

## MCULE - FRAGMENT LIBRARIES

We created two fragment libraries with HIGH and LOW sp<sup>3</sup> fractions that may be used for different purposes.

The library with HIGH sp<sup>3</sup> fraction was created from Mcule full database with the following physico-chemical property restrictions:

Property	Min	Max
Molar mass	-	300
H-bond acceptors	-	3
H-bond donors	-	3
Rotatable bonds	-	4
Heavy atom count	-	15
LogP	0	2
PSA	-	60
Ring count	1	3
Fraction of sp <sup>3</sup> carbons	0.4	-

The rows marked with orange are responsible for the pronounced 3D characteristic of the fragments. This library violates the Ro3 criteria at one point (Rotatable bonds > 4) in order to maximize the 3D character of the selected molecules.

The library with LOW sp<sup>3</sup> fraction was created from Mcule full database with the following physico-chemical property restrictions:

Property	Min	Max
Molar mass	-	300
H-bond acceptors	-	3
H-bond donors	-	3
Rotatable bonds	-	3
Heavy atom count	-	15
LogP	0	2
PSA	-	60
Ring count	1	3
Fraction of sp <sup>3</sup> carbons	-	0.4

The rows marked with green cover the Ro3 criteria so the library complies with these rules. The last row marked with orange is responsible for the low (<0.4) sp<sup>3</sup> fraction and accordingly the pronounced 2D characteristic of the fragments.

No further restrictions were made. 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](mailto: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