

Updates 12/2024



by Elisabeth M.-L. Janssen

19. December 2024

Department of Environmental Chemistry, Swiss Federal Institute of Aquatic Science and Technology (Eawag),
8600 Dübendorf, Switzerland

CyanoMetDB and curation

CyanoMetDB is a comprehensive database of secondary metabolites from cyanobacteria made openly-accessible as a dataset, which is highly curated with an international team of experts (listed below). CyanoMetDB is presented as a flat-file database comprising the following core fields: compound identifier code, compound name, compound class, molecular formula, molecular weight, monoisotopic mass, reference(s) related to the structure elucidation, SMILES string, InChI string, InChIKey, IUPAC name, whether nuclear magnetic resonance spectroscopy (NMR) was used for the structure elucidation, and the cyanobacterium or field sample type used to extract the compound from for structure elucidation.

New Dataset 2024

CyanoMetDB Version03 (2024). We successfully published Version03 of CyanoMetDB presenting the structural information of **3085 metabolites** from **1156 primary references** published between 1967 and early 2024. The dataset can be downloaded from Zenodo since September 2024: DOI [10.5281/zenodo.4551528](https://doi.org/10.5281/zenodo.4551528). In December 2024, we have surpassed **5000 downloads** directly from Zenodo!

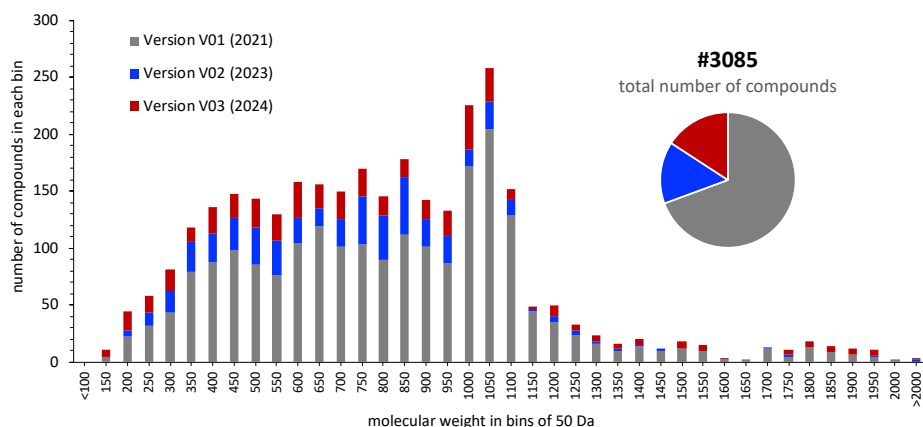


Figure 1: Distribution of molecular weights for all cyanobacterial secondary metabolites reported in CyanoMetDB, ranging from 100 to more than 2000 Da with 50-Da bin size, showing the contribution of Version 01 from 2021 (grey), Version 02 from 2023 (blue) and Version 03 from 2024 (red).

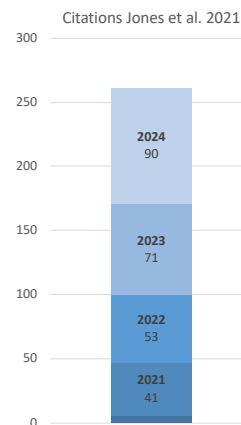


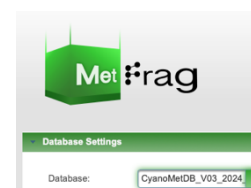
Figure 2: Citations of Jones et al. (2021, DOI: [10.1016/j.watres.2021.117017](https://doi.org/10.1016/j.watres.2021.117017)) reached 263 citation by 10. December 2024.

Citation of CyanoMetDB

To cite the use of content of CyanoMetDB we recommend to refer to the accomodating publication by Jones et al. (2021) with DOI: [10.1016/j.watres.2021.117017](https://doi.org/10.1016/j.watres.2021.117017) describing the curation of the database, together with the respective dataset version used from Zenodo by Janssen et al. (2024) with DOI [10.5281/zenodo.4551528](https://doi.org/10.5281/zenodo.4551528).

Collaborations ongoing in 2024

MetFrag and Pubchem. We coordinate the upload of CyanoMetDB Version03 on [MetFrag](#) to allow checking mass spectra against *in silico* fragmentation predictions to assist spectra annotation. Since the first Version01 of CyanoMetDB in 2021, the content is also merged with **PubChem** greatly expanding molecular information including meta data for cyanobacterial metabolites through NORMAN Suspect List Exchange Classification: "[S75 | CyanoMetDB | Comprehensive database of secondary metabolites from cyanobacteria](#)" currently displaying 3013 entries. We thank [Emma Schymaski](#) for coordinating the collaboration with MetFrag, Norman List Exchange and PubChem!



The Natural Products Atlas. Our collaborations with [The Natural Products Atlas](#) through the [Linington Research Group](#) is a fantastic example how to join forces and support each other's progress. We exchange updates of CyanoMetDB ahead of time with the Linington Group and receive cyano-related metabolite updates from them to ensure that both our databases are up-to-date (see also <https://doi.org/10.1093/nar/gkab941> from 2022) and note their [NP-MRD database](#) containing NMR spectra.



