

A COLLECTION OF SMALL MOLECULES FOR FRAGMENT-BASED SCREENING

Fragment Library

Introduction

ChemBridge's Fragment Library now offers more than 6,000 compounds. These compounds can be individually selected based on your criteria or pre-selected diversity sub-sets can be purchased. This exemplary collection of small molecules is designed for fragment-based screening by high throughput X-ray crystallography, NMR, SPR and high concentration bioassay methodologies. The Fragment Library was chosen based upon the commonly accepted Astex Rule of Three¹ plus additional property filters and using proprietary ChemBridge substructure filters.

Fragment Library Selection

Compounds are selected according to Astex Rule of Three considerations ($MW \leq 300$, H-bond donors ≤ 3 , H-bond acceptors ≤ 3 , $cLogP \leq 3$), rotatable bond count, calculated tPSA, and a cLogSw filter that has been applied for improved aqueous solubility. The commonly publicized cLogSw (predicted aqueous solubility) lower limit can be as low as -3.50, however, the -2.50 limit (approx. 3mM) applied by ChemBridge ensures a higher predicted aqueous solubility.

Fragment Library Specs & Filters

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

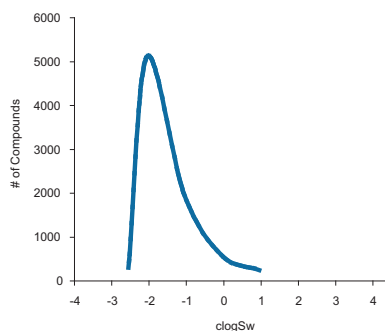
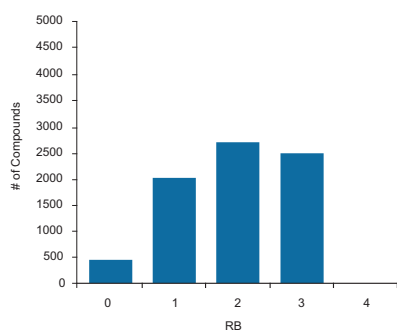
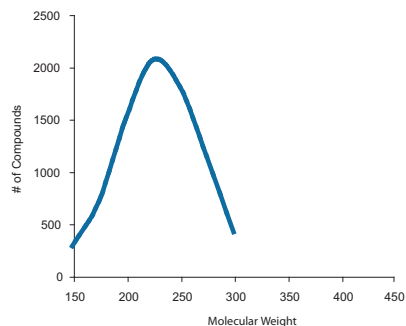
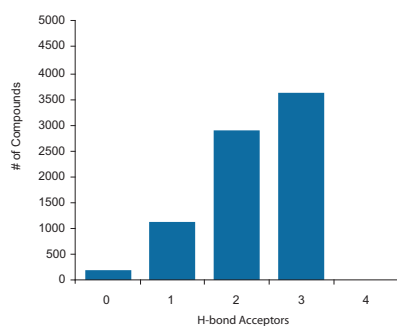
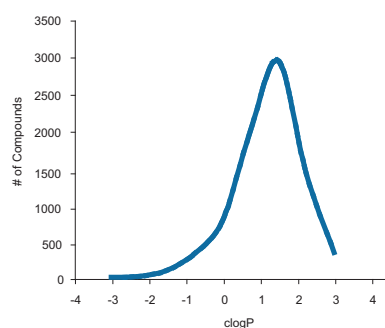
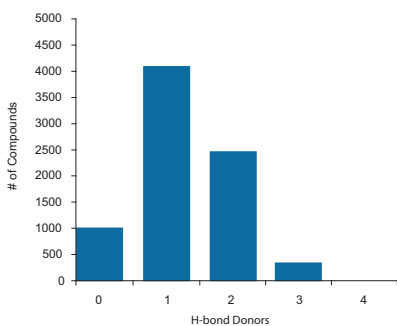
Molecular Weight	225.06
H-donors	1.22
H-acceptors	2.33
cLogP	1.27
Rotatable Bonds	2.01
cLogSw	-1.68
tPSA	49.66

¹Carr, R.A.E. *et al.*, *Drug Discovery Today*, 2005, **10**, 987-992.

Format

- Request MDL structure-data files (SDfiles) or ISIS Database (db) files for the Fragment Library.
- Select individual compounds or purchase pre-selected, diversity sub-sets of different sizes (500, 1,000 or more compounds).
- Compounds are available in milligram or micromole amounts in powder form or dissolved in DMSO and plated to your requirements.
- All compounds have a minimum purity of 90% by $^1\text{H-NMR}$, and analytical data is provided with any order.
- Follow-up stock is available for resupply, subject to availability.

Physiochemical Properties



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