

MCULE - COVALENT LIBRARY

We created two covalent libraries with **fragment** and **druglike** properties.

Both libraries contain molecules with at least one of the following structural elements:

Epoxide
Aziridine
Beta_lactame
Beta_lactone
Sulfonyl_ester
Carbamates
Vinyl_sulfone
Vinyl_sulfonamide
Boronic_acids
Boronic_esters
Boranes
Allenamide
Propiolonitrile
Isothiocyanate
Sulfonimidoyl_fluoride

Oxaziridine
Cyanide
Alkylthiol
Maleimide
Ketoamide
2-chloro-heterocycles
2-ethynyl-heterocycles
2-vinyl-heterocycles
Acrylamide
Acrylonitrile
Alkylhalide
Haloester
Haloamide
Haloketone
VA_michael_acceptors

The druglike 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

MCULE LIBRARY DATASHEET

The fragment library was created from Mcule full database with the following physico-chemical property restrictions (Ro3):

Property	Min	Max
Molar mass	-	300
H-bond acceptors	-	3
H-bond donors	-	3
Rotatable bonds	-	3

No further restrictions were made. The files contain the molecules in SMILES (*SMILESID*) format.

If you would prefer other molecular format or further filtering - feel free to contact us at support@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 LIBRARY DATASHEET