

Compound collections



For any high throughput screening laboratory, the “jewel in the crown” is manifested by the compounds, or compound libraries, used in screening experiments. The Drug Discovery Facility holds an “in house” 37,000 lead-like diversity library.

The diversity of the library is demonstrated by 13,000 individual Bemis-Murcko frameworks. We also have access to the fully FDA approved library (approx 1200 compounds) of active drug molecules.

Property	Value
Mol. Weight	< 500 Da
Rotational bonds	≤ 10
H-bond donors	≤ 5
H-bond acceptors	≤ 10
Topological molecular polar surface area (tPSA)	$\leq 140.0 \text{ \AA}^2$
Partition coefficient (logP)	≤ 5.0
Aqueous solubility (logS)	≥ -7.0