early Career Award in Computational Metabolomics**
 - *Dr. Aleksander Smirnov*, University of North Carolina at Charlotte
- **MANA Metabolomics Service Cores Best Presentation Awards – 2 awardees**
 - *Wasim Sandhu*, University of California, Davis
 - *Mr. Brady Anderson*, University of Michigan
- **MANA Early Career Members Lightning Talk Awards – 2 awardees**
 - *Dr. Xinyu Fu*, Michigan State University
 - *Dr. Matthias Klein*, The Ohio State University
- **MANA Early Career Members Lightning Talk Awards – 2 awardees**
 - *Dr. Xinyu Fu*, Michigan State University
 - *Dr. Matthias Klein*, The Ohio State University
- **MANA Early Career Members Best Poster Awards – 12 awardees**
 - *Dr. Yuanyue Li*, University of California, Davis
 - *Dr. Eléna Legrand*, McGill University
 - *Dr. Dorsa Varshavi*, University of Alberta
 - *Dr. Armando Alcazar Magana*, Oregon State University
 - *Dr. Lisaura Maldonado-Pereira*, Michigan State University
 - *Mr. Russel Fling*, Michigan State University
 - *Mr. Nathan Stevens*, University of California, Davis
 - *Mrs. Alexandra Cheney*, Montana State University
 - *Ms. Yue Han*, Georgia Institute of Technology
 - *Mr. Nick Rigel*, The Ohio State University
 - *Ms. Ya-Chun Chan*, University of Alberta
 - *Mr. Jerry Chen*, University of North Carolina at Charlotte

NOVEMBER 2021

Metabolomics Society News

Nordic Metabolomics Society

Visit www.nordicmetsoc.org.

The new board of the Nordic Metabolomics Society was elected on October 4-10, 2021 in an online vote, with a two-year mandate. This year, several of the founding members have completed their second two-year term. The new board members are:

- Nils Joakim Færgeman (University of Southern Denmark, Odense, Denmark)
- Tone Frost Bathen (Norwegian University of Science and Technology, Trondheim, Norway)
- Guro F. Giskeødegård (Norwegian University of Science and Technology, Trondheim, Norway)
- Daniel Globisch (Uppsala University, Uppsala, Sweden)
- Katharina Herzog (Novo Nordisk A/S, Bagsværd, Denmark, and Lund University, Lund, Sweden). Early-career member.
- Tuulia Hyötyläinen (Örebro University, Örebro, Sweden)
- Olli Kärkkäinen (University of Eastern Finland, Kuopio, Finland)
- Otto Savolainen (Chalmers University of Technology, Gothenburg, Sweden) Early-career member.
- Margrét Thorsteinsdóttir (University of Iceland, Reykjavik, Iceland)

The officers in the new Board will be selected on November 11th, 2021, at the time of the first meeting of the new Board as well as of General Assembly of the Society.

The Nordic Metabolomics Society will hold its next conference in Copenhagen, September 6-9, 2022.



lipotype

Webinar
Why Population Health Studies Must Include Lipidomics

December 2, 2021
5:00 pm CET/11:00 am EST
Join us via Zoom Ap

REGISTER

Free Admission

Photo: iStock/Jake Atcher



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

General Enquiries

info@metabolomicssociety.org

Membership Enquiries

membership@metabolomicssociety.org

Metabolomics South Africa

Visit www.metabolomics-sa.co.za.

The second Annual Metabolomics Symposium – Metabolomics South Africa, in partnership with African Center for Gene Technologies (ACGT), held a two-day symposium from 20th – 21st, October 2021.

This virtual event was sponsored by Leco, Microsep, Sciex, Biocrates, Separations, Waters, Diplomics and Shimadzu South Africa. Since its establishment in 2018, MSA has grown with 250 signed-up members, with the majority from South Africa and 17% from other African countries. This year the symposium, with about 120 attendees, was an opportunity for principal investigators, postgraduate students, and interested parties to share their metabolomics research, applications, (minimum) standards procedures, and emerging technologies. Additionally, the event intended to foster further collaboration amongst metabolomics researchers within South Africa (SA) and across Africa and Europe by providing a platform for researchers to network and to identify synergies. A wide range of topics were showcased including (i) natural products from South African marine invertebrates, (ii) validation of metabolomics data, (iii) application of metabolomics in agriculture, (iv) molecular networking tools (in GNPS) and applications in natural product research, (v) metabolomics as an indispensable tool in South Africa medicinal plant research and (vi) applications of metabolomics in COVID-19 and cancer research. These topics were covered by local and international speakers and can be viewed on the Metabolomics South Africa YouTube channel <https://www.youtube.com/channel/UC1b62HhEVbETDlwz4w6YAbw>.

