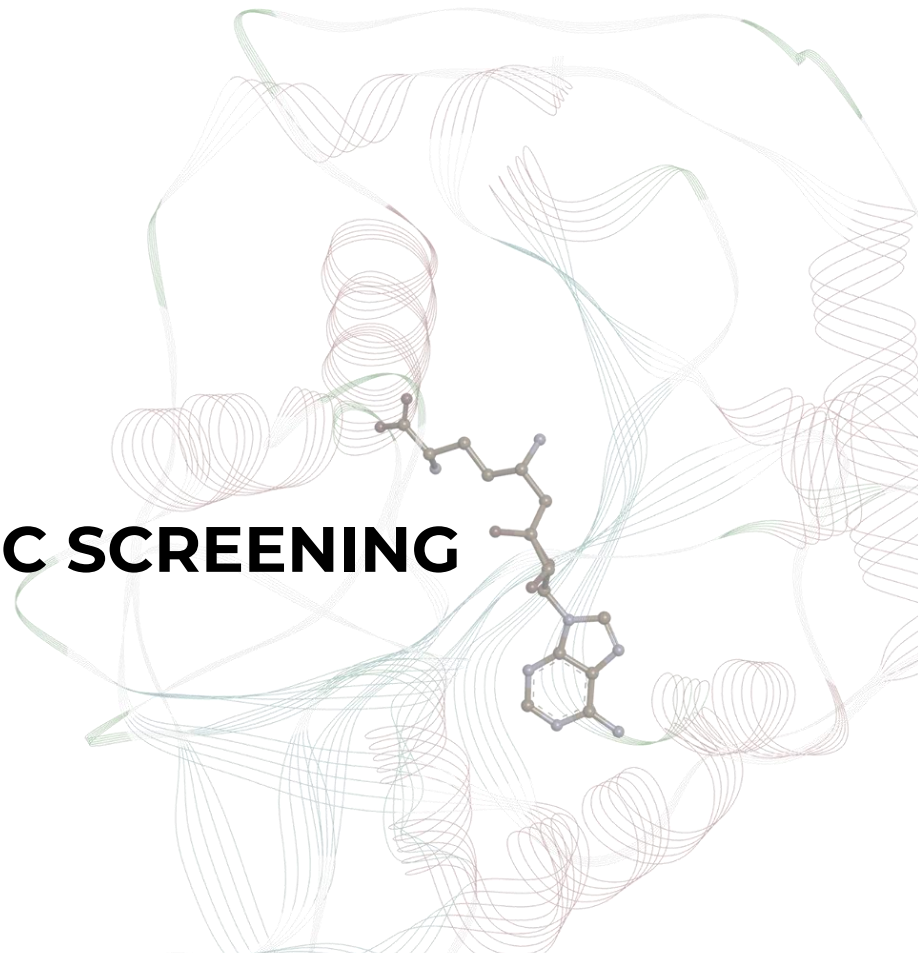
OTAVA chemicals

Compounds for HTS
Chemical building blocks
Fragment libraries
Targeted libraries
Drug discovery services



PHENOTYPIC SCREENING LIBRARY

OTAVA offers Phenotypic Screening Library. The Phenotypic Screening Library represents a multi-purpose set of compounds for different goals such as cellular assays, bacterial assays, tissue assays, animal models, screening against various molecular targets including with unknown structures, multiple biological targets. This library contains a set of compounds with maximal biological and chemical diversity (more than 1000 chemical scaffolds including nature-like).
The library consists of **4, 068 compounds***.

