OctoChemDB: An Integrated Platform for HRMS-Based Small Molecule Dereplication

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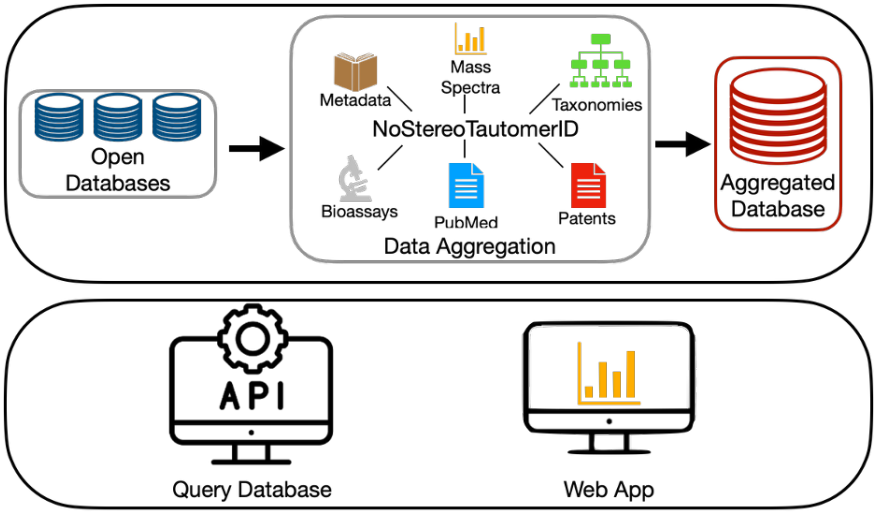
High-resolution mass spectrometry (HRMS) is routinely applied to small molecule identification and dereplication, but the interpretation of MS and MS/MS data is often hindered by the dispersion of reference information across multiple resources. We present OctoChemDB (octochemdb.cheminfo.org), a web-based tool supporting HRMS-based identification through accurate mass calculations and MS/MS data analysis with integrated access to chemical, spectral, and literature-based reference information within a single environment. The OctoChemDB platform is described in detail in a manuscript accepted for publication in Analytical Chemistry.

OctoChemDB enables monoisotopic mass–based searches with defined mass accuracy, molecular formula generation, isotopic pattern comparison, MS/MS fragment analysis, and spectral similarity matching against literature-reported spectra. Reference data accessed through the application include chemical structures, PubMed abstracts, patent information, bioactivity records, and taxonomic annotations.



OctoChemDB relies on an automated framework that aggregates chemical, spectral, and associated reference data from open resources and exposes them through a web-based application. The approach is demonstrated through the identification of known compounds, including widely used reference molecules such as caffeine and MDMA, from HRMS and MS/MS data, highlighting its utility for rapid and informed dereplication in analytical chemistry workflows.

[1] Silvestre, R., Patiny, L., & Zasso, M. OctoChemDB: A Comprehensive Web Service for Chemical Data Integration [Computer software]. https://doi.org/10.5281/zenodo.5091586