Prizes were awarded to the best postgraduate student presentations, and the two winners were Ms. Anza T. Ramabulana and Mrs. Chanel Pretorius, both PhD candidates at the University of Johannesburg, SA.

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SpOtlight

Visualizing chemical relationships of metabolites based on their mass fragmentation spectra with mass spectral embeddings

Spotlight Article contributed by Dr. Justin J.J. van der Hooft, Artur van Bemmelen, Joris Louwen and Niek de Jonge of the Bioinformatics Group, Wageningen University, Wageningen, the Netherlands

Nature is full of fascinating structural diversity of which we know only a small portion both in terms of structures and their functions. Mass spectrometry (MS) has become an important method to chart nature's structure diversity. More recently, MS fragmentation approaches that result in MS/MS spectra (also referred to as tandem or MS² spectra) are starting to become indispensable to study complex natural mixtures. Fragmented molecules often break into diagnostic mass fragments that can be linked to substructures or scaffolds. However, even with this very useful spectral information in hand, it is still very difficult

to puzzle together complete structures from the building blocks observed by the mass spectrometer; also, because many of the building blocks are not yet structurally solved. The understanding of metabolites' functions and roles in ecological systems will prove to be very difficult if not impossible without knowing their structures. To overcome the current bottlenecks in untargeted metabolomics analyses, in the Van der Hooft Computational Metabolomics Group (embedded within the Bioinformatics Group at Wageningen University & Research, WUR), we develop and apply computational metabolomics bioinformatics tools to enhance the analysis of MS/MS spectra. With current methods, only a fraction of MS/MS spectra can be reliably annotated by matching spectra to public spectral libraries. However, spectra that do not have a direct match to your spectral data but are structurally related, for example sharing a scaffold or substructures, often referred to as analogues, can still inform you about structural properties of metabolites in your sample. In our group we currently focus on retrieving relevant structural information from MS/MS spectra for which no fully identical match can be found in a library. Examples of tools from our group trying to achieve this goal are MS2LDA for detecting spectral patterns caused by substructures in MS datasets of your samples and MotifDB to match MS/MS spectra to annotated substructure patterns. Currently, we are in the process of building tools that exploit the novel mass spectral embeddings produced by Spec2Vec and MS2DeepScore to recognize analogues based on MS/MS spectra.

Understanding chemical relatedness of metabolites based on their MS/MS spectra

Spec2Vec and MS2DeepScore are two methods developed in and with our group that use machine learning to compare MS/MS spectra and predict their chemical similarity. Inspired by natural language processing, Spec2Vec is an unsupervised approach that can learn from any dataset how mass fragments and neutral losses in MS/MS spectra are related. In contrast, MS2DeepScore is a supervised approach that is trained to obtain a mass spectral similarity score from an MS/MS spectral pair that reflects the structural similarity of the fragmented molecules, i.e., using the Tanimoto score based on molecular fingerprints. These methods both use MS/MS spectra as an input and return mass spectral embeddings (300 dimensional vectors) that can be used to find and locate chemically similar compounds. The models will return similar positions in the embeddings for spectra of compounds with chemical similarity. The supervised aspect of MS2DeepScore means that it will only provide useful results if the model was trained with spectra that sufficiently resemble your sample.



Photo by Eric Scholten

Spec2Vec on the other hand, will work with any MS/MS dataset. We demonstrated that these approaches outperform current methods such as the modified cosine score when determining mass spectral similarity, and thus result in improved library matching as well as faster and more scalable analogue searches. Here, we provide an outlook into the possibilities our mass spectral embeddings offer in the direction of data visualization to better understand these approaches and better study chemical relatedness of metabolites.

Visualization of mass spectral embeddings

With the growing amount of MS/MS data that is currently being generated, it becomes more important to have good methods for data visualization of MS/MS data of entire samples, instead of single spectra. Here, we explore visualizations of the mass spectral embeddings created by Spec2Vec and MS2Deepscore to study the chemical similarity of MS/MS spectra in datasets. In Figure 1, an example of a mass spectral embedding visualization (after dimensionality reduction) is provided. Each dot represents a spectrum and is colored based on the chemical class they belong to, since we used GNPS public library spectra with known structures that could be classified. We can observe how similarly colored dots are often grouped together, showing that chemically similar compounds are often located relatively close together, thus proving that mass spectral embeddings can learn chemistry based on information that is present in the MS/MS spectra.

