

MCULE CNS TARGETING LIBRARIES

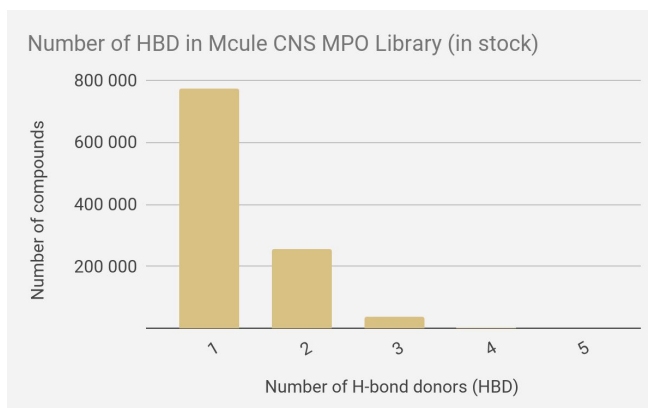
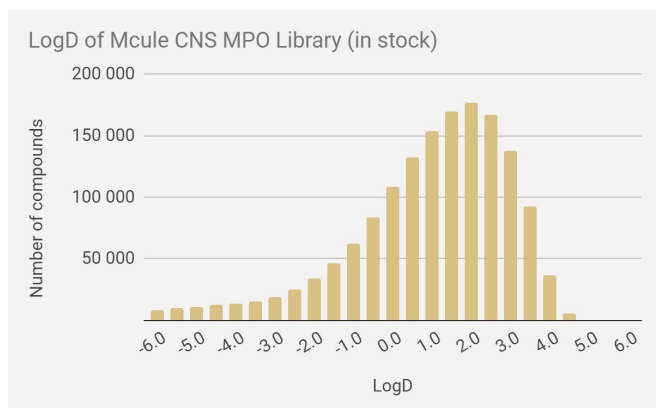
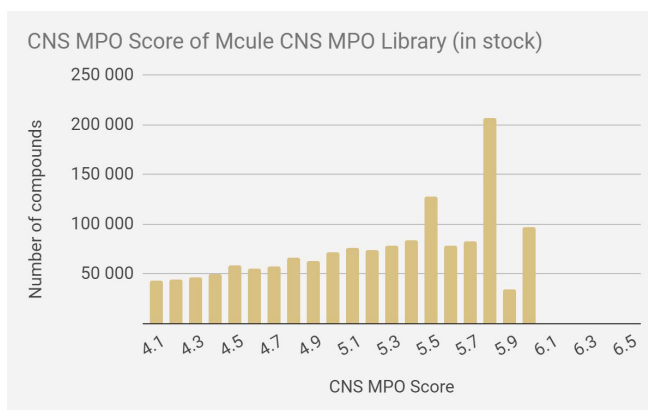
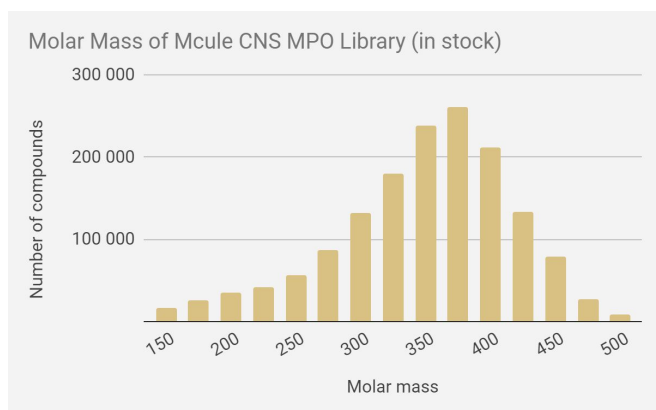
The targeted delivery of active ingredients to specific areas of the central nervous system (CNS), protected by the blood-brain barrier (BBB), enables innovative treatment strategies for neurological disorders. To achieve this, potential candidate molecules must possess specific properties that facilitate penetration of the BBB. We calculated the underlying physicochemical properties, as well as the [CNS Multiparameter Optimization \(MPO\)](#) and [BBB](#) scores, for all purchasable compounds in the Mcule Database. After applying CNS MPO and BBB filtering, focused libraries with an enhanced potential to reach CNS targets were generated.

THE MCULE CNS TARGETING LIBRARIES ARE LISTED BELOW:

- **Mcule CNS MPO Library:** this collection includes molecules with CNS MPO score ≥ 4 .

The CNS MPO score is based on physicochemical properties that strongly correlate with the pharmacokinetic profile of compounds, including lipophilicity (logP), distribution coefficient at pH 7.4 (logD), molecular weight (Mw), topological polar surface area (TPSA), number of hydrogen-bond donors (HBD), and the pK_a value of the most basic center.