All compounds are:

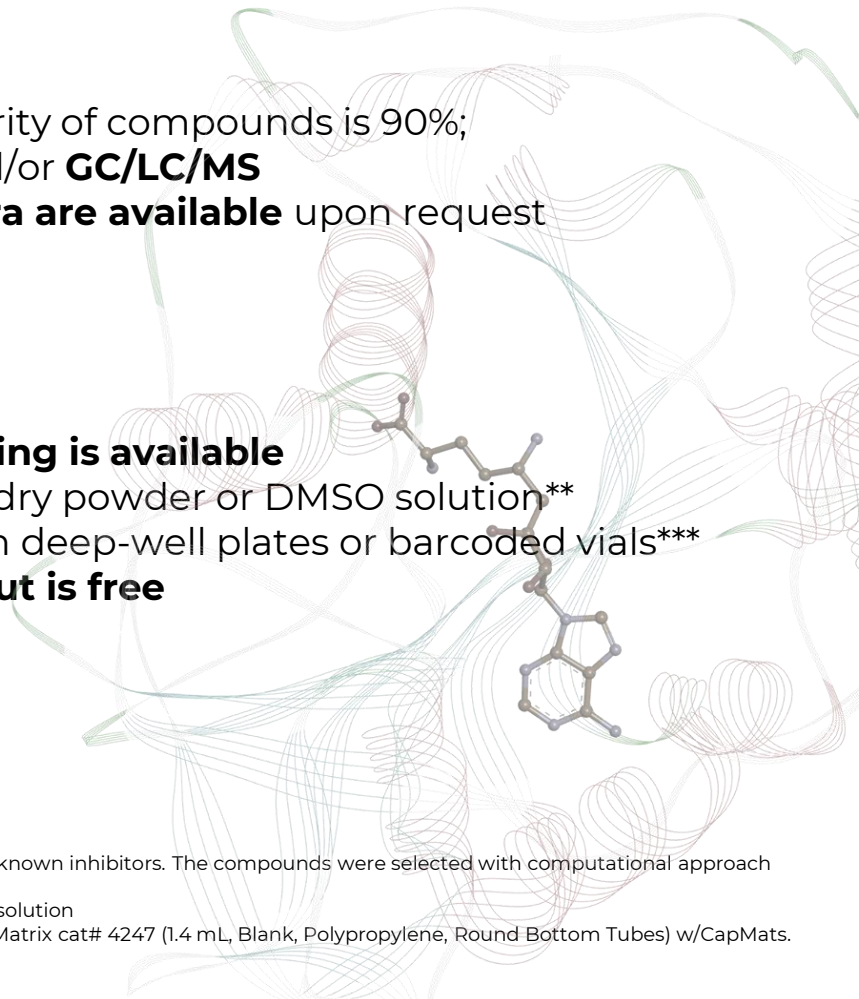
- **in stock**; available amounts: 1 – 50 mg
- ***Drug-like* only**; reactive, pan-assay interference (PAINS), redox-active and aggregator compounds were removed from the library.

QA/QC passed:

- minimal purity of compounds is 90%;
- by **NMR** and/or **GC/LC/MS**
- **NMR spectra are available** upon request

Frendly packing services:

- **Cherry-picking is available**
- Supplied as dry powder or DMSO solution**
- Packaging in deep-well plates or barcoded vials***
- **Weighing out is free**



*Please note that the library does not contain known inhibitors. The compounds were selected with computational approach and are intended for screening projects

