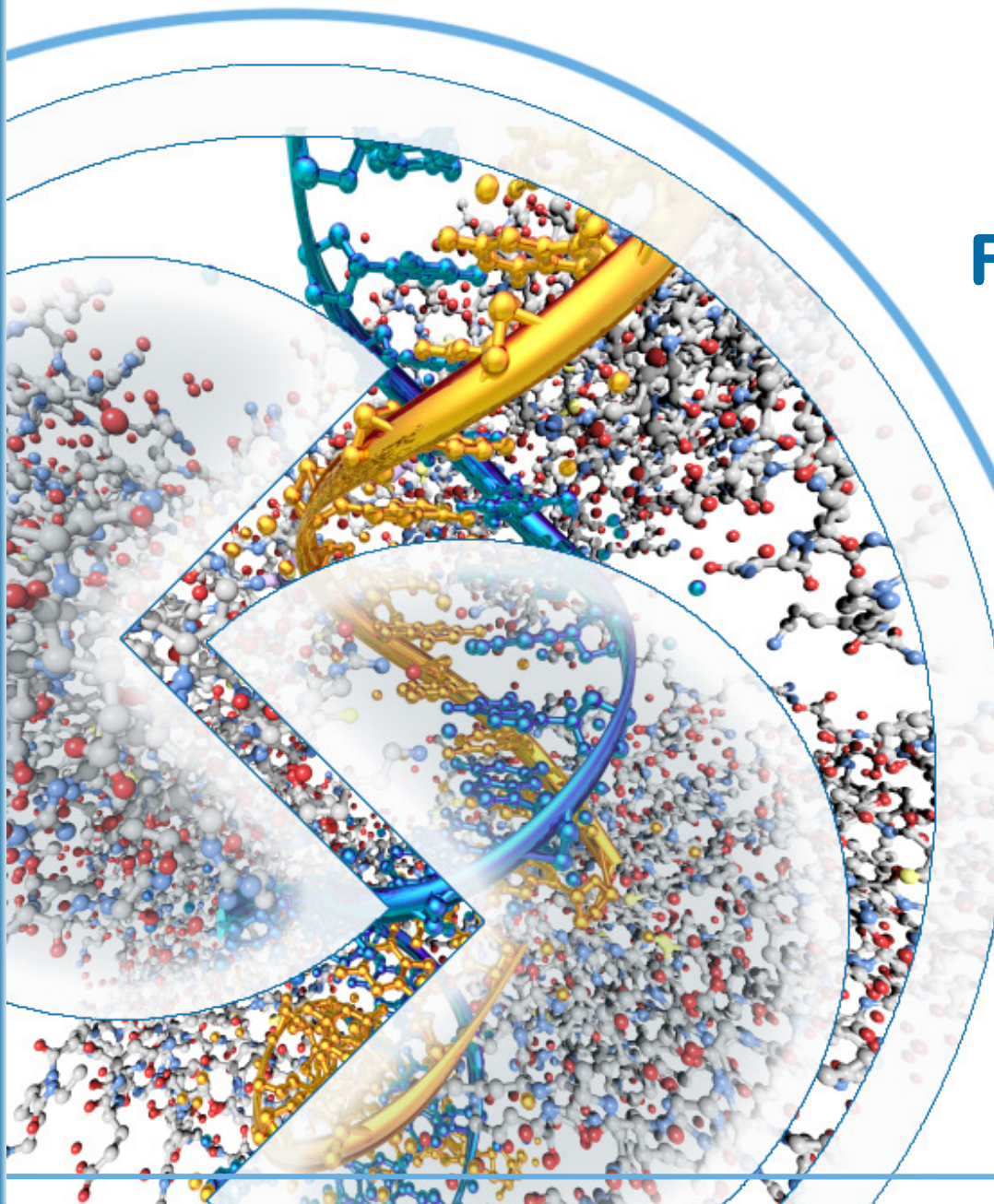


Fragment Library for Fragment-Based Lead Discovery (FBDD)



6605 Nancy Ridge Drive, San Diego, CA 92121
Tel.: 858-794-4860, Fax: 858-794-4931
E-mail: chemdiv@chemdiv.com

ChemDiv Fragment Library

Key Features:

