Enamine Brominated Fragments

1280 compounds

Deliverable as entire set or as selected compounds.

The increasing number of clinical candidate drugs developed by fragment based drug discovery (FBDD) has already approved the effectiveness of this approach in medicinal chemistry [1, 2]. X-Ray crystallography is one of the most spread screening techniques in FBDD due to such advantages as absence of false positive results, finding of weak interactions [3]. The anomalous scattering of X-Rays inherent to bromine atoms and permitting their unambiguous identification [4] makes brominated compounds very convenient for X-Ray screening. Recent researches concerning targeting HIV-1 protease [5] and identifying ligand-binding hot spots in proteins [6] at screening of brominated compounds have initiated the formation and studying of new libraries of bromo-containing compounds.

Accounting mentioned above **Enamine Brominated Fragment** Library was designed from our screening and building blocks collections. All compounds contain one aromatic bromine, correspond to main “Rule of three” criteria identifying fragments [7] (the upper limits for MW and logP are 350 and 3.5 correspondingly to account Br contribution, see the Table) and pass internal Enamine structural filters considering PAINS [8], high reactive and toxic motifs.

Parameter	Enamine Brominated Fragments
MW	170 … 350
HAC	8 … 21 (90.2 % <19 HA)
clogP	-0.5 … 3.5
HBD	≤ 3
HBA	≤ 3
RotB	≤ 3
TPSA, Å	≤ 90
Chiral centers	≤ 2
No of Br	1
Purity	90+ %
Availability	>10 mg

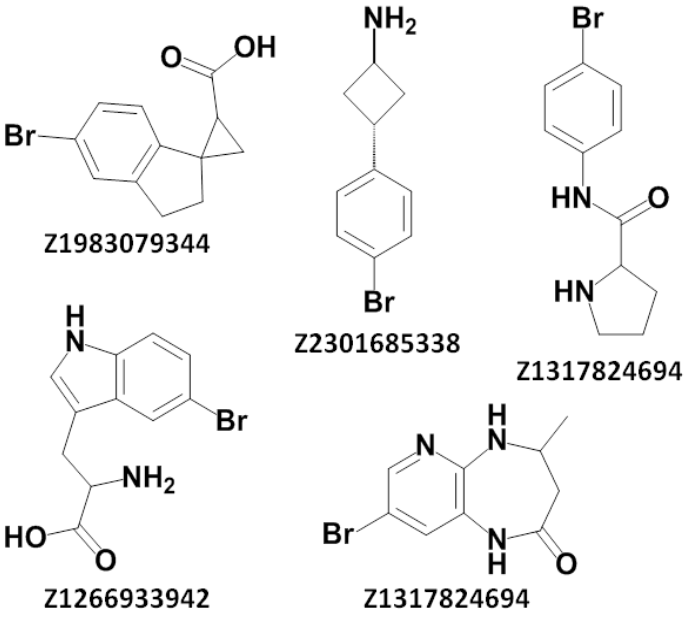

Figure 1. Representative set of **Brominated Fragments**.

The diversity coefficient of **Enamine Brominated Fragments** is **0.76**, structural diversity is described with **569** different Bemis-Murcko loose frameworks [9], physical chemical profile is summarized on the Figure 2.

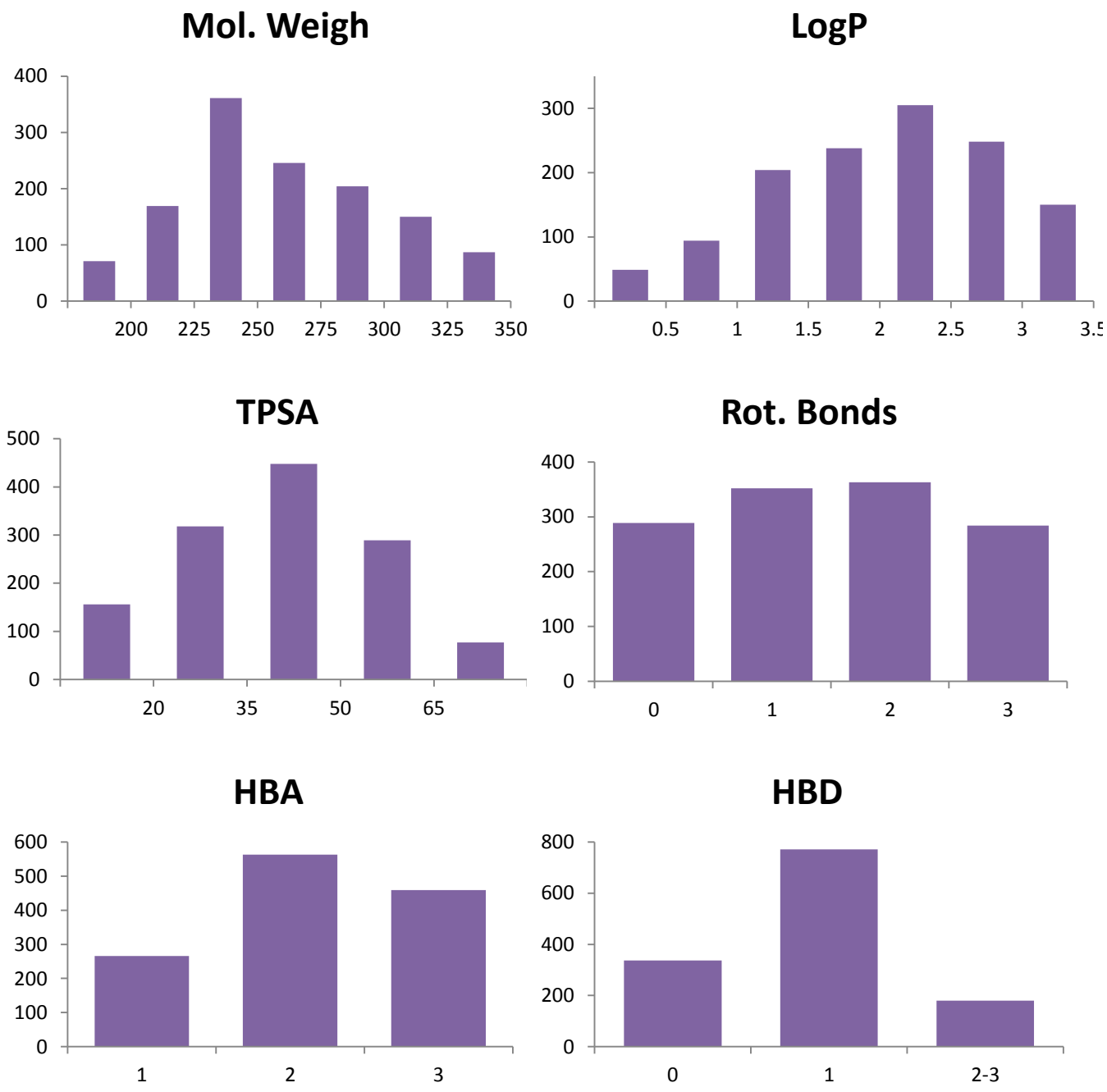

Figure 2. Physical chemical profile for **Enamine Brominated Fragments**.

Also Enamine **Golden Fragment Library**, general **Enamine Fragments** as well as different focused fragment libraries (Enamine **PPI, Fsp^3-enriched, Fluorinated 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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