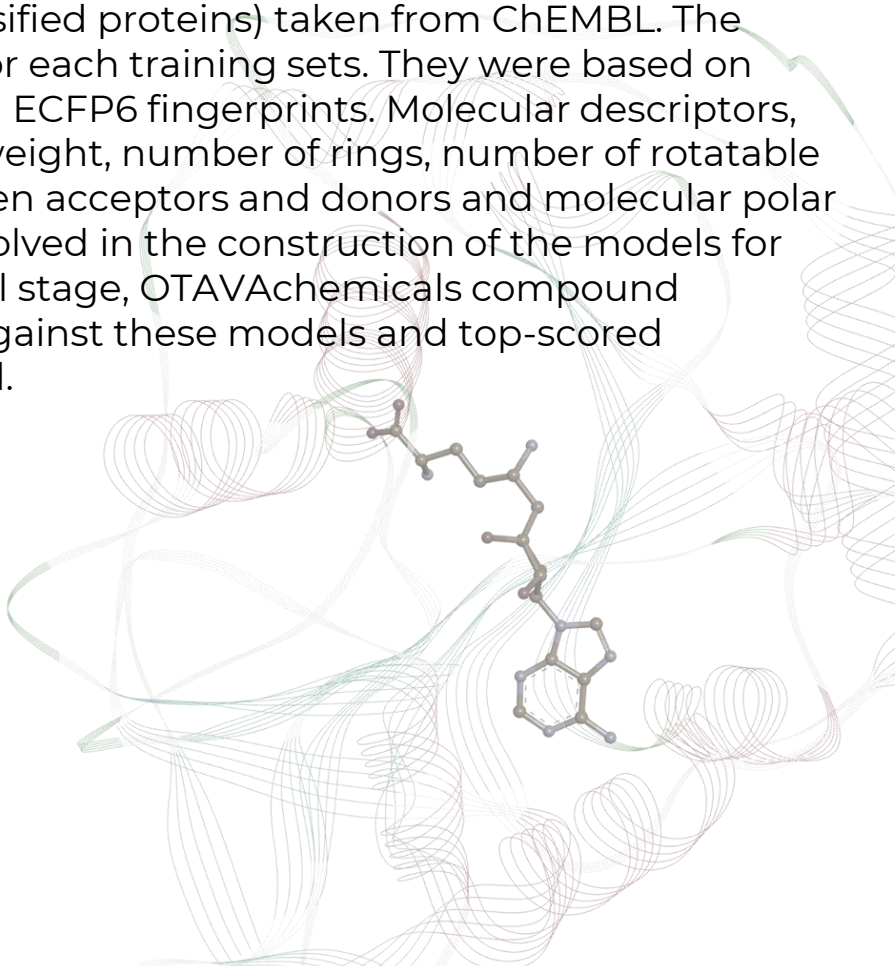
**there is additional fee for preparation of the solution

***4 ml amber glass vials or Deep-well plates: Matrix cat# 4247 (1.4 mL, Blank, Polypropylene, Round Bottom Tubes) w/CapMats. Or plates and vials provided by customer.

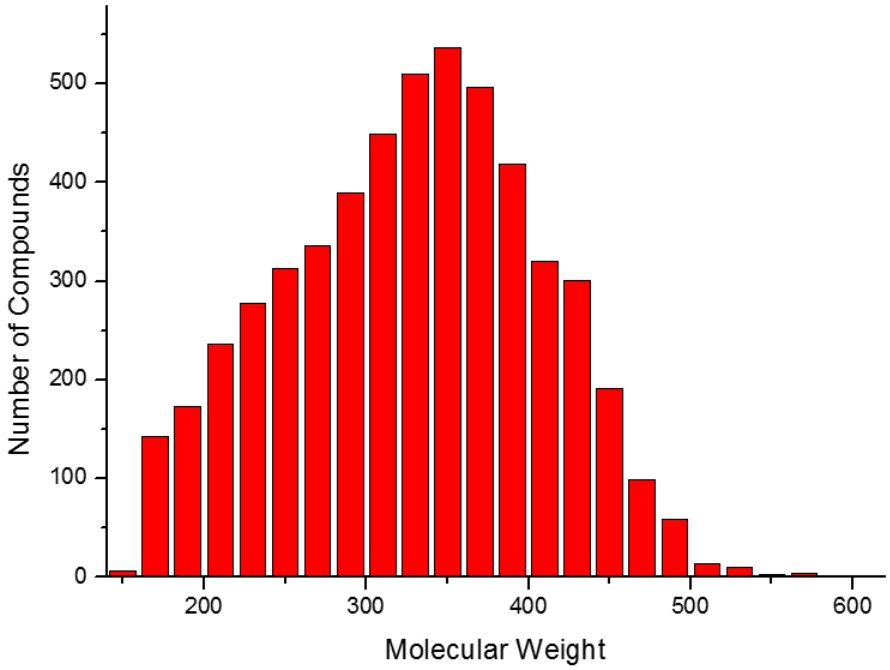
Design speciality:

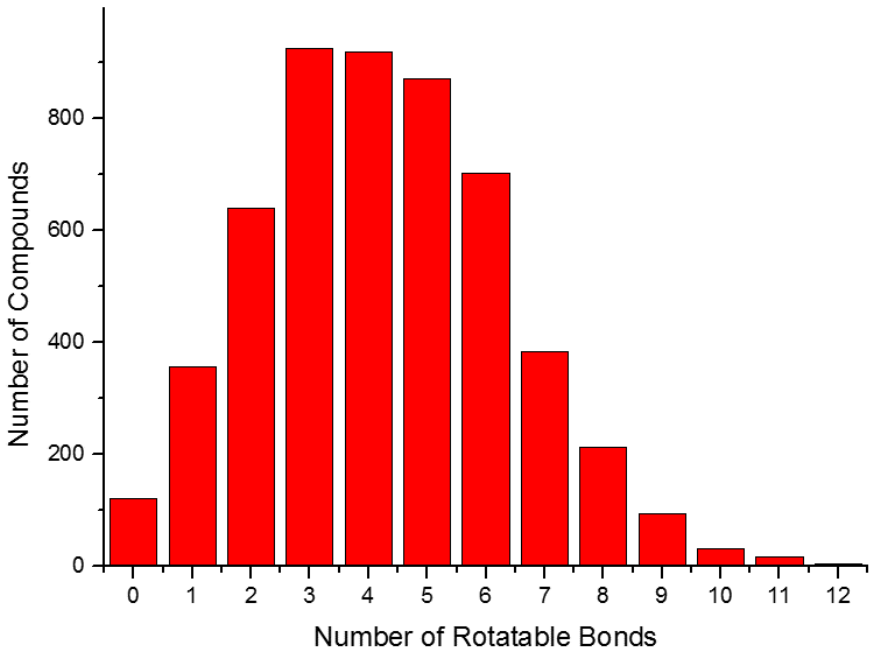
Given the potential applications of a Phenotypic Screening Library, the focus of the compounds selection strategy lies on biodiversity, screening-compliant physicochemical properties and maximal coverage of chemical space, aimed at providing hits for a wide spectrum of biological goals. The library has been designed by clustering of biologically relevant chemical database (50,000 small organic compounds). The database contained compounds selected on the base of approved drugs templates and templates of ligands with known activity against main classes of biological targets taken from ChEMBL and also included compounds from OTAVAchemicals targeted libraries.

Approved drugs were taken from DrugBank and clustered to several sets served as templates for Bayesian models. Also it was used sets of bioactive reference molecules (activity cutoff was 10 nM, only for the most numerous groups – 1 nM and for small groups – 100 nM) towards major subclasses of protein target classes (enzymes, membrane receptors, ion channels, transporters, transcription factors, proteins involves in adhesion, auxiliary transport proteins, epigenetic regulators, secreted proteins, structural proteins, surface antigens, other proteins and unclassified proteins) taken from ChEMBL. The models were developed for each training sets. They were based on FCFP4, ECFP4, FCFP6 and ECFP6 fingerprints. Molecular descriptors, such as LogP, molecular weight, number of rings, number of rotatable bonds, number of hydrogen acceptors and donors and molecular polar surface area were also involved in the construction of the models for more accuracy. At the final stage, OTAVAchemicals compound collection was screened against these models and top-scored compounds were selected.



The summary of the library characteristics:





