MCULE FRAGMENT LIBRARY

We created the Mcule Fragment Library with two subsets, that can be used for different purposes.

- **3D fragments (high fsp3)**: this subset contains sp3-rich carbons to maximize the 3D character of the fragments, thereby increasing the binding specificity of any identified hits.
- **2D fragments (low fsp3)**: this collection includes fragments with a low sp3 carbon atom ratio, which favors rigid molecules, thus, facilitates co-crystallization.

The subset of 3D fragment with a high sp3 fraction was created from the Mcule Full Database using the following physicochemical 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	3
PSA	-	60
Ring count	1	3
Fraction of sp3 carbons	0.4	-

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

The subset of 2D fragments with a low sp3 fraction was created from the Mcule Full Database with the following physicochemical 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	3
PSA	-	60
Ring count	1	3
Fraction of sp3 carbons	-	0.4

The rows marked in green cover the Ro3 criteria, indicating that the library complies with these rules. The last row marked in orange is responsible for the low (<0.4) sp3 fraction, resulting in the pronounced 2D characteristic of the fragments. No further restrictions were made.

Click here to access the downloadable data file of Mcule Fragment Library. This ZIP file contains two SMI.GZ files that include the molecules in SMILES format (*SMILES ID*).

Additionally, 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'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.

MCULE FRAGMENT LIBRARY DATASHEET

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