**F*sp*3 Fragment Library**

In accordance to current trends and requirements in the field of FBDD Princeton Biomolecular designed the library of *qualitative Fsp3 enriched Fragments* that comprises over **11,000 on-the-shelf compounds**. Favor of Fsp3 enriched small molecules in drug design is due to strong correlation between degree of carbon bonds saturation, higher aqueous solubility, lower melting point and as result correlation with successful drug candidates. According to recently reported mean F*sp*3 value for approved drugs of 0.471, we applied cut of Fsp3 > 0.46 to preselected set of fragments. Besides, small molecules in current library passed through precision MedChem structure filters including PAINS (A, B, C) and REOS.

Physicochemical parameters applied for fragments selection are listed below:

1. 150 ≤ MW ≤ 300
2. -2 ≤ ClogP ≤ 3
3. RotBonds ≤ 3
4. HBD ≤ 3
5. HBAcc ≤ 3
6. Carbocyclic aromatic rings ≤ 1
7. No more than 3 fused rings and no more than 2 aromatic rings
8. Br, Sulfo, Cyano, Nitro groups total count ≤ 1
9. S and Cl atoms total count ≤ 2
10. 15 Å2 < TPSA < 100 Å2
11. **F*sp*3** > **0.46**

1 F. Lovering, J. Bikker and C. Humblet*, J. Med. Chem*., **2009**,52, pp 6752–6756.