SMALL MOLECULES FOR FRAGMENT-BASED SCREENING

Fragment Library

Introduction

The ChemBridge® Fragment Library set offers more than 5,000 compounds that can be individually selected based on your criteria, allowing researchers to build fragment sets of size and composition best suited to their research objectives and methodologies. ChemBridge can also assist in the selection of diverse sub-sets. This collection of small molecule fragments provides compounds for use in fragment-based screening and drug discovery using high-throughput X-ray crystallography, NMR, SPR and high concentration bioassay methodologies. Compounds can be provided in mg or umol equivalent amounts and delivered undissolved or as DMSO solutions.

Selection

Compounds included in the Fragment Library set were chosen based upon the commonly accepted Astex Rule of Three[1], additional physiochemical property filters, and proprietary ChemBridge substructure filters. ChemBridge has applied Rule of Three considerations (MW ≤ 300, H-bond donors ≤ 3, H-bond acceptors ≤ 3, cLogP ≤ 3) along with rotatable bond count, calculated tPSA, and a cLogSw (predicted aqueous solubility) filter for a first-pass aqueous solubility filter (-2.50 or higher corresponding to a predicted aqueous solubility of approx. 3mM or higher). The Fragment Library set is further divided into the High Solubility Set (HSS) composed of approx. 2,500 fragments with minimum DMSO solubility of 100mM and minimum solubility in phosphate buffered saline (PBS; pH 7.4) of 200uM (with many fragments soluble at 1mM) and a set of approx. 2,500 fragments with solubility below one or both of the HSS criteria.

Specifications

ChemBridge Cutoff Values	
Molecular Weight	150 to 300
H-donors	≤ 3
H-acceptors	≤ 3
cLogP	≤ 3
Rotatable Bonds	≤ 3
cLogSw	≥ -2.50
tPSA	≤ 120

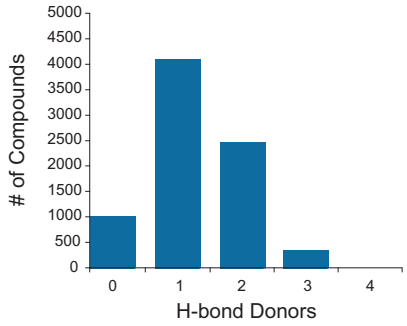
Average Property Values	
Molecular Weight	225.06
H-donors	1.22
H-acceptors	2.33
cLogP	1.27
Rotatable Bonds	2.01
cLogSw	-1.68
tPSA	49.66

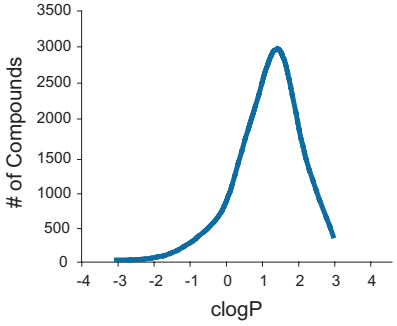
[1] Carr, A.E.; Congreve, M.; Murray, C.; Rees, D.; Fragment-based lead discovery: leads by design, *Drug Discovery Today*, 2005, 10, 987-992

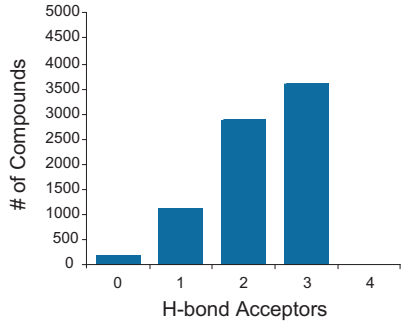
Format

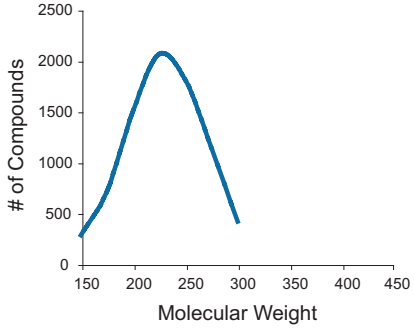
- Download structures and custom select from the approximately 5,000 Fragment Library compounds.
- Compounds are available in mg or umol amounts undissolved (mostly powders, some oils) or dissolved in DMSO and plated to your requirements.
- All compounds have a minimum purity of 90% by NMR or by LC-MS/ELSD.
- Follow-up stock is available for resupply, subject to availability.

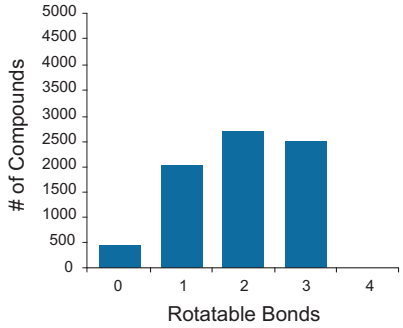
Physiochemical Properties

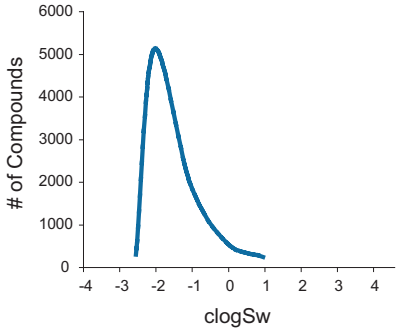


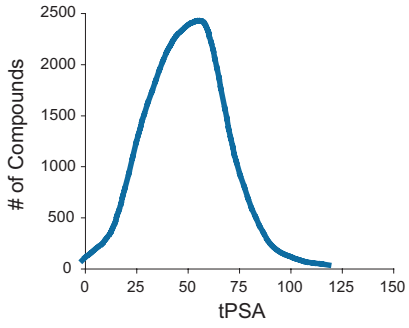












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