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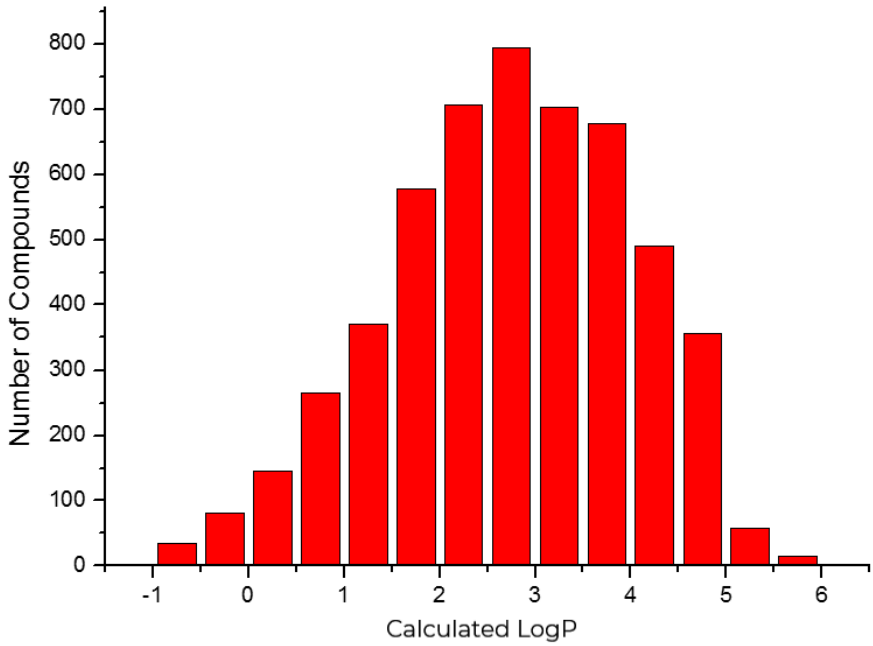