- *Consists of more than 15,700 fragments;*
- *The most recent update – more than 7,300 fragments;*
- *More than 6,400 fragments meet strict Astex Rule of Three criteria [1] (MW ≤ 300, cLogP ≤ 3, H-bond donors ≤ 3, H-bond acceptors ≤ 3)**
- *Assured chemical diversity (diversity coefficient 0.87)*

**Note: The authors of Ro3 have agreed that the latter two criteria are questionable and have not been widely adopted [2]. Therefore, we at ChemDiv use softened filters H-bond donors ≤ 7 and H-bond acceptors ≤ 7 for Fragment Library.*

References:

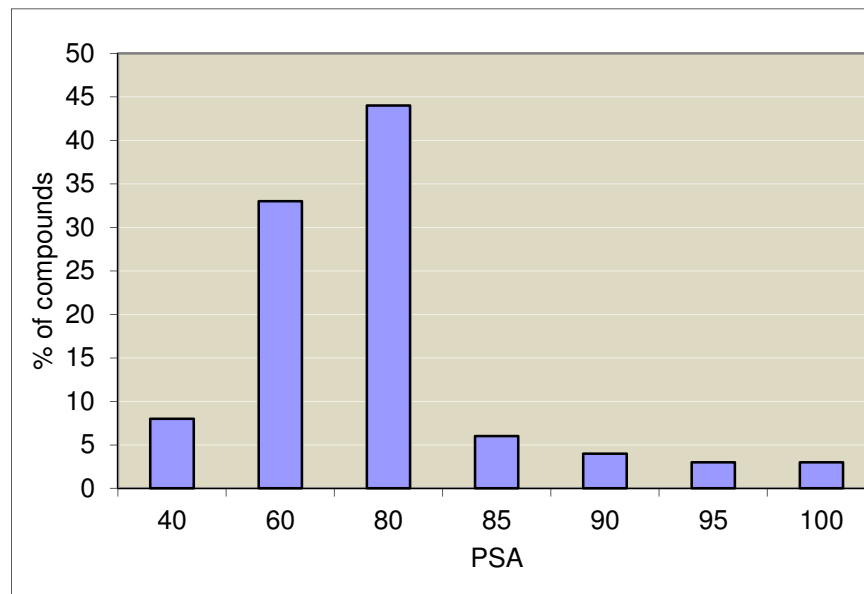
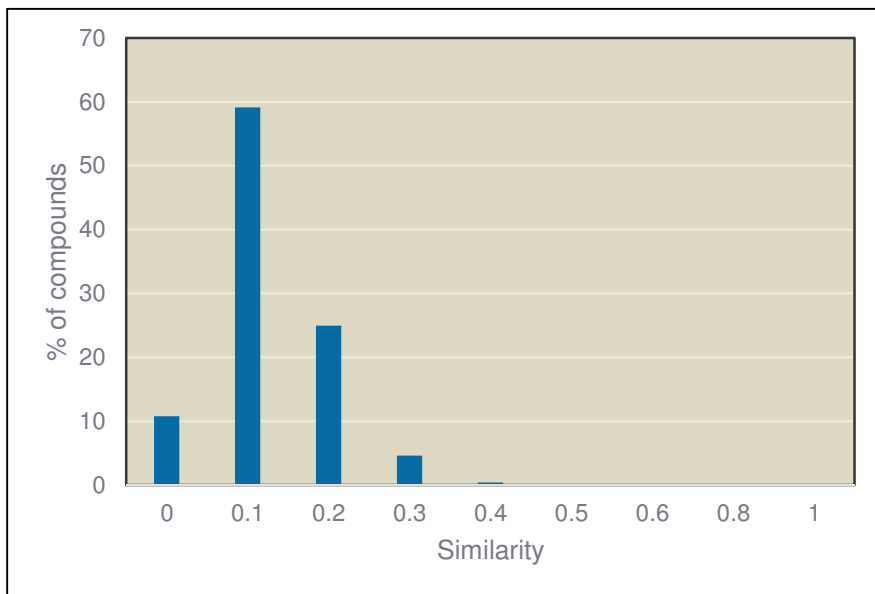
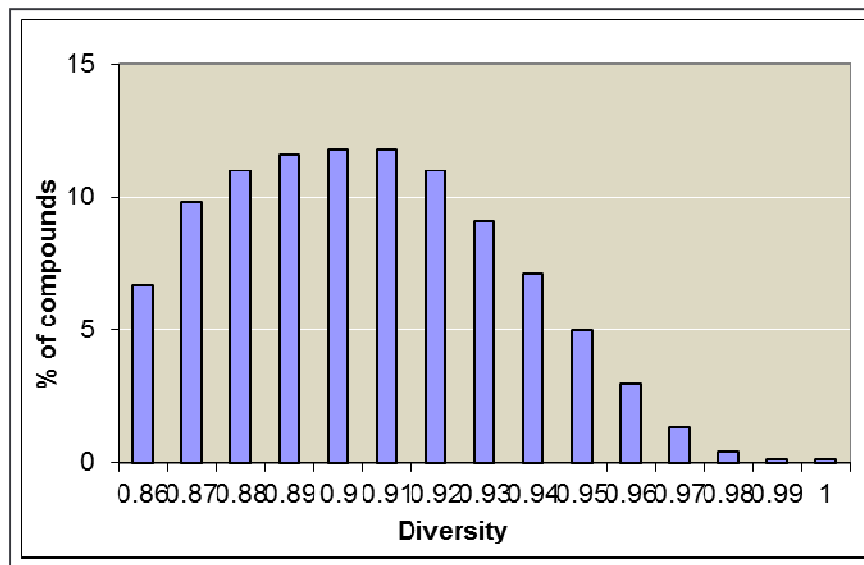
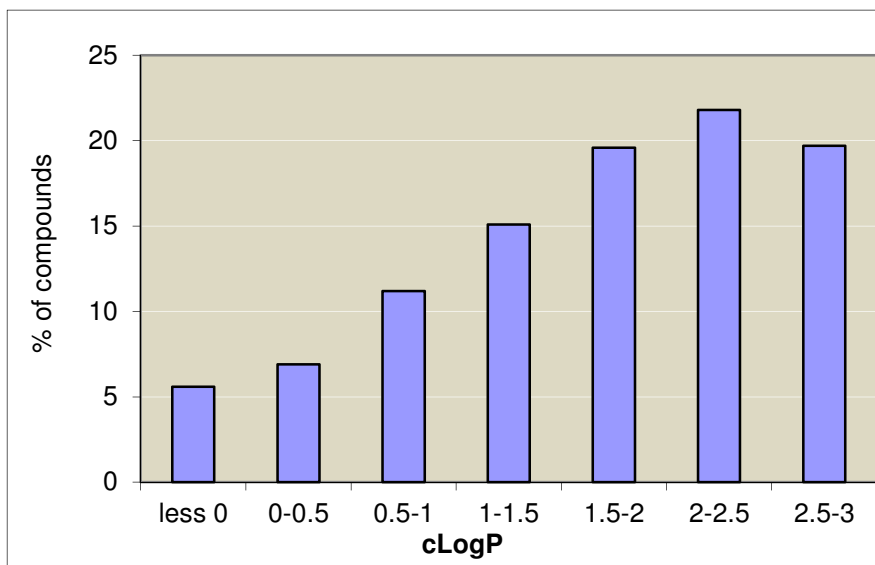
- [1] Congreve, M., Carr, R., Murray, C., Jhoti, H. A 'Rule of Three' for fragment-based lead discovery. *Drug Discov. Today* **8**, 876–877 (2003).
- [2] Jhoti, H.; Williams G.; Rees D.C.; Murray C.W. The 'rule of three' for fragment-based drug discovery: where are we now? *Nat. Rev. Drug Discov.* **12**(8), 644-5 (2013).

