

## Workshop

### Sunburst in the metabolome - Chemical Compound Class Annotation Using Sirius and MetIgel

- Date: 29.06.2023 3-5pm + 05.07.2023 9am -3pm
- Mode: Hybrid
- Location: iDiv (Puschstraße 4, Leipzig) / Zoom
- Teacher: Dr. Henriette Uthe (EcoMetEoR/iDiv/FSU)
- Guest: Dr. Markus Fleischauer (AG Böcker/Bioinformatics/FSU)
- Charge: Free
- Registration Deadline: 31.05.2023

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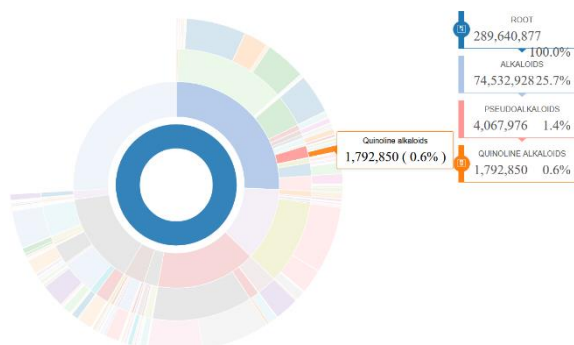
<https://www.idiv.de/de/forschung/plattformen-und-netzwerke/ecometeor.html>

The analysis of plant metabolomic data can be extremely challenging, particularly when it comes to metabolite annotation. The lack of standard reference spectra and the complexity of plant metabolism mean that many compounds cannot be accurately annotated. However, chemical compound class annotation can provide valuable insights into the metabolomic data, even in the absence of detailed annotation. SIRIUS is a powerful software tool that can be used to annotate the chemical compound classes of plant metabolites. It integrates a collection of tools developed by the group of Sebastian Böcker (FSU), including CSI:FingerID (with [COSMIC](#)), [ZODIAC](#) and [CANOPUS](#). The resulting chemical compound classification can be used to describe the changes in the chemical profile of plants for example with sunburst plots. However, it is important to handle this tool and the results with care and to question them. For example, having a thorough understanding of the scoring system can aid in evaluating the results.

In this hands-on workshop, our aim is to introduce you to SIRIUS and guide you through the process of analyzing your dataset to obtain chemical compound classes. We will also engage in discussions with Dr. Markus Fleischauer on evaluating the results, providing you with the opportunity to directly ask him questions about SIRIUS.

During the second part of the workshop, we will explore the utilization of MetIgel, an R-based Shiny App, to generate sunburst plots.

If you're interested to join this workshop or if you have further questions please contact [Henriette.uth@idiv.de](mailto:Henriette.uth@idiv.de)



iDiv is a central facility of Leipzig University within the meaning of Section 92 (1) of the Act on Academic Freedom in Higher Education in Saxony (Sächsisches Hochschulfreiheitsgesetz, SächsHSFG). It is run together with the Martin Luther University Halle-Wittenberg and the Friedrich Schiller University Jena, as well as in cooperation with the Helmholtz Centre for Environmental Research – UFZ. The following non-university research institutions are involved as cooperation partners: the Helmholtz Centre for Environmental Research – UFZ, the Max Planck Institute for Biogeochemistry (MPI BGC), the Max Planck Institute for Chemical Ecology (MPI CE), the Max Planck Institute for Evolutionary Anthropology (MPI EVA), the Leibniz Institute DSMZ–German Collection of Microorganisms and Cell Cultures, the Leibniz Institute of Plant Biochemistry (IPB), the Leibniz Institute of Plant Genetics and Crop Plant Research (IPK) and the Leibniz Institute Senckenberg Museum of Natural History Görlitz (SMNG).

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