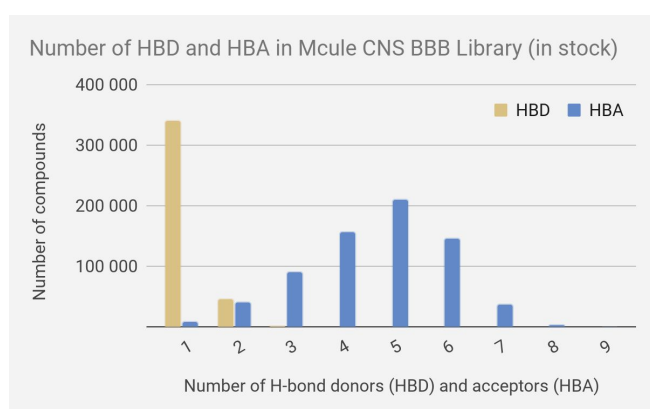
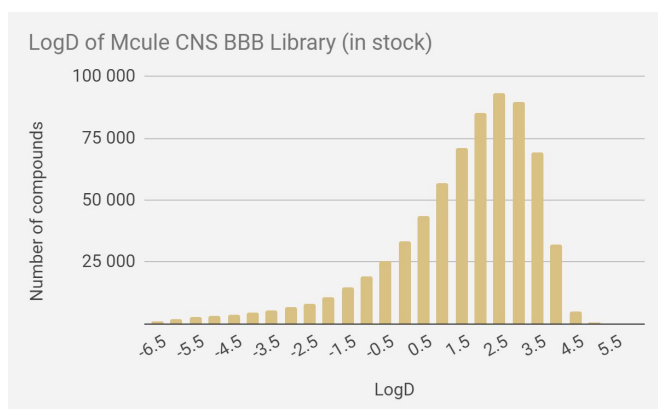
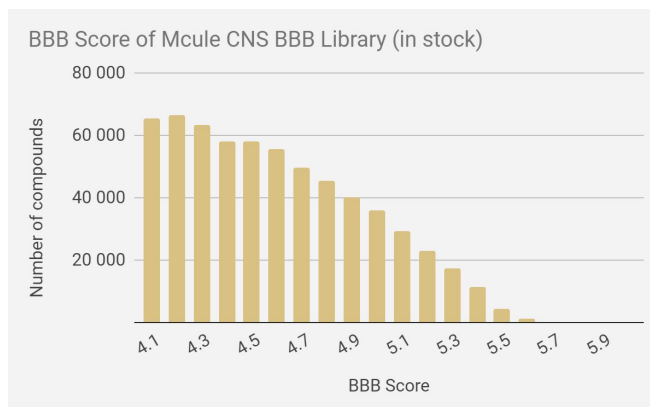
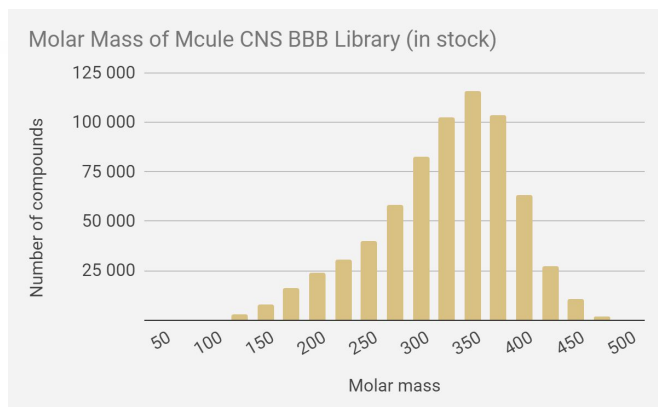
THE PROPERTY DISTRIBUTIONS OF MCULE CNS MPO LIBRARIES (In-stock subset):



- **McuLe CNS BBB Library:** this collection contains molecules with BBB score ≥ 4 .

The BBB score is a powerful alternative to CNS MPO for estimating BBB permeability. Like CNS MPO, it relies on critical physicochemical properties such as the number of aromatic rings, heavy atoms, MWHBN (a descriptor comprising Mw, HBD, and hydrogen bond acceptors (HBA)), TPSA, and pK_a .

THE PROPERTY DISTRIBUTIONS OF MCULE CNS BBB LIBRARIES (In stock subset):



The Mcule CNS Targeting Libraries were further filtered against more than 1,000 SMARTS-based substructure patterns, including PAINS, and other MedChem filters to avoid toxic or promiscuous functional groups.¹⁻⁴

- [1] Baell, J. B. & Holloway, G. A. New Substructure Filters for Removal of Pan Assay Interference Compounds (PAINS) from Screening Libraries and for Their Exclusion in Bioassays. *J. Med. Chem.* 2719-2740 (2010).
- [2] Saubern, S., Guha, R. & Baell, J. B. KNIME Workflow to Assess PAINS Filters in SMARTS Format . Comparison of RDKit and Indigo Cheminformatics Libraries. *Mol. Inform.* 30, 847-850 (2011).
- [3] Pearce, B. C., Sofia, M. J., Good, A. C., Drexler, D. M. & Stock, D. A. An Empirical Process for the Design of High-Throughput Screening Deck Filters. 1060-1068 (2006).
- [4] Bruns, R. F. & Watson, I. A. Rules for Identifying Potentially Reactive or Promiscuous Compounds. *J. Med. Chem.* 55, 9763-9772 (2012).

Please click [here](#) to access the downloadable data files of Mcule CNS Targeting Libraries. The ZIP file contains CSV.GZ compressed files that include the molecules in SMILES format, along with their properties such as molar mass, LogP, PSA, LogD, etc., as well as CNS MPO and BBB scores.

Mcule's professional laboratory services include:

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

Mcule's cheminformatics services include:

- Custom screening library design and selection,
- Generation of synthetically feasible chemical libraries 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.