

**Библиотеки, содержащие
фармакофорные
фрагменты**

**Fragment Library for
Fragment-Based Lead
Discovery (FBDD)**

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] ($MW \leq 300$, $cLogP \leq 3$, $H\text{-bond donors} \leq 3$, $H\text{-bond acceptors} \leq 3$)***
- **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 $H\text{-bond donors} \leq 7$ and $H\text{-bond acceptors} \leq 7$ 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).

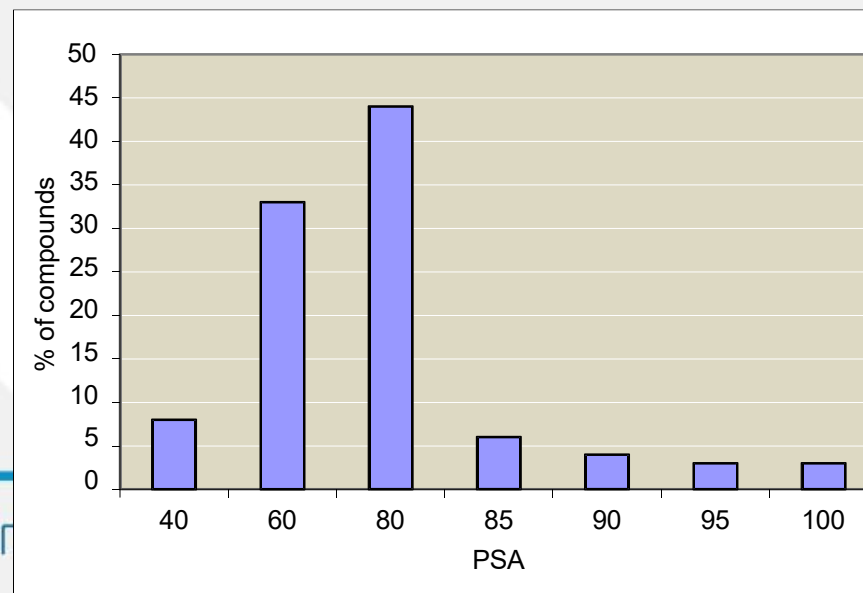
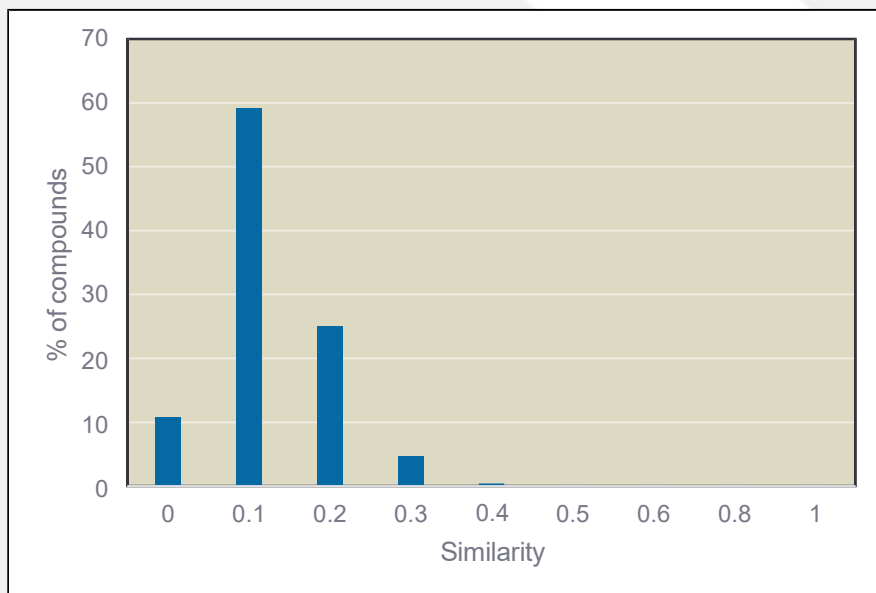
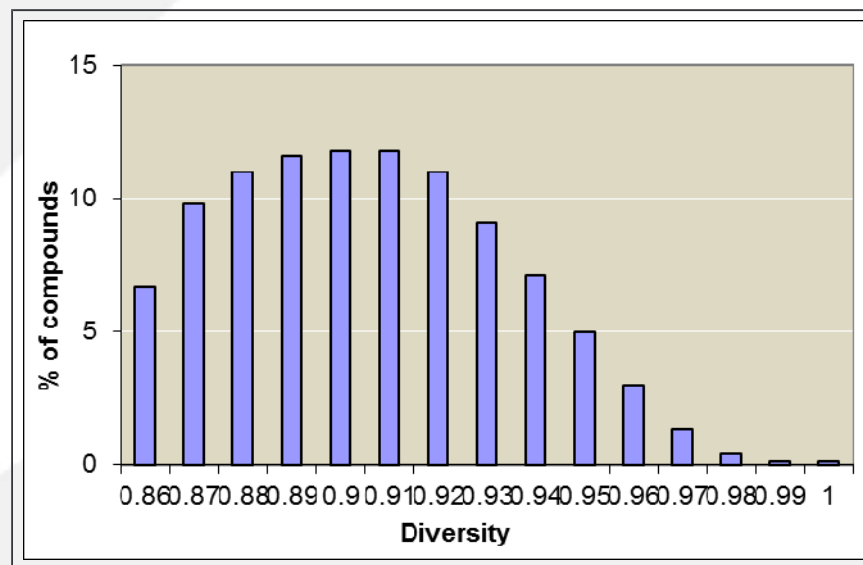
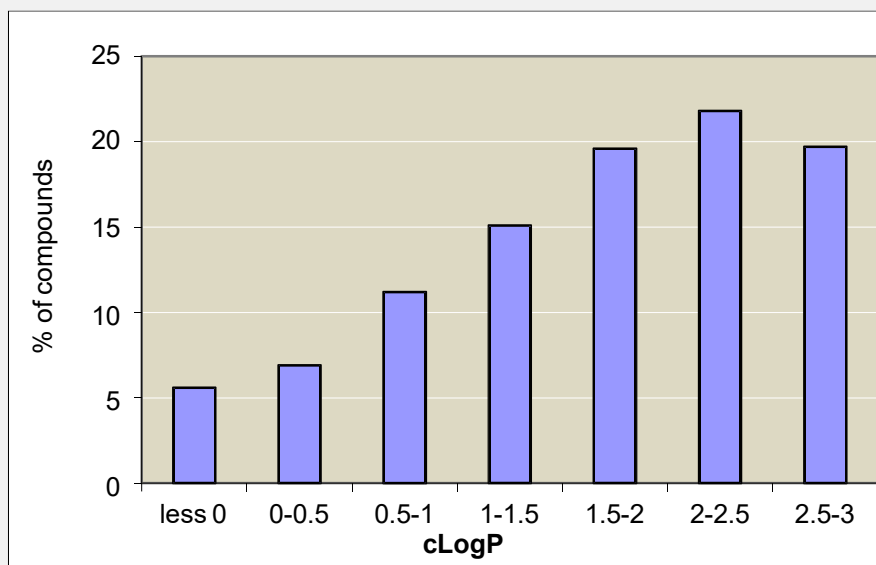
2 Jhoti, H.; Williams G.; Rees D.C.; Murray C.W. The 'rule of three' for fragment-based drug discovery: where are we now? *Nat. Rev. Drug Discov.* 12(8), 644-5 (2013).

