

Enamine Fsp³-enriched Fragments

1817 compounds

Deliverable as entire set or as selected compounds.

The utilization of fragment based drug discovery (FBDD) approach has already been proved by more than 30 compounds entering the clinic [1]. Among the main focuses of FBDD are Fsp³-enriched fragments. Since introduction of the concept “Escape from Flatland” in 2009 implying in the increase of saturation fraction Fsp³ (Fsp³ = ratio of sp³ hybridized carbons vs total carbon count) and presence of (potential) chiral centers in libraries [2] numerous MedChem projects directed on the design and screening of more saturated fragments have been appeared [3-5]. Recently the improvement of binding selectivity and frequency toward a set of 100 proteins for diverse small molecules with high ratio of sp³-hybridized and stereogenic atoms have been shown [4].

Considering the needs for new Fsp³-enriched fragments **Enamine Fsp³-enriched Fragment** library was designed from our screening and building blocks collections. Beside the “Rule of three” requirements identifying the fragments [6] the criterion Fsp³ > 0.4 as well as internal Enamine structural filters (including PAINS [7]) were applied.

Parameter	Enamine Fsp ³ -enriched Fragments
MW	140 ... 300
HAC	9 ... 22 (88.2 % <19 HA)
clogP	-1 ... 3
HBD	≤ 3
HBA	≤ 3
RotB	≤ 3
TPSA, Å	≤ 90
Chiral centers	≤ 2
Purity	90+ %
Availability	10 mg

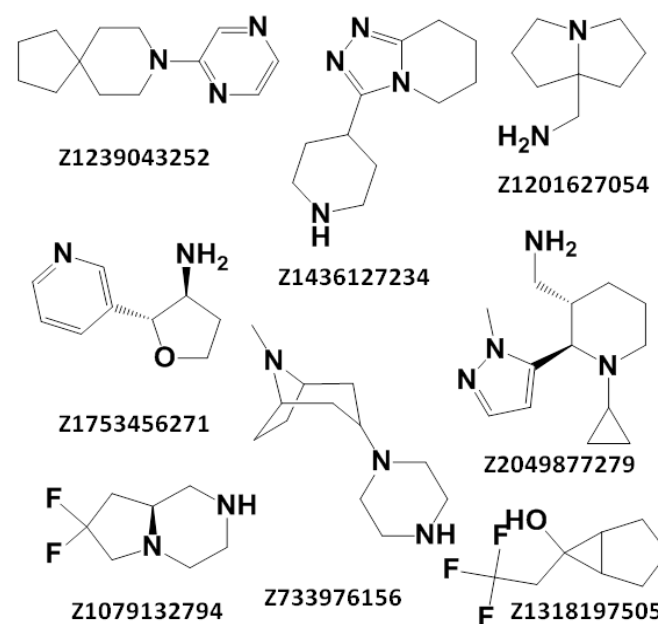


Figure 1. Representative set of Fsp³-enriched Fragments.

Enamine Fsp³-enriched Fragments are characterized by high structural diversity (the diversity coefficient is **0.89**) including novel compounds with spiro-, bridged, fused rings (see Figure 2) and are described with **1276** different Bemis-Murcko loose frameworks [8].

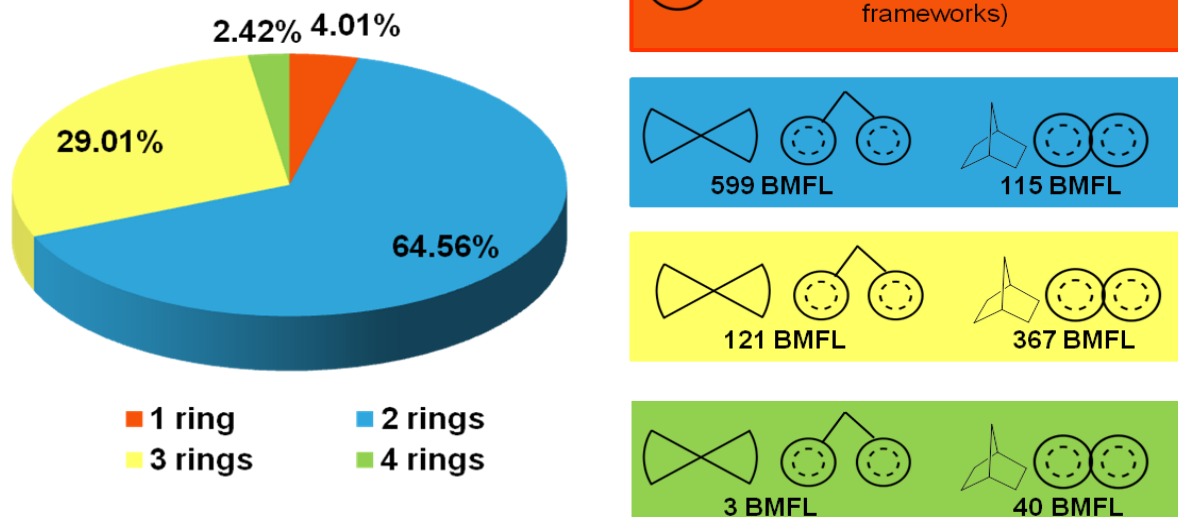


Figure 2. Analysis of structural diversity of Enamine F_{sp^3} -enriched Fragments.

