

BioBlocks Comprehensive Fragment Library

San Diego, CA, 01/31/2020

BioBlocks Comprehensive Fragment Library (CFL) is now available for Drug Discovery collaborations. BioBlocks' fragment library design was aided by our team's deep expertise in medicinal chemistry and meets very strict property criteria, making it suitable for the discovery of high quality leads. Plate 1 and Plate 2 contain compounds selected from millions of candidates for their unique combination of 3D core shapes, hydrogen patterns, solubility, and synthetic versatility.

The set provides low flexibility, low molecular weight starting points with key hydrogen bond patterns for fragment-based lead discovery (FBLD) and serves as a starting point for our Leap-to-Lead™ discovery platform. For each hit structure, a set of >1000 related 3D analogs can be generated for hit follow up, and >95% of the fragments contain handles for straightforward synthetic elaboration.

Features

- Designed using first principles to be less biased towards known targets
- Selected for diverse chemotypes, shapes, and 3D motifs
- Inclusion criteria more stringent than the rule-of-three
- Designed for limited flexibility and compact interactions with target sites
- Highly soluble (>100mM in 100% DMSO)

Screening results

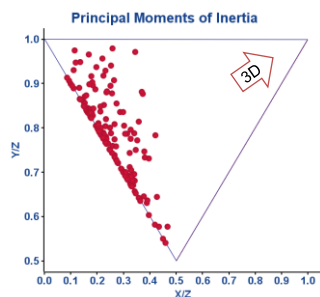
- **Hits for a diverse set of target classes**
- Hit rates typically ~5%
- Potencies for hit compounds typically range from 100-4,000 μ M

Applications

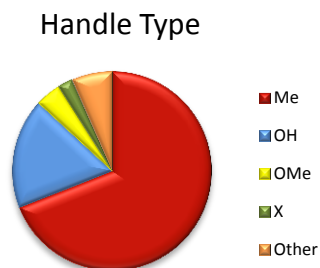
- Starting point for our Leap-to-Lead™ discovery platform
- Screened by BioBlocks and our collaborators:
 - High-concentration biochemical screens
 - SPR
 - TSA
- Screening planned for 2020 by BioBlocks and our collaborators:
 - NMR
 - MST
 - X-ray follow up
- Core shapes distributed to permit X-ray crystallography multiplexing

Property Summary	CFL Plates	CFL Design Goals	Typical Commercial
# Fragments	170	500	1700 - 30000
MW	166	175	170 - 270
AlogP	0.8	0.8	1.3 - 1.8
H Donors	0.9	1.1	≥ 1
H Acceptors	2.1	2.5	2 - 4
Rotatable Bonds	0.6	0.5	2 - 3
Unique Rings	75	100	
HBond Patterns	103	250	
% 3D	61	80	
% Commercial	54	30	
% Handles	99	98	

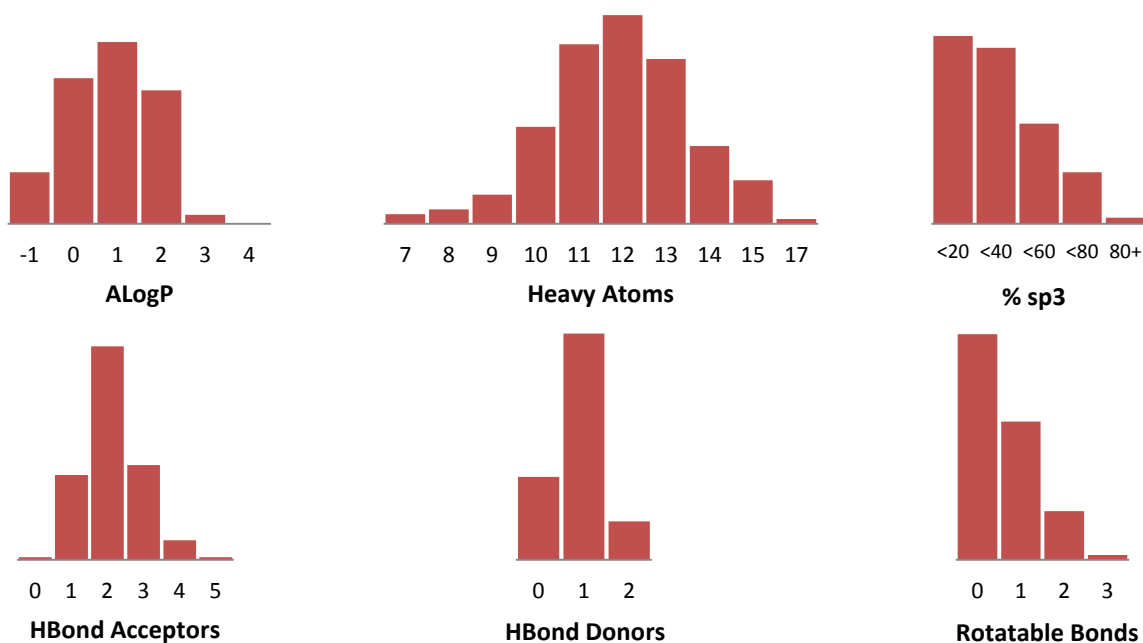
3D Distribution



Handle Distribution



Property Distributions



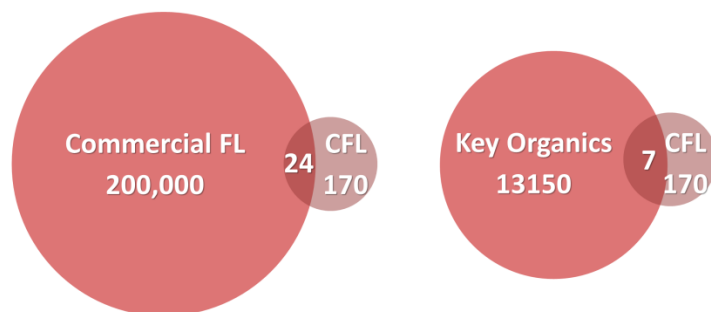
Library Format

- Solutions in DMSO arranged arrayed by mutual agreement
- Typical sample is 2-4 mg compound dissolved in 0.2 mL DMSO (200 mM solution)

Library Novelty

[Independent expert evaluation](#) shows minimal overlap with other fragment libraries:

Unique Commercial Fragments Largest Overlap



Further information is available at <http://www.bioblocks.com/l2loverview/#comprehensive-fragment-library>, by email at info@bioblocks.com or by phone 858-558-5900.