Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V.

Dortmund & online

COLLOQUIUM

Connecting the Dots: Recent Advances in Computational Metabolomics to Prioritise Relevant Metabolite Features

Speaker:

Dr Justin J.J. van der Hooft, is an Assistant Professor in Computational Metabolomics in the Bioinformatics Group at Wageningen University & Research in the Netherlands.

Time:

Thursday, June 11, 2026 – 1 pm

Venue:

ISAS Campus, Lecture Hall
Otto-Hahn-Straße 6b
44227 Dortmund

&

WebEx: https://t1p.de/9hrjk
Meeting-ID: 2781 290 7028
Password: awJpGJeW722

Mitglied der Leibniz-Gemeinschaft

Abstract

Nature has always been a rich resource of diverse chemistry. Fortunately, in recent years, technological advances in the omics fields have increased our capacity in measuring them. For example, modern mass spectrometers generate information-rich chemical profiles used for untargeted metabolomics studies. Such studies are typical examples of exploratory data analysis, as one does not a priory know what one will discover in the data. Typically, researchers do have a goal with the study: whether it is finding out differences in plant tissue metabolic content or associating antimicrobial activity to metabolites in bacterial extracts. However, the current information-rich metabolomics profiles leave researchers with the daunting task to separate valuable signals from everything else.

In this seminar, I will highlight recent advances in networking and machine learning-based strategies to organize, annotate, and prioritize metabolite features. These include the work on SpecReBoot that enhances molecular networking organization by trimming unwanted spectral links and focusing on more reliable connections, MS2LDA unsupervised substructure discovery to complement spectral library-based annotation, and FERMO for correlation-based prioritization of metabolite features. I will briefly highlight how interactive visual dashboards support informative desicion making in metabolomics analysis workflows. These current developments allow researchers to use statistics and phenotype information such as bioactivity to filter and select for relevant metabolite features and network connections. To demonstrate this, I will show examples using case studies from various natural origins.

I will finish the seminar with highlighting the important role of Open Science and Software in stimulating community-based science. Altogether, I expect

that the presented progress in computational metabolomics tools will empower metabolomics researchers navigating their increasingly complex datasets to find and annotate relevant and novel chemistry in nature.

Short Bio Speaker:
Justin J.J. van der Hooft is an Assistant Professor in Computational Metabolomics in the Bioinformatics Group at Wageningen University & Research, NL, and an author of >100 peer-reviewed articles in the metabolomics field. Justin is very fascinated by the ingenuity of nature in creating marvellous chemical structures. He obtained his PhD (2012) in Systematic Metabolite Annotation and Identification at the Biochemistry and Bioscience groups in Wageningen. After a postdoctoral period in Glasgow, UK, studying both analytical and computational aspects of metabolite structure annotation, and together with Joe Wandy & Simon Rogers coining MS2LDA unsupervised substructure discovery, he returned to Wageningen. Since 2020, his team has been developing computational metabolomics strategies to decompose mass spectral data 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. Recently developed tools and frameworks include SpecReBoot for confidence-aware molecular networking, MS2Query to perform analogue search, FERMO to prioritize metabolite features and profiles by enabling effective and reproducible data integration and data filtering strategies, and NPLinker to handle multi-omics data for natural products discovery. Since 2022, he is also a Visiting Professor in Johannesburg. Got interested? Find out more and meet the team here: https://vdhooftcompmet.github.io. You can find his contributions to the metabolomics field here: https://scholar.google.nl/citations?user=zv9seLwAAAAJ&hl=en&oi=ao