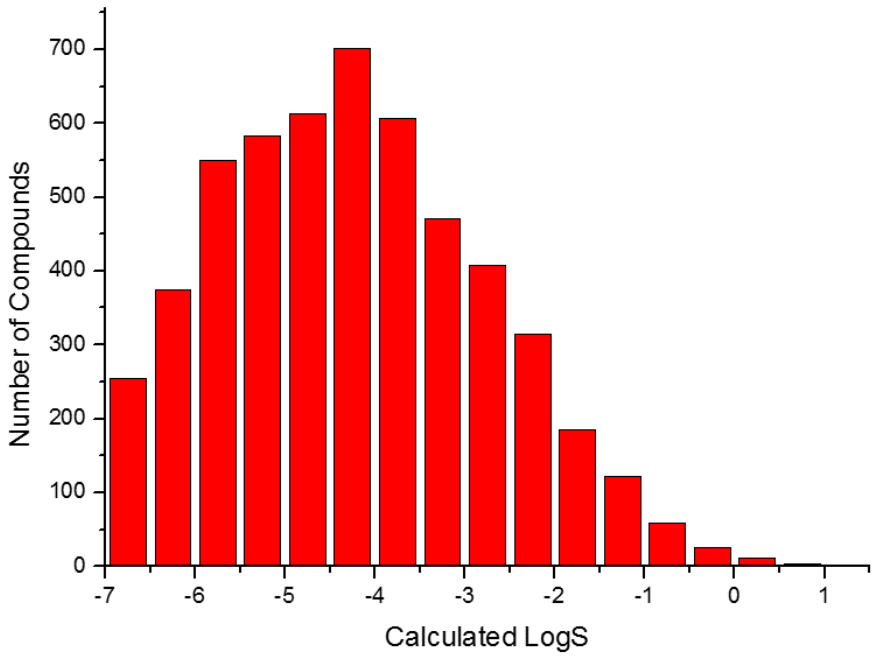

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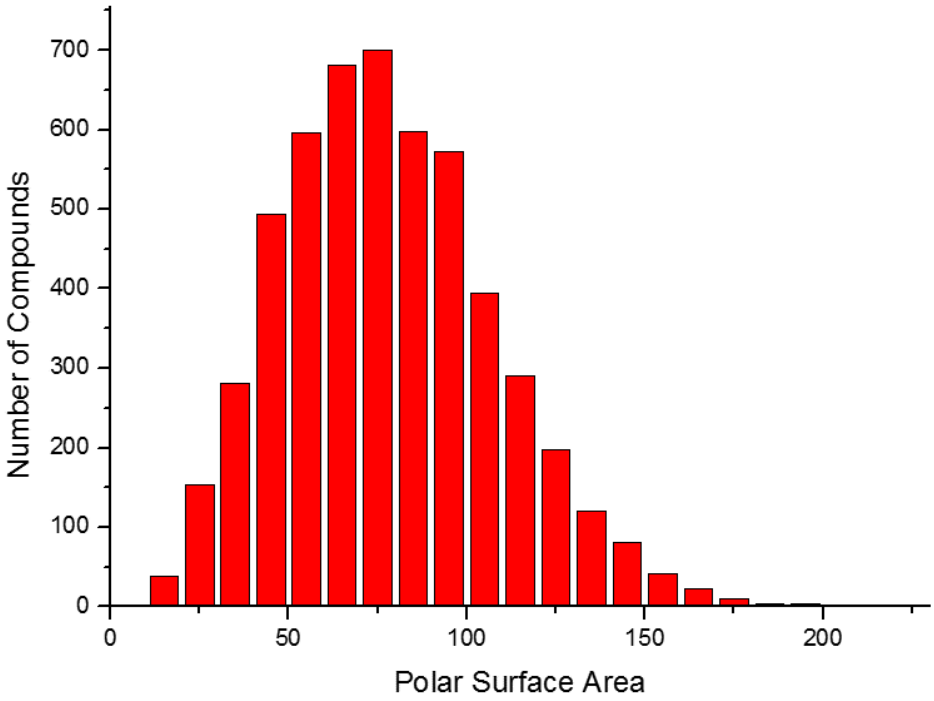

