

MCULE MACROCYCLE LIBRARY

THE MCULE MACROCYCLE LIBRARY WAS ESTABLISHED WITH THE AIM OF FACILITATING THE DIRECT TARGETING OF MACROMOLECULES, BOTH FOR PROMOTING AND INHIBITING THEIR INTERACTIONS.

Although the physicochemical properties of macrocycles often surpass the rule of five, they still exhibit favorable pharmacokinetic characteristics, including permeability and oral bioavailability. As a result, these molecules can lead us to previously unexplored regions of the chemical universe, where ligands for yet undruggable targets may exist.

In order to assemble a substantial pool of compounds, the selection criteria were as follows:

- The molecule must possess a primary ring with a minimum of ten atoms.
- Additionally, the ring must contain at least one heteroatom.

Full collection

In stock collection

Please access the downloadable data files of the Mcule Macrocyclic Library on our [webpage](#). Here, you can find the SMI.GZ files for both the full and in stock collections, provided separately. The SMI.GZ files contain the molecules in SMILES format (*SMILES ID*).

Additionally, our professional laboratory services can help you by:

- Transferring samples to plates/vials as solid or DMSO solution,
- Solubility characterization,
- Temperature controlled shipping,
- Quality control via LC-MS & NMR (on demand).

Please also reach out to our cheminformatics experts with projects related to:

- Screening library building/expansion,
- Generation of synthetically feasible chemical spaces based on your building blocks,
- Filtering the Mcule database based on your criteria.

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.