

Enamine Covalent Fragment Library

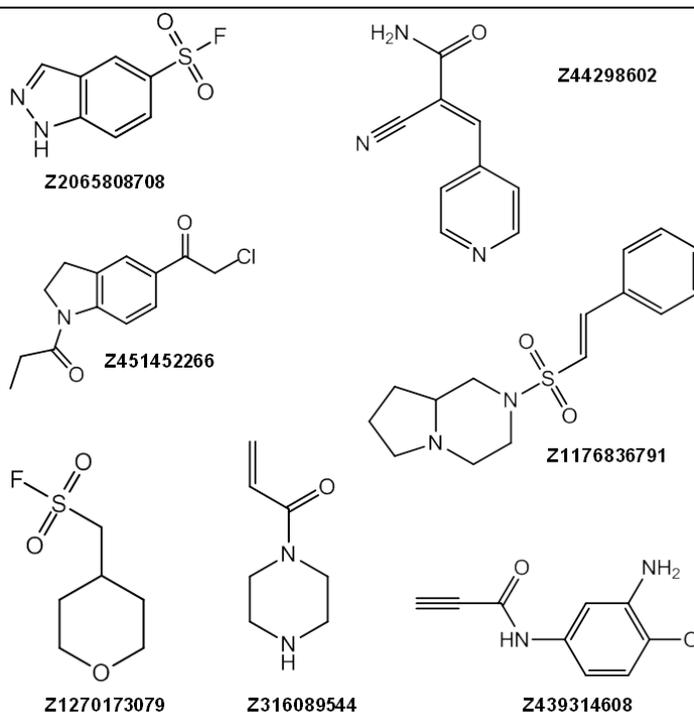
Number of compounds	1,460
Number of Bemis-Murcko loose frameworks	541
Diversity coefficient	0.768

Identifying electrophilic ligands able to form covalent bonds with specific biological targets is a promising approach to Fragment Based Drug Discovery (FBDD). High biochemical potency and selectivity via targeting of specific amino acid residues are among the main advantages of this approach.

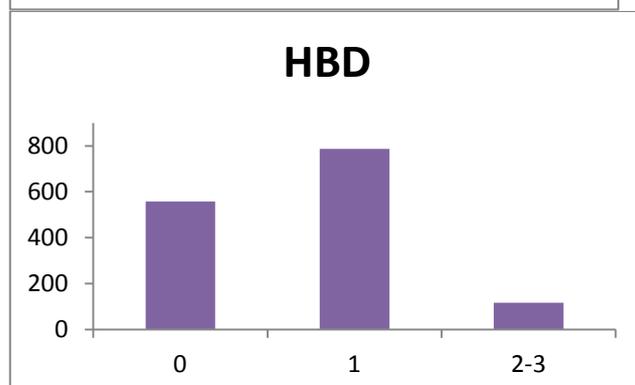
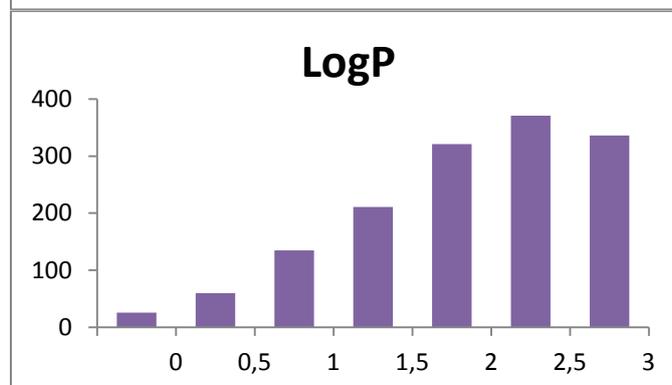
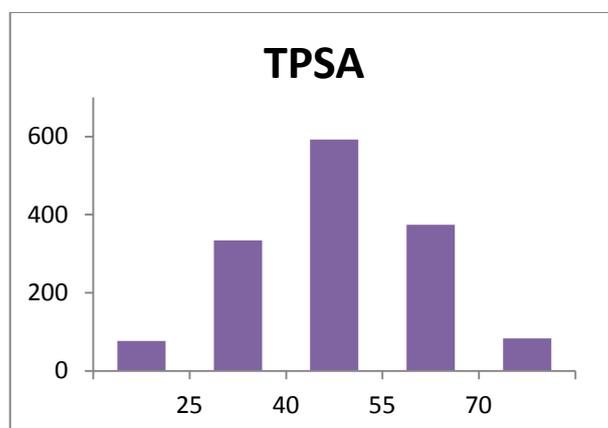
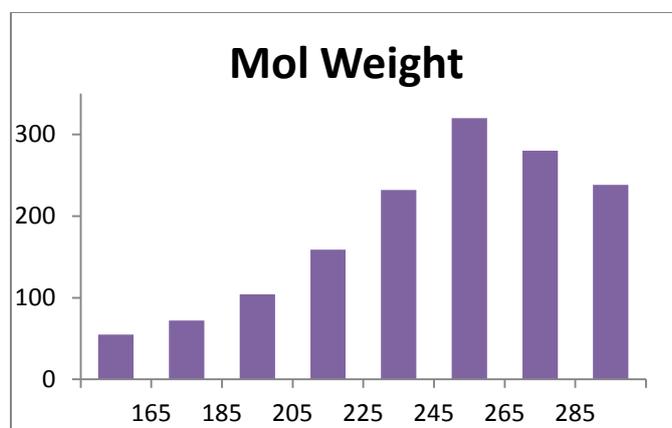
We have selected 1,460 electrophilic fragments containing the majority of vinyl, halomethyl ketones, sulfonyl fluorides, acrylonitriles and vinyl sulfones able to form covalent bonds with cysteine, serine and tyrosine residues. All fragments correspond to “Rule of three” criteria and selected Enamine’s internal filters for highly reactive and toxic motives. Not all reactivity filters, however, were applied in order to allow for maintaining electrophilic nature as a key property of this fragments set.

MW	140 ... 300
No of heavy atoms	8 ... 22
clogP	-0.5 ... 3
HBD	≤ 3
HBA	≤ 3
RotB	≤ 3
TPSA, Å	≤ 100
N+O	1...6

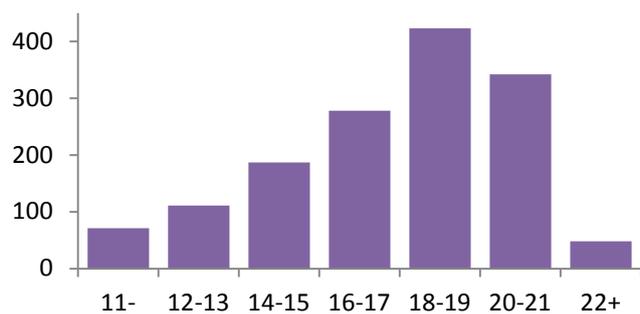
Molecular criteria used in selection of the covalent fragment.



Examples of compounds from Enamine **Covalent Fragment Library**.



HeavyAtomCount



HBA