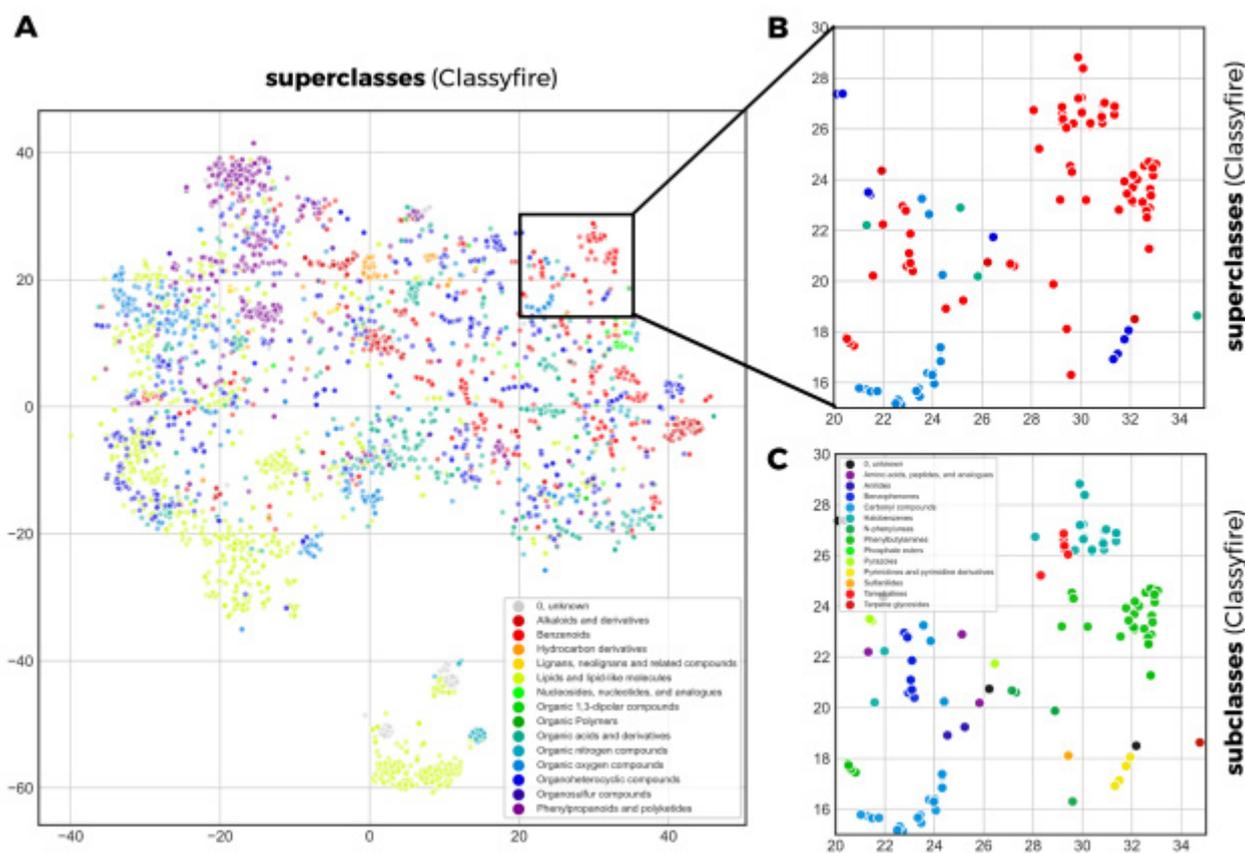


Figure 1: (A) 3601 GNPS public library spectra are plotted as colored dots with x,y positions derived through t -SNE based on the MS2Deepscore mass spectral embeddings. Dots are colored according to 14 compound superclasses provided by ClassyFire (large panel). (B) zooms into a small region for which (C) also the ClassyFire subclasses are highlighted.

Source: Huber et al., 2021, *J. of Cheminformatics*, <https://jcheminf.biomedcentral.com/articles/10.1186/s13321-021-00558-4>.

Benefits of mass spectral embeddings for metabolomics analyses

The use of mass spectral embeddings has benefits for visualization as compared to methods that rely on calculating similarity scores between two spectra, e.g., (modified) cosine score. The first benefit is speed; library matching and analogue search are much faster because only a single embedding must be calculated for each spectrum, instead of similarity score for every spectrum pair. Since the created embeddings are already trained to reflect the chemical differences, they can be used directly for plotting, using methods like T-SNE or UMAP that (further) reduce the number of dimensions from a few hundreds to 2 or 3 to allow for graphical display. To show the scalability of this method, in Figure 2 we show a plot where more than 180,000 spectra from GNPS public spectral libraries are visualized together. Again, the colors represent chemical compound classes, and we can observe that similar colors (classes) tend to cluster together.