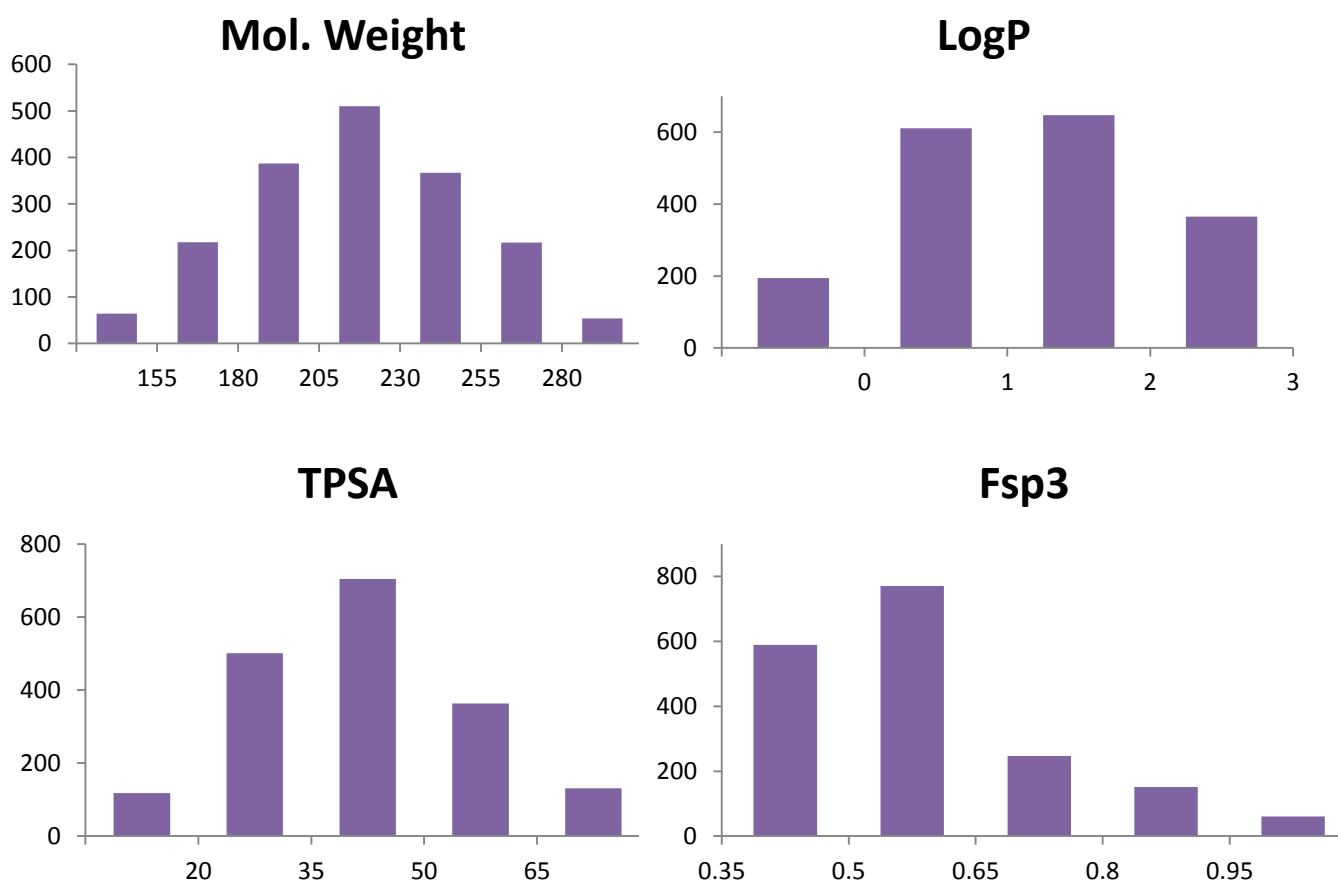


Figure 3. Physical chemical profile for Enamine F_{sp^3} -enriched Fragments.

Novelty, high chemical and structural diversity of Enamine F_{sp^3} -enriched Fragments will make easier any search of new ligands for challenging targets.

Also Enamine **Golden Fragment Library**, general **Enamine Fragments** as well as different focused fragment libraries (**Enamine PPI**, **Fluorinated**, **Brominated Fragments**) were developed

exploiting the same filters and approaches. Furthermore the database of **Enamine Feasible Fragments** calculating near 465 k compounds and representing the biggest offered on the market “fragment space” was prepared by applying fragment identifying criteria to Enamine REAL DataBase collection. For further information please visit www.enamine.net.

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