



MCULE - NUCLEOTIDE LIBRARY

In this library we collected molecules from the Mcule full database - that contain at least one of the 5 naturally occurring nucleotide basis: Adenine, Guanine, Thymine, Cytosine, Uracil. Phosphate or ribose moieties were not required.

The library fulfills the following physicochemical property criterion:

Property	Min	Max
Molar mass	100	800

The library has also been filtered against more than 600 SMARTS-based structural including PAINS^{1,2}, and other MedChem filters³ rules.

If you would prefer other molecular format or further filtering - feel free to contact us at support@mcule.com.

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).

MCULE LIBRARY DATASHEET

Our professional laboratory services include

- 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