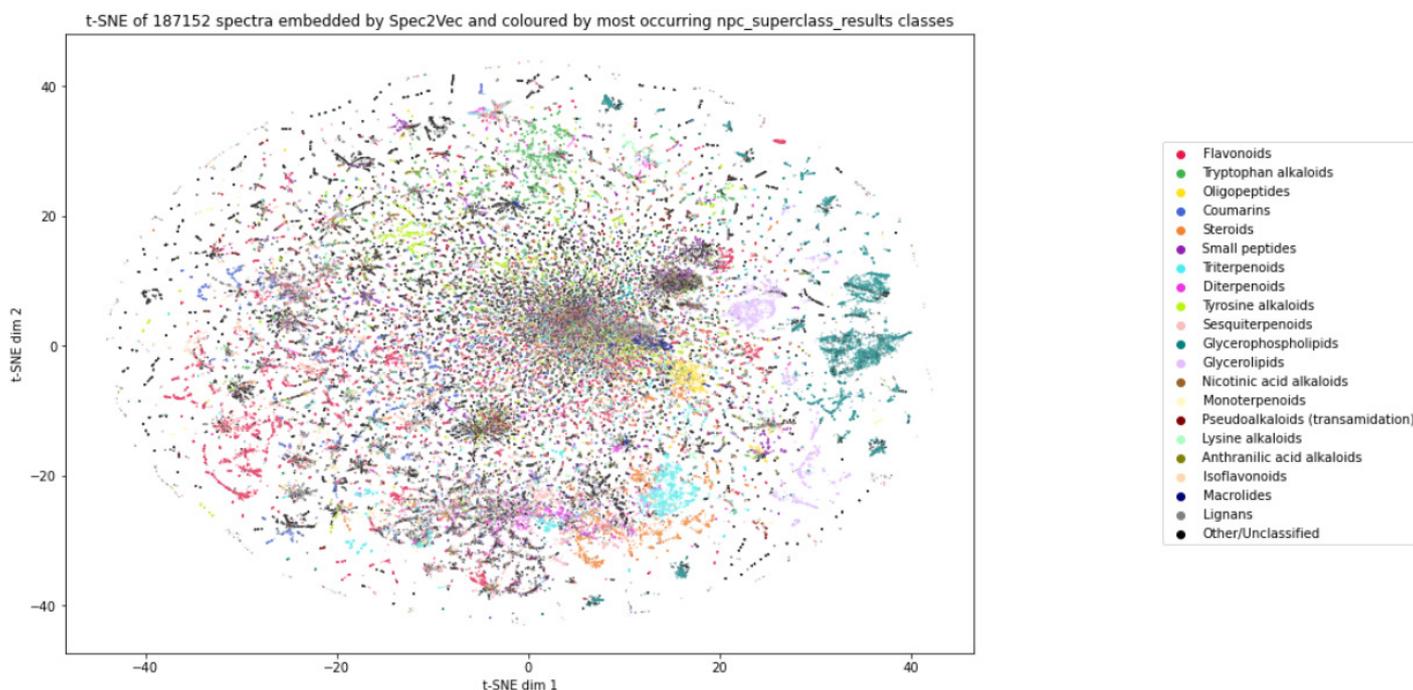


Figure 2: t-SNE plot of 187152 GNPS public library spectra based on Spec2Vec embeddings. The MS/MS spectra are colored based on the most occurring NPClassifier super classes that represent main natural product related categories.

Another benefit is that embeddings of spectra can be generated for every spectrum even if no good library match or analog can be found in the existing databases of spectra. Since the embeddings are learned or trained to represent chemical similarity, it is expected that embeddings contain features that reflect relevant chemical information. Thus, by visualizing the location of MS/MS spectra of yet unknown structures relative to other already known compounds, and further studying the chemical information captured by the 300 dimensions of the mass spectral embeddings, based on its MS/MS spectrum, we could obtain an indication of the kind of molecule that was fragmented without knowing its exact structure. Furthermore, the relative chemical distance between compounds from your sample can be visualized with this method, which makes it possible to still identify groups of metabolites in your natural mixtures that are chemically similar even when they cannot be matched to a library. Such metabolite groups could then be annotated, and these annotations can be saved within the mass spectral embeddings for future use.

Challenges of visualizing the chemical space

One of the challenges with visualizing embeddings is that the embeddings are stored in 300 dimensions while the visualization is done in 2 dimensions (x and y axis). The challenging part is that you will always get a visualization that has not all distances visualized correctly. Fortunately, some work in this regard has already been done, which resulted in methods like t-SNE and UMAP. We are currently in the process of further optimizing the settings of these methods to get a method that is reliable and has good results for our research goals. Additionally, we are also experimenting with 3-dimensional visualization methods that make it easier to separate similar compounds and study the chemical relation of molecules as inferred from their MS/MS spectra. Figure 3 shows a screenshot of a prototype 3D visualization of a t-SNE representation of a mass spectral embedding. Different forms and shapes of metabolite clusters can now be observed that cannot be appreciated as such in 2D visualizations.



