

Mcule - 'True Positive' High Throughput Screening library

The library was created from Mcule full database with the following physico-chemical property restrictions:

Property	Min	Max
Molar mass	160	450
H-bond acceptors	2	9
H-bond donors	0	2
Rotatable bonds	2	8
Heavy atom count	8	-
LogP	-0.4	3.5
PSA	20	120
Aromatic ring count	-	4
Aliphatic ring count	1	-
Fraction of sp ³ carbons	0.2	-
O and N atom count	1	-
Non-organic atom count	-	0
Heteroatom ratio	0.1	1.5
Acidic group count	-	2
Basic group count	-	2

Chiral centers	-	2
Acidic and basic group count	-	3
Non cyclic amide count	-	1
Refractivity	40	130

It was further filtered by more than 600 SMARTS-based substructure filters including PAINS^{1,2}, and other MedChem filters³ to avoid toxic or promiscuous functional groups.

It is also completely novel against ChEMBL⁴ and SureChEMBL molecules.

It contains the molecules in SMILES (SMILES ID) format.

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).

4, Gaulton A, Hersey A, Nowotka M, Bento AP, Chambers J, Mendez D, Mutowo P, Atkinson F, Bellis LJ, Cibrián-Uhalte E, Davies M, Dedman N, Karlsson A, Magariños MP, Overington JP, Papadatos G, Smit I, Leach AR. — *Nucleic Acids Res.* 2017; 45(D1):D945-D954. doi: 10.1093/nar/gkw1074

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