Fragment Library

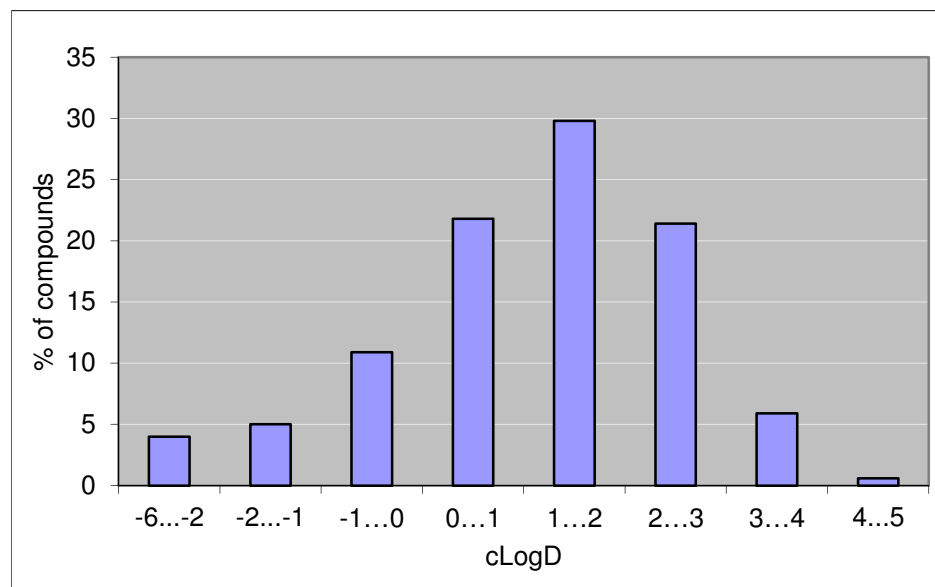
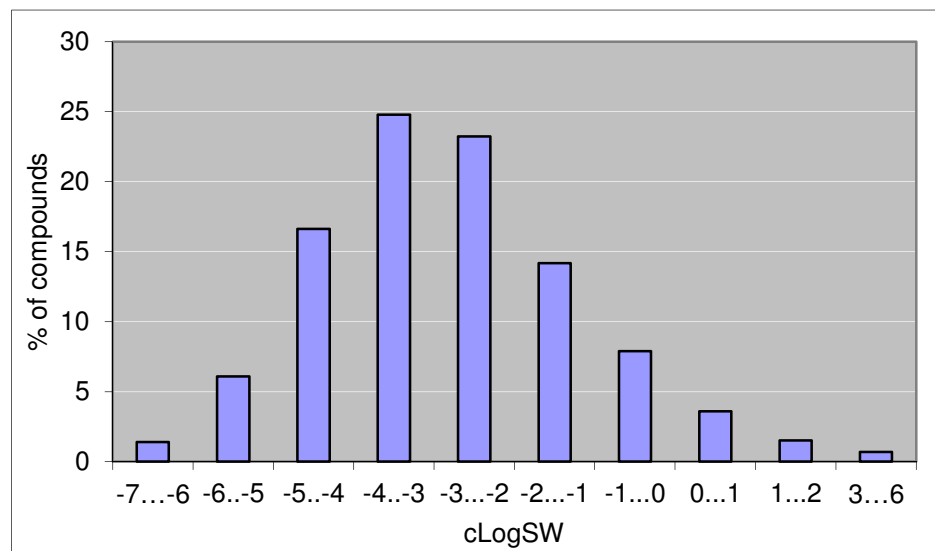
Library Members Properties:

Parameter	Range	Average
MW	96...300	253
cLogP	-2.7...3.0	1.7
NRB	0...3	1.5
HBA	0...7	3.6
HBD	0...6	1.0
PSA	3.2...109	62
cLogD (pH 7.4)	-8.0...7.2	1.6
cLogSW (pH 7.4)	-7.4...5.64	-2.4

Key parameters distribution for Fragment Library



Key parameters distribution for Fragment Library



ChemDiv Fragment Library

Further Information

- *We provide structure data file (MDL sdf or db) or SMILE upon request;*
- *You can choose entire library or set of selected of fragment compounds; we will be happy to assist you with selection (e.g. by applying custom filters, by core diversity etc,);*
- *All fragments are available in ≥ 1 mg quantities and can be delivered as custom weighted dry powders or as solutions in DMSO. Custom formatting is available;*
- *We provide analytical data with all orders.*

**Thank you for considering ChemDiv
Fragment Library!**