MIBiG 4.0. Our CyanoMetDB member [Paul D'Agostino](#) included CyanoMetDB accessions in the newest version of [MIBiG 4.0](#) which is up and running now. MIBiG facilitate the standardized deposition and retrieval of biosynthetic gene cluster data and CyanoMetDB now complements entries for cyanobacteria with more complete metadata for the respective metabolites. Working together in the future will further ensure that both databases represent the most up-to-date datasets publicly available regarding cyanobacterial metabolites.



Under development

Several satellite projects and collaborations keep developing through the network of CyanoMetDB members! We encourage to reach out when you seek project partners to achieve the best synergies within our research community.

Transformation Products. One expansion of the current database will include transformation products of cyanobacterial metabolites in future versions of CyanoMetDB. These newly added compounds can include natural transformation products produced biologically (e.g., enzymatic) or abiotically (e.g., naturally produced reactive oxidants, irradiation) as well as products formed during engineered processes of water treatment (e.g., oxidation, disinfection). *Reach out if you are interested to contribute!*

Mass Spectra Reference Data on MassBank. Identification of cyanobacterial metabolites in new samples is challenging as we lack available reference standards. For that reason, CyanoMetDB members started to work on recording reference mass spectra. We have systematically measured spectra for **346 metabolites** in the Janssen Lab and Niedermeyer Lab with similar MS platforms (ESI Orbitrap) and instrument methods. For each compound, spectra in positive and negative mode both with 9 collision energies each were recorded (i.e., **18 spectra types**) and for each spectra type **5-10 replicate spectra** were gathered. The obtained raw data were processed using an open source R package RMassBank, which is responsible for automatic MS and MS/MS recalibration, clean-up and intensity correction, as well as gathering spectral meta data to generating exports that can be deposited as new entries in [MassBank](#). In total the stringent data processing approved spectra of **165 metabolites for upload**. The teams providing the material for these compounds, cyanobacterial extract or (semi)purified compounds, assigned their confidence level for the validity of the compound identification and additional meta data for the MassBank entry. We are currently organizing a publication of the workflow and the overview of these newly available reference spectra to give credit to all participating teams. The spectra will be publicly available once the accompanying manuscript is published.



CyanoMetDB Members 2024 – A Fantastic Team !

Elisabeth M.-L. Janssen¹, Martin R. Jones², Ernani Pinto³, Fabiane Dörr⁴, Mariana A. Torres⁴, Fernanda Rios Jacinavicius⁴, Hanna Mazur-Marzec⁵, Karolina Szubert⁵, Robert Konkel⁵, Luciana Tartaglione⁶, Carmela Dell'Aversano⁶, Antonella Miglione⁶, Pearse McCarron⁷, Daniel G. Beach⁷, Christopher O. Miles⁸, David P. Fewer⁹, Kaarina Sivonen⁹, Jouni Jukela⁹, Matti Wahlsten⁹, Timo H. J. Niedermeyer¹⁰, Franziska Schanbacher¹⁰, Pedro Leão¹¹, Marco Preto¹¹, Paul M. D'Agostino¹², Martin Baunach¹³, Elke Dittmann¹⁴, Maria Miguel-Gordo¹⁴, Raphael Reher¹⁵, Simon Sieber¹⁶

(1) Department of Environmental Chemistry, Swiss Federal Institute of Aquatic Science and Technology (Eawag), 8600 Dübendorf, Switzerland; (2) School of Biosciences, University of Birmingham, Edgbaston, Birmingham, B15 2TT, United Kingdom; (3) Centre for Nuclear Energy in Agriculture, University of São Paulo, CEP 13418-260 Piracicaba, São Paulo, Brazil; (4) School of Pharmaceutical Sciences, University of São Paulo, CEP 05508-900, São Paulo, Brazil; (5) Department of Marine Biology and Biotechnology, University of Gdansk, 81-378 Gdynia, Poland; (6) University of Napoli Federico II, School of Medicine and Surgery, Department of Pharmacy, 80131 Napoli, Italy; (7) Biotoxin Metrology, National Research Council Canada, Nova Scotia, Halifax B3H 3Z1, Canada; (8) Norwegian Veterinary Institute, Ås, Norway; (9) Department of Microbiology, University of Helsinki, 00014 Helsinki, Finland; (10) Pharmaceutical Biology, Freie University Berlin, Germany; (11) Interdisciplinary Centre of Marine and Environmental Research (CIIMAR/CIMAR), University of Porto, Portugal; (12) Helmholtz Institute for Pharmaceutical Research Saarland, 66123 Saarbrücken, Germany; (13) Institute of Pharmaceutical Biology, University of Bonn, 53115 Bonn, Germany; (14) Institute for biology and biochemistry, University of Potsdam, Germany; (15) Department of Pharmacy, University Marburg, Germany; (16) Department of Chemistry, University Zurich, 8001 Zurich, Switzerland.

Join the team! We welcome any enthusiast who likes to contribute to working together on CyanoMetDB.
Please contact Elisabeth.janssen@eawag.ch for more information.