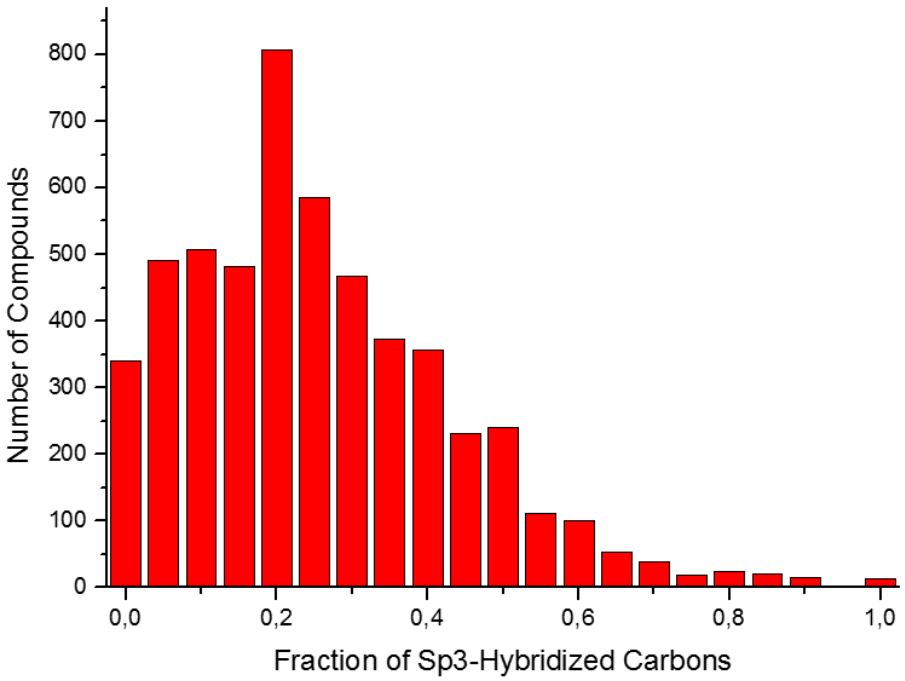

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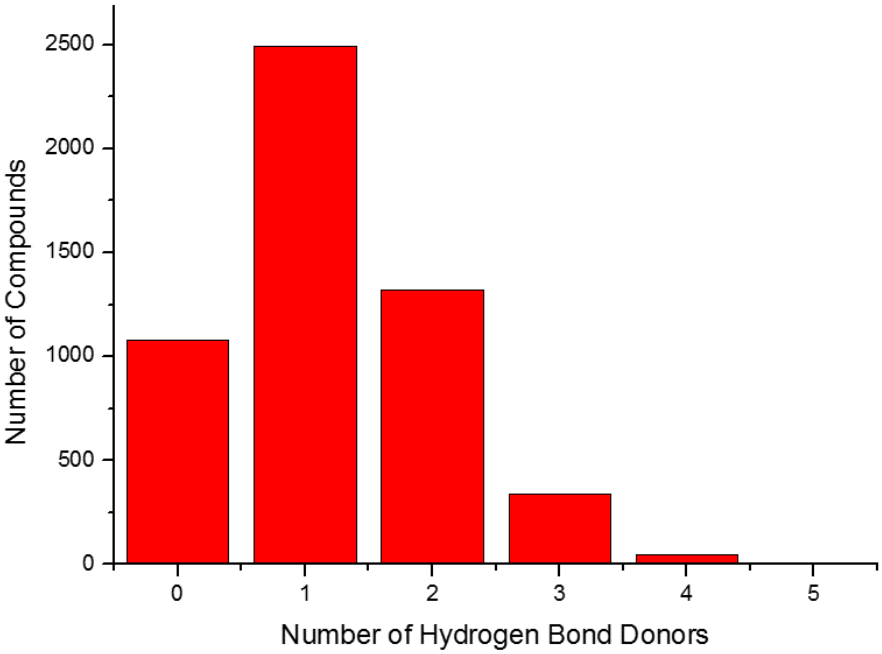