Fragment Library

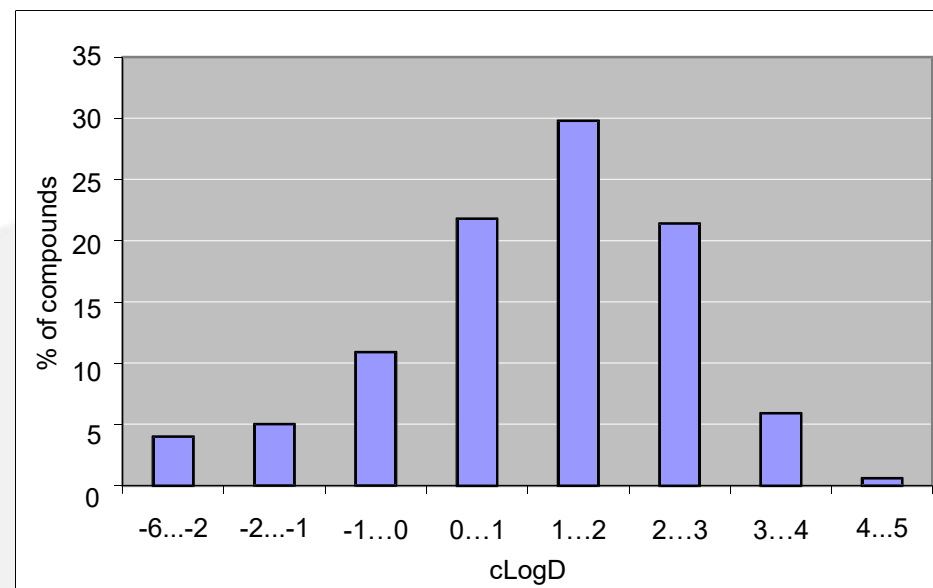
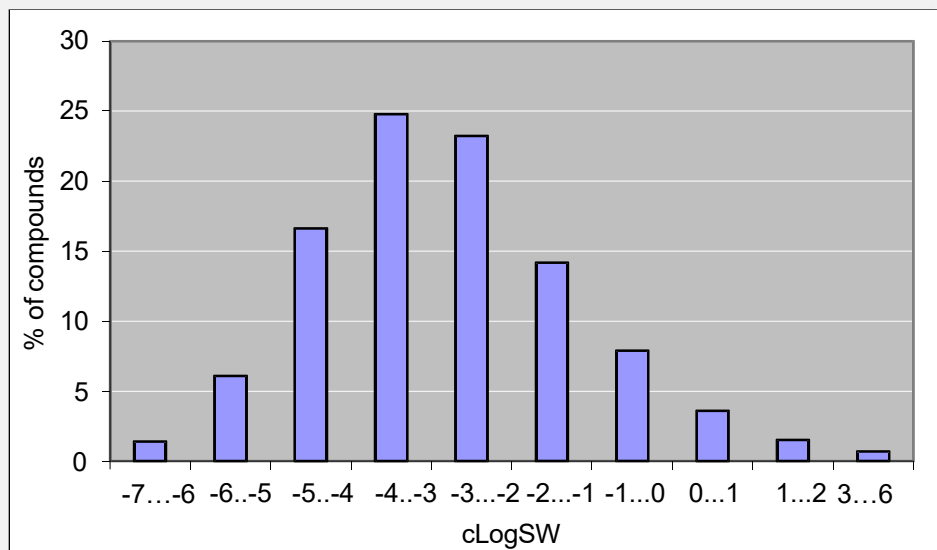
Library Members Properties:

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



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.*



Благодарим за внимание

Инструкция по заказу соединений из библиотеки «ХимРар»:

Наш сайт: <https://chemrar.ru/library-full-list/>

Направьте список интересующих соединений на email: vvk@chemrar.ru

В соответствии с вашим запросом менеджер выполнит подборку соединений и направит информацию о наличии. Имеется возможность сделать поиск по структуре/буквенному идентификатору (ID, CAS, MFCD), а также импортировать файл в различных форматах: SMILE, sdf, txt.