Figure 3: Zoomed in screenshot of 3D visualization of a t-SNE plot created from a Spec2Vec mass spectral embedding as shown in Fig. 2. Produced in collaboration with Dienke Stomph and Bart Knuiman of the WANDER team that is part of WUR.

Chemical compound classification

Chemical compound classification represents a prominent use case of mass spectral embeddings as this would represent a fast and scalable alternative for existing methods. Such classification could be done by creating a scatterplot of library spectra with known classifications in the mass spectral embedding and plotting your own spectra on top of this plot. In Figure 4, you can find a visualization of what such a plot could look like in the future. Classification can then be done by judging the distance of your sample to various compound class clusters, even if spectral libraries do not contain an exact match to metabolite spectra from your sample. To make this possible, it will be necessary to find a way to create good clusters of these compound classes. The machine learning methods, however, are not (yet) perfect at predicting chemical distances, and there can be large differences between how chemically similar compounds are within a chemical class. Some chemical classes have much more structural variety within their group than other classes. Thus, to overcome the mentioned challenges, we are currently investigating which approach is most suitable for chemical compound classification based on mass spectral embeddings.

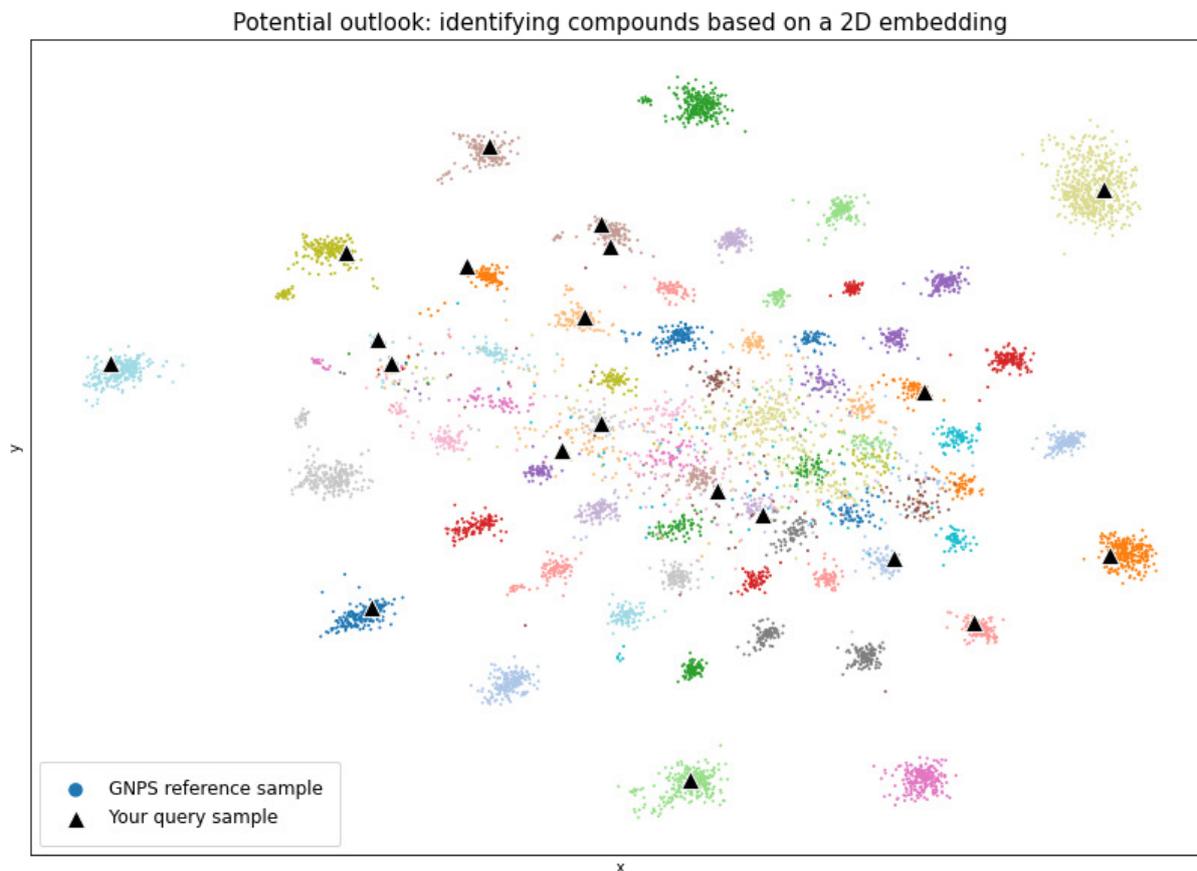


Figure 4: Outlook into how visualization of mass spectral embeddings could be used to gain a quick overview of the chemical compound classes and thus the type of metabolites that are present in your sample. We note that this is still a work in progress. Each color represents a chemical compound class, such as from ClassyFire or NPClassifier. The triangles represent MS/MS spectra from a query sample that could then be classified based on their positions in the mass spectral embedding.

