**Fluorine Fragment Library**

HTS screening performed with 19F NMR spectroscopy is becoming increasingly popular in early Drug Discovery. Rapid growth of versatile 19F NMR methodologies lead to increasing role of fluorine containing compounds in hit identification and lead optimization phases of drug discovery projects. Our Fluorine Fragment Library of over **9,600 small molecules** was designed with aim to best meet of even most sophisticated demands of contemporary FBDD. Strict MedChem filtering criteria and Ro3 PhysChem parameters were combined to rich the set of small molecules perfect for fragment-based screening. Furthermore, our Library of Fluorine containing fragments has been subjected to chemotype control to secure proper quality of the product.

Restriction of Physicochemical parameters used for selection are summarized below:

120 < MW < 300

-2.0 < ClogP < 3.0

HbAcc ≤ 4

HbD ≤ 3

RotBonds ≤ 4

Sulfone, Cyano and Nitro groups count ≤ 1

Br count ≤ 1

S and Cl atoms count ≤ 2

Structure filters applied to the Library:

Amide count ≤ 1

Carbocyclic aromatic rings count ≤ 1

Eli Lilly MedChem rules1, PAINS (A, B, C)2, REOS3

1. Bruns R.F., Watson I.A. (Eli Lilly), *J. Med Chem.,* **2012**, 55(22), pp 9763–72.
2. Bell J.B., Holloway G.A. (Cancer Therapeutics), *J. Med. Chem*., **2010**, 53 (7), pp 2719–2740.
3. Walters P.W., Namchuk M. (Vertex), *Nat. Rev. Drug Discov*., 2003, 2, pp259–266.