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.

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 and calculated TPSA limits.

High Solubility Subset

Approximately half of the Fragment Library compounds meet the criteria for the High Solubility Subset (HSS). These fragments have a minimum DMSO solubility of 200mM and minimum solubility in phosphate buffered saline (PBS; pH 7.4) of 200uM (with many fragments soluble at 1mM in PBS). The remaining fragments have DMSO solubility of less than 200mM or PBS solubility of less than 200uM.

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

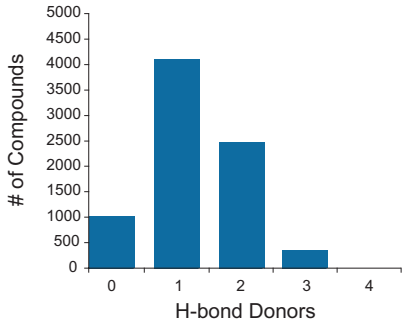
Molecular Weight	225.06
H-donors	1.22
H-acceptors	2.33
cLogP	1.27
Rotatable Bonds	2.01
cLogSw	-1.68
TPSA	49.66

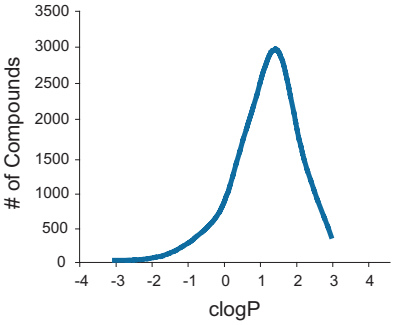
[1] Carr, A.E.; Congreve, M.; Murray, C.; Rees, D.; Fragment-based lead discovery: leads by design, *Drug Discovery Today*, 2005, 10, 987-992

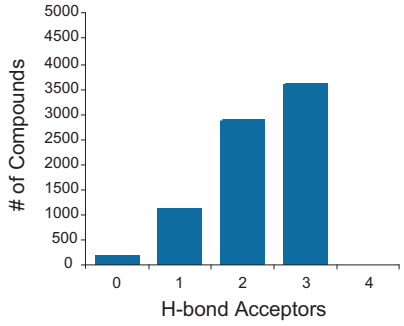
Format

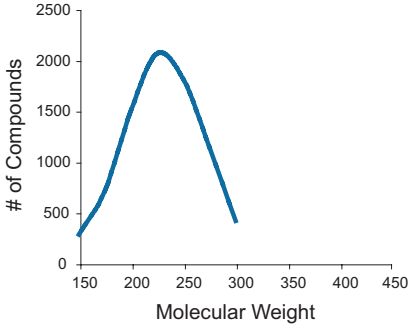
- Download structures and custom select from more than 5,000 Fragment Library compounds.
- Compounds are available in mg or umol amounts undissolved (mostly powders, some oils), as DMSO solutions in standard or deuterated DMSO or as dry film and formatted to your requirements.
- All compounds have a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

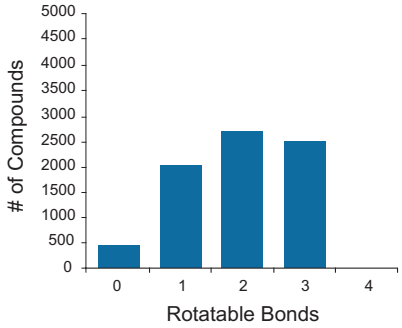
Physiochemical Properties

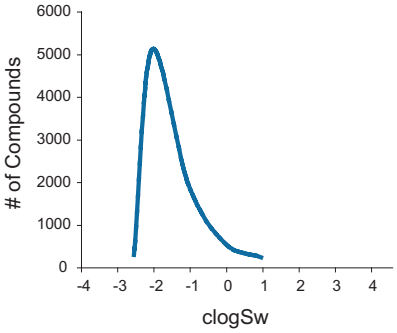


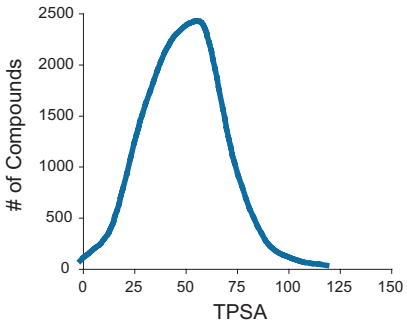












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