

MCULE NATURAL PRODUCTS LIBRARY

The Mcule Natural Products Library is designed to provide comprehensive coverage of the natural product (NP) chemical space and its synthetic expansions. It is organized based on supplier-provided classifications and divided into three main sections:

- **Natural Products:**

This subset exclusively contains compounds with structures of natural origin, collected from 7 supplier catalogs. The entries are labeled as natural products by their respective suppliers, ensuring high-confidence classification and diversity within naturally occurring scaffolds.

- **Natural Product Derivatives:**

A broader collection compiled from over 13 supplier catalogs, this subset includes compounds whose core structures are derived from natural products. These molecules often retain key structural features of the parent natural compounds while offering even higher diversity or enhanced properties through chemical modification.

- **Natural-like Products:**

This is the broadest of the three sets, sourced from over 17 supplier catalogs. It includes all previously mentioned compounds, as well as those with structures that occur in nature but are synthetically produced.

Please access the downloadable data files of the Mcule Natural Product Library on our [webpage](#). In the ZIP file you will find files of **CSV.GZ** format. The compressed files contain the compounds together with other relevant information in the following format*:

SMILES, compound mcule ID, product mcule IDs, delivery time (wdays), purity %, stereo label

* If the compounds are available from multiple suppliers the product mcule IDs are separated by ";". In such case the lowest "delivery time (wdays)" (wdays = working days) is shown and the "purity %" value of this specific product. Other suppliers might offer the product with different delivery time and purity values.

If you would prefer another molecular format or a further customized library contact us at support@mcule.com.

Did you know?

Mcule provides professional laboratory services including:

- **Mcule Express Compound Inventory System™** - powered by robotized cold room sample storage
- **Custom formatting** - Solid weighing, robotized dissolution and pipetting
- **Experimental sample characterization** - Structure identity, purity, solubility and reactivity analysis
- **Comprehensive logistic services**- Compound procurement, sample management, customs clearance and worldwide delivery

Mcule provides professional cheminformatics services including:

- **Custom library design** - using a wide range of ligand- and structure-based molecular modeling and cheminformatic approaches including physicochemical property calculations, molecular fingerprint based similarity and substructure searches, diversity selection, similarity clustering, scaffold hopping, toxicity filtering, PAINS and other unwanted substructure filters, molecular docking, etc. Custom library generation workflows can be applied on the Mcule Database or Mcule ULTIMATE database
- **Generation of synthetically feasible chemical universes** - based on specific building blocks and reaction rules

Mcule's Custom Solution Experts are ready to guide you through the selection and ordering process free of charge! If you have any questions or need any help, please feel free to contact us at support@mcule.com.