MCULE - PHENOTYPIC LIBRARY

In this library you can find purchasable molecules with Mcule IDs and ChEMBL[1] IDs that have an activity on a known target in the submicromolar (<1,000 nM) range.

The salt forms/stereoisomers/charges may be different from the published molecules.

If you would like to check the forms of the original CHEMBL molecules - you can do a look-up at https://www.ebi.ac.uk/chembl/g/#search_results/all using the enclosed ChEMBL IDs.

The CSV files contain the canonical SMILES strings, Mcule IDs and ChEMBL IDs in the first three columns.

SMILES,Mcule_ID,ChEMBL_ID,

Subsequently, the bioactivity data are listed. Column names in the header are identical to the names used in the ChEMBL database:

TargetDictionary_target_type_0,ProteinClassification_pref_name_0,Assays_chembl_0,
TargetDictionary_pref_name_0,TargetDictionary_organism_0,

In the **max100activity** file we made an upper cap for the number of activities per compound because there are structures in the ChEMBL database with more than 200 activities (the max is above 1,200). This file can be more easily opened by Excel as a table.

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

1, 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

mcule.com Kft. ● H-1115 Budapest, Bartok Bela ut 105-113. Building II/A, Hungary, EU ● 535 Everett Ave #410, Palo Alto, CA 94301, USA ● www.mcule.com

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

mcule.com Kft. ● H-1115 Budapest, Bartok Bela ut 105-113. Building II/A, Hungary, EU ● 535 Everett Ave #410, Palo Alto, CA 94301, USA ● www.mcule.com