Outlook into the role of mass spectral embeddings in metabolomics data analysis

Our main vision is to enable the use of mass spectral embeddings for scalable multi-sample comparisons. An example of a future use case would be if one has two or more samples with a few hundred MS/MS spectra that can be compared directly, by visualizing the embeddings of these spectra in the same space and incorporating quantitative information about the molecules. Differentially expressed metabolites and their chemical relationships can then be highlighted. Moreover, overlaying comparative results onto a plot with already annotated library spectra that are colored based on chemical compound class can give a quick overview of the type of metabolites that are likely present in your samples and which type of metabolites differ between samples. Moreover, it will also help to prioritize likely novel chemistry in your samples: if MS/MS spectra are placed far away from metabolite groups that contain MS/MS spectra with known structures. We expect that the data visualization approaches presented here will become a valuable first step in analyzing mass spectrometry fragmentation data to chart nature's chemical diversity. This in turn will enable us to start to understand the function and roles that molecules play in ecological systems.

Contact

If you are interested in learning more about our work on mass spectral embeddings for MS/MS spectra and their visualization, or if you have suggestions, or are interested in collaborating on this topic you can contact us via justin.vanderhooft@wur.nl or niek.dejonge@wur.nl and follow our group on Twitter: [@vdHooft_CompMet](https://twitter.com/vdHooft_CompMet)

Further reading

Comprehensive review on substructure-based and network-based analyses using mass spectrometry, NMR spectroscopy, or a combination thereof: <https://pubs.rsc.org/en/content/articlehtml/2021/np/d1np00023c>

MS2LDA substructure discovery:

- Concept: <https://www.pnas.org/content/113/48/13738>
- Web application: <https://academic.oup.com/bioinformatics/article/34/2/317/4158166>
- Website: <http://www.ms2lda.org>

MotifDB: <https://pubs.rsc.org/en/content/articlelanding/2019/fd/c8fd00235e>

MS2LDA+: <https://pubs.acs.org/doi/10.1021/acs.analchem.7b01391>

Spec2Vec unsupervised embedding:

Concept & Structural Similarity Measure: <https://journals.plos.org/ploscompbiol/article?id=10.1371/journal.pcbi.1008724>

MS2DeepScore supervised embedding:

Concept: <https://jcheminf.biomedcentral.com/articles/10.1186/s13321-021-00558-4>



The Metabolomics Society's President's Award goes to an elected scientist between 5 and 10 years after PhD graduation who significantly shaped the metabolomics field.

This year, the Society recognized Justin's academic achievements in metabolomics and his contributions to the Metabolomics Society as well as support for early-career scientists in metabolomics.

Photo by Dr. Justin J. J. van der Hooft.

Recent Publications

Recently published papers in metabolomics

- [AdipoAtlas: A reference lipidome for human white adipose tissue](#)
- [Applying metabolomics to veterinary pharmacology and therapeutics](#)
- [Comparison of Fecal Collection Methods on Variation in Gut Metagenomics and Untargeted Metabolomics](#)
- [Discovering metabolite quantitative trait loci in asthma using an isolated population](#)
- [A DMS Shotgun Lipidomics Workflow Application to Facilitate High-Throughput, Comprehensive Lipidomics](#)
- [Graph Convolutional Networks for Improved Prediction and Interpretability of Chromatographic Retention Data](#)
- [Improved Sample Preparation for Untargeted Metabolomics Profiling of Escherichia coli](#)
- [Integrative analysis of the Inflammatory Bowel Disease serum metabolome improves our understanding of genetic etiology and points to novel putative therapeutic targets](#)
- [Lipidomics Reveals Dysregulated Glycerophospholipid Metabolism in the Corpus Striatum of Mice Treated with Cefepime](#)
- [Metabolite discovery through global annotation of untargeted metabolomics data](#)
- [Metabolomics in degenerative brain diseases](#)
- [Metabolomics in Exercise and Sports: A Systematic Review](#)
- [Metabolomics-based engineering for biofuel and bio-based chemical production in microalgae and cyanobacteria: A review](#)
- [Metabolomics to Predict Acute Kidney Injury in Cirrhosis](#)
- [Metabolomics Signatures of SARS-CoV-2 Infection](#)
- [NMR-based metabolomics associated with chronic kidney disease in humans and animals: a one health perspective](#)
- [Nontargeted Serum Lipid Profiling of Nonalcoholic Steatohepatitis by Multisegment Injection-Nonaqueous Capillary Electrophoresis-Mass Spectrometry: A Multiplexed Separation Platform for Resolving Ionic Lipids](#)
- [Plasma Lipidomics Identifies Unique Lipid Signatures and Potential Biomarkers for Patients With Aortic Dissection](#)
- [The state of the art in plant lipidomics](#)
- [Targeted and Nontargeted Metabolomics of Amino Acids and Bioactive Metabolites in Probiotic-Fermented Unhopped Beers Using Liquid Chromatography High-Resolution Mass Spectrometry](#)
- [Transcriptomics, Epigenetics, and Metabolomics of Primary Aldosteronism](#)
- [Untargeted metabolomics analysis by gas chromatography/time-of-flight mass spectrometry of human serum from methamphetamine abusers](#)
- [Untargeted metabolomics identifies succinate as a biomarker and therapeutic target in aortic aneurysm and dissection](#)



