MCULE 'TRUE POSITIVE' HIGH THROUGHPUT SCREENING LIBRARY

Based on multiple successful compound selection projects for high throughput screening (HTS) with our pharma partners, we collected the Mcule 'True Positive' HTS Library, which could serve an optimal starting point for HTS scenarios.

The library was created from the Mcule Database using the following physicochemical 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 sp3 carbons	0.2	-
O and N atom count	1	-
Non-organic atom count	0	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

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After the physicochemical property-based selection, the subset was further filtered using more than 600 SMARTS-based substructure filters, including PAINS[1,2], and other MedChem filters[3], to exclude toxic or promiscuous functional groups. The Mcule True Positive HTS Library is entirely novel in comparison to ChEMBL[4] and SureChEMBL molecules.

Please access the downloadable data files of the Mcule 'True Positive' HTS 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) If you would prefer another molecular format or a further customized library contact us at **support@mcule.com**.

Did you know?

Mcule provides professional laboratory services including:

- Mcule Express Compound Inventory System™ - powered by robotized cold room sample storage
- Custom formatting - Solid weighing, robotized dissolution and pipetting
- Experimental sample characterization - Structure identity, purity, solubility and reactivity analysis
- Comprehensive logistic services- Compound procurement, sample management, customs clearance and worldwide delivery

Mcule provides professional cheminformatics services including:

- Custom library design - using a wide range of ligand- and structure-based molecular modeling and cheminformatic approaches including physicochemical property calculations, molecular fingerprint based similarity and substructure searches, diversity selection, similarity clustering, scaffold hopping, toxicity filtering, PAINS and other unwanted substructure filters, molecular docking, etc. Custom library generation workflows can be applied on the Mcule Database or Mcule ULTIMATE database
- Generation of synthetically feasible chemical universes - based on specific building blocks and reaction rules

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.**

REFERENCES

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[3] An Empirical Process for the Design of High-Throughput Screening Deck Filters, Pearce, B. C., Sofia, M. J., Good, A. C., Drexler, D. M. & Stock, D. A., *J Chem Inf Model* **2006**, 46 (3), 1060-1068., DOI: 10.1021/ci050504m.

[4] The ChEMBL database in 2017, 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