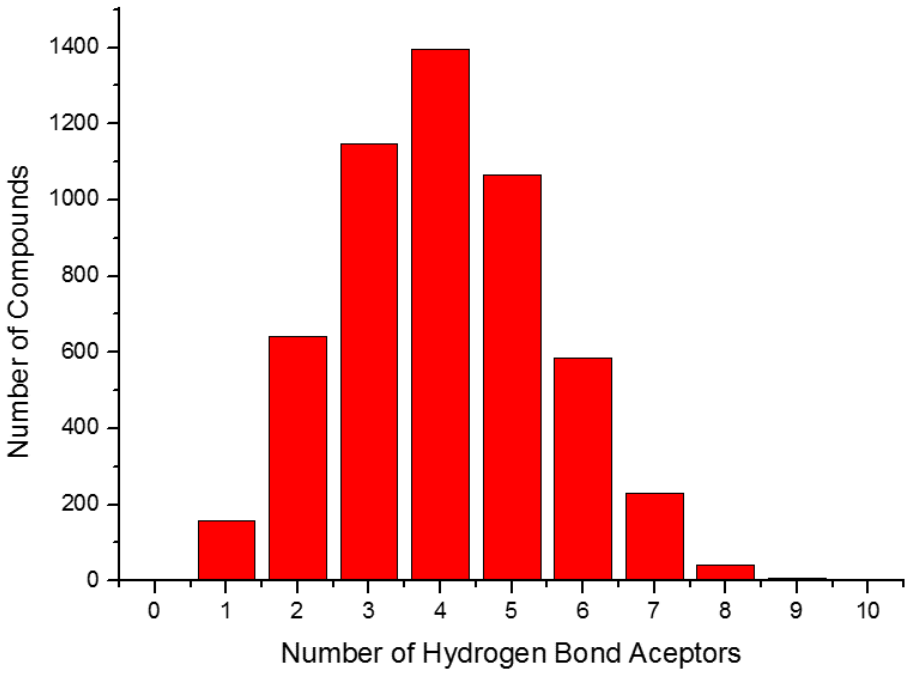

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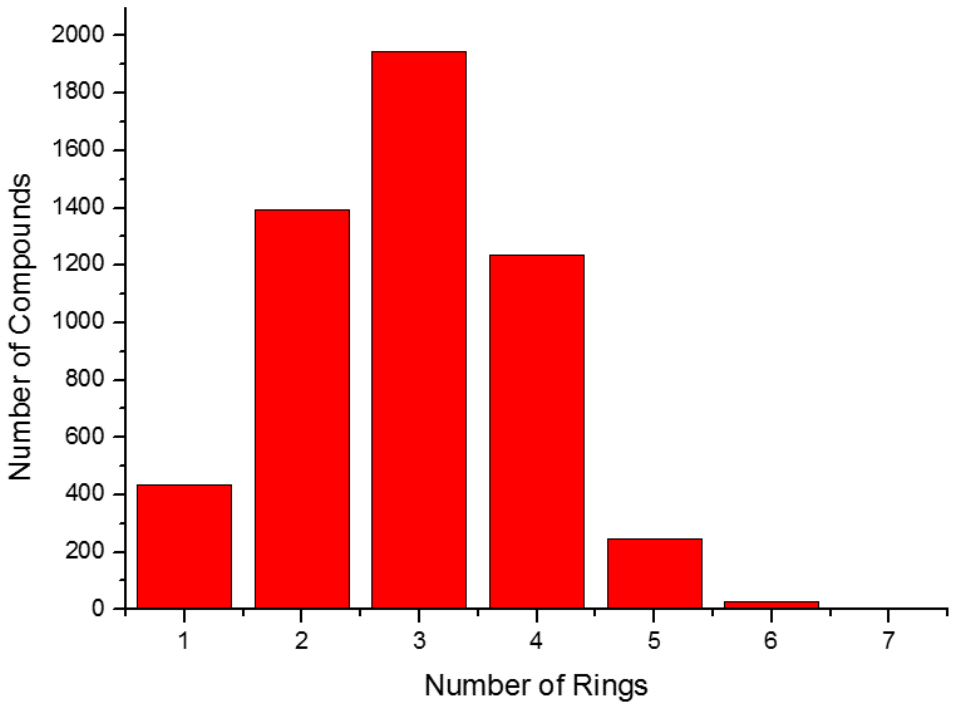

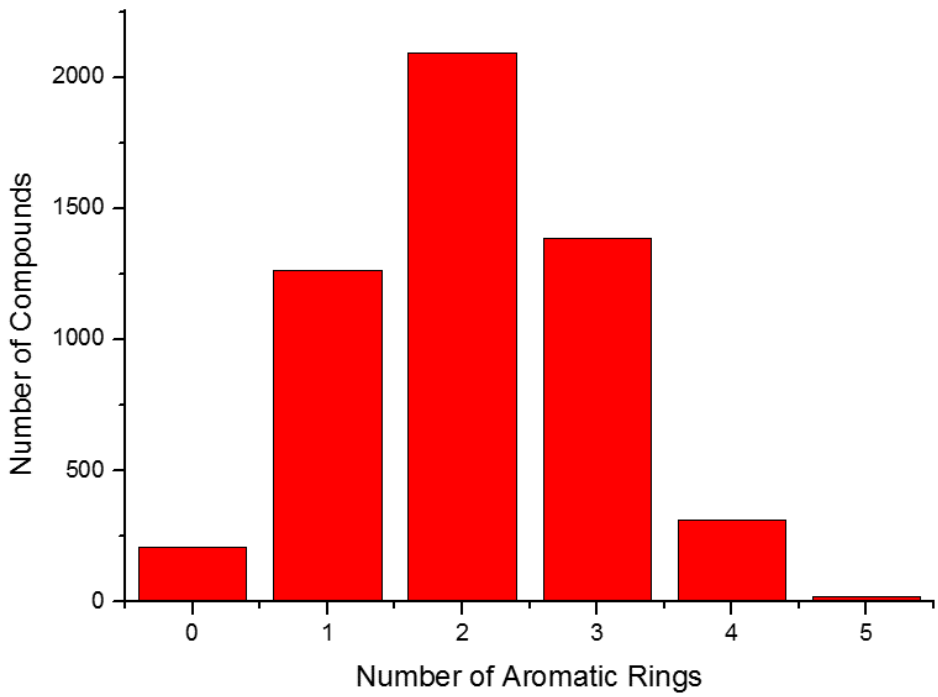

The library can be expanded or narrowed based on physicochemical and other properties.

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