Metabolomics Events

FEATURED
EVENT



2 December 2021

Why Population Health Studies Must Include Lipidomics

Venue

5:00pm CET (Berlin)/11:00am EST (NYC)

Zoom Webinar

Overview

Cohort studies frequently rely on omics technology but biomarker identification studies benefit only if the data are of high quality and reproducible.

The 3rd session of “The Lipidomics Webinar”: Christian Klose will discuss biomarker studies, multiomics analyses, and clinical challenges. After this 30 minute talk, he will answer questions. Register to join our webinar for free!



lipotype Webinar
Why Population Health Studies Must Include Lipidomics
December 2, 2021 | 5:00 pm CET / 11:00 am EST
Free Admission
REGISTER HERE

19-20 Nov 2021

World Endocrine & Obesity Conference

Venue

Bangkok, Thailand

Overview

The 2021 World Endocrine and Obesity Conference (2021WEOC) will be organized around the theme ‘Endocrine Care through Innovation & Discovery’ and will be run as a hybrid model allowing a Virtual and Physical platform.

Local and international speakers will share insights on advancing Endocrinology, Obesity, Diabetes and Metabolism Quality Improvement through Patient and Family Experiences that will present new concepts, technologies, management protocols, and clinical experiences in their respective disciplines.

It will be a wonderful opportunity for all the delegates as it provides an international networking opportunity to collaborate with the world-class trauma and critical care and medical associations.

Additional information [here](#). [Conference Flyer](#)

21-25 November 2021

28th ANSZMS Biennial Conference

Venue

Virtual, Australiand and New Zealand Society for Mass Spectrometry

Overview

Participants of ANZSMS28 will discuss contemporary aspects of mass spectrometry relating to chemistry, biology, earth science, archaeology, environmental science, forensics, physics and the latest advancements in mass spectrometry technology and techniques. The program will also include panel discussion forums for early career researchers and mass spectrometry careers in academia and industry. The Australian Core MS Facilities Annual Meeting will be held as a satellite meeting and will use the highly reputable cloud-based OnAir virtual conference portal from EventsAIR to provide the best possible experience to all participants.

This is an event not to be missed!

Additional information [here](#).

24 November 2021

Cambridge Cheminformatics Meeting

Venue

4:00-6:00pm GMT, Cambridge Cheminformatics Network

Overview

Join the Cambridge Cheminformatics Network to hear Jack Scannell on Models in Drug R&D, Anton Martinsson on Human PK, and Mehmet Aziz Yirik on Structure Generation.

Register [here](#).

29 November - 2 December 2021

Virtual Podium Asia Pacific 2021

Venue

8:00am CST / 8:00pm SGT

Virtual Conference

Overview

Virtual Podium Asia Pacific (VPAP) 2021 free event was established to promote scientific discussion and engagement in Proteomics, Metabolomics and Lipidomics in the Globe during this COVID-19 pandemic.

The virtual podium is a way to connect with our omics community. To facilitate this networking opportunity, we have two sessions in four days with 16 keynote speakers and 40 lightening talks.

This is an opportunity for you to present and submit an abstract to present in 5-minute lightening talks. We are giving away 8 cash awards and few more encouragement awards during the virtual event.

Additional information [here](#).

2 December 2021

Think Big: From Study Design to Metabolomics Data Interpretation

Venue

9:00am PST, UC Davis - West Coast Metabolomics Centre
Virtual

Overview

In this short course, we will discuss pitfalls in study designs that may severely hamper metabolomic studies, shortly reviewing power analyses, bias in studies, biological and chemical controls. We will very briefly review the types of metabolomic assays that give investigators data and problems associated with the choice of assays. Most of the time will be allotted to data interpretation, i.e. what to do once you have received metabolomics data, once data have been curated and once statistics have been completed: how can you then further interpret the data, how to generate new hypotheses, how to link biological data and other -omics data, and how to utilize databases that are available for free online.

