Fsp³-enriched Fragment Library

The mean saturation degree Fsp^3 (calculated as number of sp^3 hybridized carbons / total carbon count) was shown to increase from 0.36 for 2.2 million molecules at the development stage to 0.47 for 1,179 of approved drugs. A higher Fsp^3 count together with low molecular weight and ClogP values, leads to higher bioavailability and specificity of compounds, thus making them attractive for drug discovery process.

In response to these new trends in drug discovery, involving comprehensive structural analysis of approved drugs and determination of relationships between molecular complexity and pharmacological promiscuity of drug-like compounds [1–5], Life Chemicals has extrapolated the results of described investigations to its Fragment Library design.

Applying the Fsp^3 cut-off at 0.45 to the Life Chemicals General Fragment Library resulted in our **Fsp³-enriched Fragment Library** of around **19,900** sp^3-rich screening compounds. Physicochemical parameters are summarized in the table below:

Parameter	MW	ClogP	Fsp^3	TPSA	RotB	HBD	HBA	Benzene rings
Selection range	≤ 300	< 3	≥ 0.45	< 90 Å²	≤ 3	≤ 3	≤ 3	≤ 1
Average value	247.5	1.1	0.6	59.2	3.4	1.4	2.9	≤ 1

Additionally, a **Diversity Screening Set** of **1,600** structurally-diverse sp^3-rich fragments was prepared to provide the most-promising drug-like screening compounds for fragment-based lead discovery in a convenient manner. These fragment-like molecules possess a wide range of chemical structure dissimilarity and are compliant with in-house MedChem and PAINS structural filters [6-7].

The compound selection can be customized based on your requirements, cherry-picking is available.

Please, contact us at orders@lifechemicals.com for any additional information and price quotations.

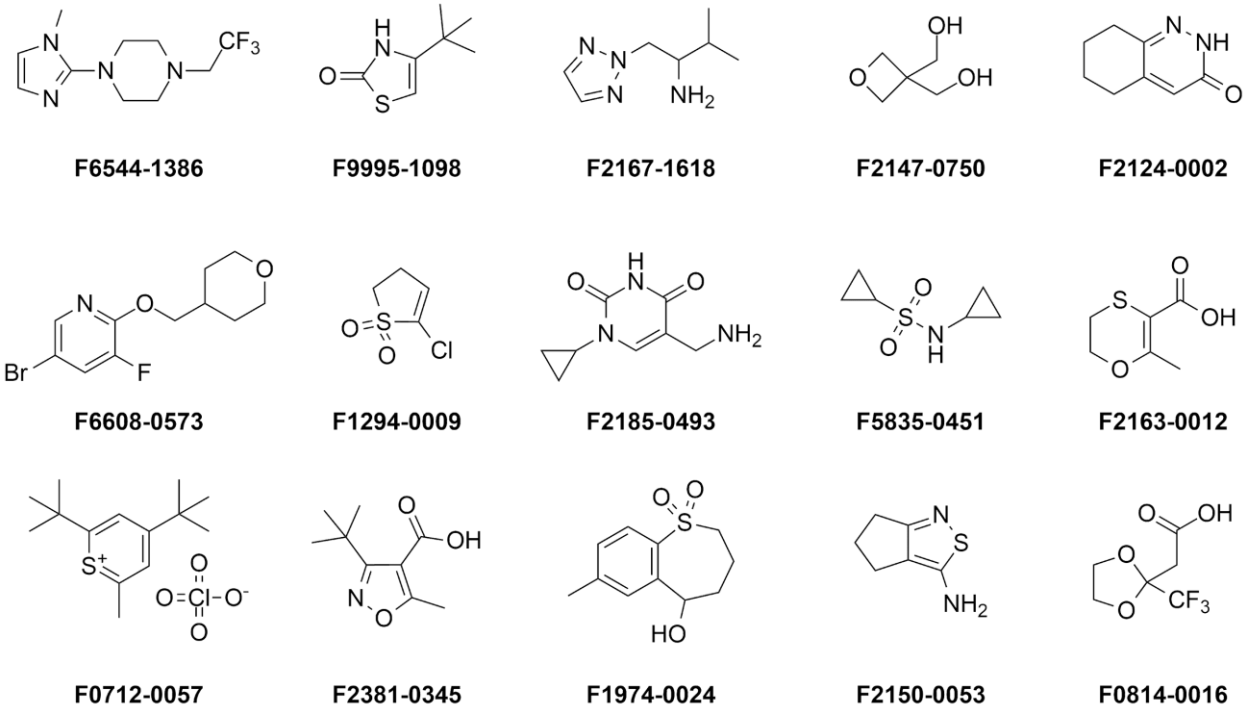

Figure 1. Representative compounds from the Fsp³-enriched Fragment Library

References

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