Additional information [here](#).

7 December 2021

Possibilities and Limitations of GC-MS in Metabolomics

Venue

4:00-6:00pm CET / 7:00-9:00am PST
Zoom, Polish Metabolomics Society

Overview

Attend the first in a series of expert meetings hosted by the Polish Metabolomics Society. The first meeting will be dedicated to GC-MS based metabolomics: "Possibilities and limitations of GC-MS in metabolomics" with Olivier Fiehn, Fernanda Rey-Stolle, and Christina Troyer as speakers.

Registration is required. Additional information [here](#).

13-16 May 2022

2nd Metabolism in Health and Disease Conference

Venue

Fiesta Americana Condesa, Cancun, Mexico

Overview

Topics will span diverse areas such as cancer metabolism, organismal metabolism in disease, metabolic pathway engagement in cell function, metabolites as signaling molecules, mitochondrial biology, nutrient sensing, metabolism in tissue homeostasis and repair, neurometabolism, and metabolism in host-microbe interactions.

Additional information [here](#).

20-24 June & 20-23 September 2022

CliMetabolomics

Venue

20-24 June, Leipzig and Halle, France / 20-23 September, Saale, Germany

Overview

CliMetabolomics is a Franco-german Research Workshop that aims to better understand the plasticity of plants and to develop sustainable plants adapted to climate change. CliMetabolomics offers training in analytical tools and an innovation management method to early career scientists. The workshop lasts two weeks and consists of seminars, discussions and many practical courses.

Additional information [here](#).

26-27 October 2022

2nd International Diabetes and Metabolic Surgery Summit

Venue

Tel Aviv, Israel, IDMSS

Overview

The focus of the forthcoming IDMSS 2022 will be the relationship between obesity and type 2 diabetes and their associated complications and the beneficial results obtainable from metabolic/ bariatric surgery. This Summit is vital to increase the international knowledge of these procedures and stimulate the investigation and development of new and more effective treatments. The Summit will bring together many of the world experts in the fields of metabolic surgery and medicine and is a must for all clinicians caring for patients suffering from metabolic diseases.

Additional information [here](#).

Metabolomics Jobs

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

Jobs Offered

Job Title	Employer	Location	Posted	Closes	Source
Various Positions	Various	Various	12-Nov-21	Various	Metabolomics Association of North America Job Board
Sr. Marine Education Specialist - Science Technology Centre (STC)	Woods Hole Oceanographic Institution	Massachusetts, USA	4-Oct-21	Until Filled	Careers@WHOI
Digital Coordinator	Woods Hole Oceanographic Institution	Massachusetts, USA	4-Oct-21	Until Filled	Careers@WHOI
PDF Position	Fernandez Lab, School of Chemistry and Biochemistry, Georgia Institute of Technology	Georgia, USA	Sep-21	Until Filled	MetaboNews Jobs
Team Leader for Computational Metabolomics	Pacific Northwest National Library (PNNL)	Washington, USA	Sep-21	1-Dec-21	Careers at PNNL



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-  **Research collaboration**

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Metabolomics Jobs

Job Title	Employer	Location	Posted	Closes	Source
Senior Computational Metabolomics Scientist	Pacific Northwest National Library (PNNL)	Washington, USA	Sep-21	1-Dec-21	Careers at PNNL
Metabolomics of Algae - Post-doctoral Fellowship	Cawthron Institute	Nelson, New Zealand	10-Jun-21	Until Filled	Cawthron Institute
PhD Student and Post-doctoral Fellow Positions in Mass Spectrometry Metabolomics and Proteomics	Technion – Israel Institute of Technology	Haifa, Israel	29-Mar-21	Until Filled	MetaboNews Jobs
Postdoctoral R&D Scientist - NMR-based metabolomics	Lesaffre	Loos, France	16-Mar-21	Until Filled	SmartRecruiters.com
PhD Research Project Opportunities, Centre for Integrative Metabolomics and Computational Biology	Edith Cowan University	Joondalup, Australia	16-Mar-21	Until Filled	MetaboNews Jobs

Jobs Wanted

This section is intended for very highly qualified individuals (e.g., lab managers, professors, directors, executives with extensive experience) who are seeking employment in metabolomics.

We encourage these individuals to submit their position requests to your MetaboNews team at (metabolomics.innovation@gmail.com). Upon review, a limited number of job submissions will be selected for publication in the Jobs Wanted section.

- [Dr. Paulina Samczuk](#) - Seeking an interesting Postdoc offer or other position which would allow her to develop herself.