TargetMol®

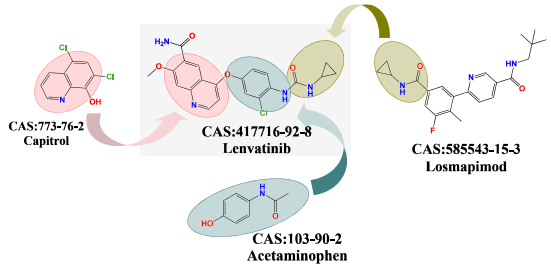
A DRUG SCREENING EXPERT

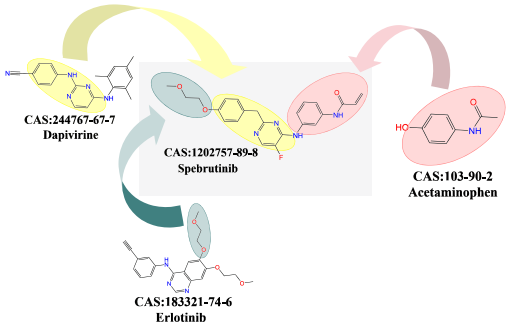
Drug-Fragment Library-Cat.No.L8800

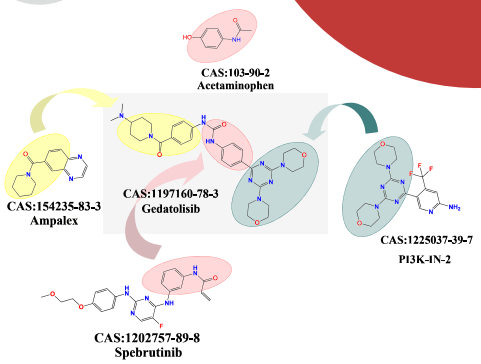
In recent years, Fragment-Based Drug Discovery (FBDD) has received a lot of attention from pharmaceutical researchers. Three marketed drugs (Vemurafenib, Venetoclax and Erdafitinib) and more than 30 clinical phase drugs have been successfully produced using the FBDD method. This demonstrates the promising application of this technology.

Fragment structures of one drug can appear in other drugs, there is a clear structure-activity relationship (SAR) between the structure of these fragments and drug properties. Using these fragment molecules to perform FBDD screening can increase the probability of Hits attainment, resulting in a subsequent structural development that is more likely to generate small molecules with desirable ADMET properties.

A fragment library with high quality can improve the hit rate of FBDD screening and hence increase the success rate of drug screening. Through structural analysis and screening of 2342 marketed drugs and 1487 clinical phase drugs, TargetMol® has constructed a Drug-Fragment Library consisting of 1159 fragments.



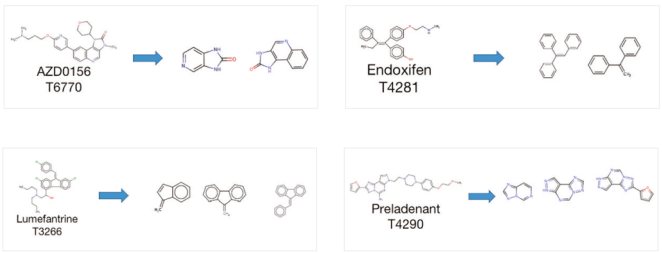




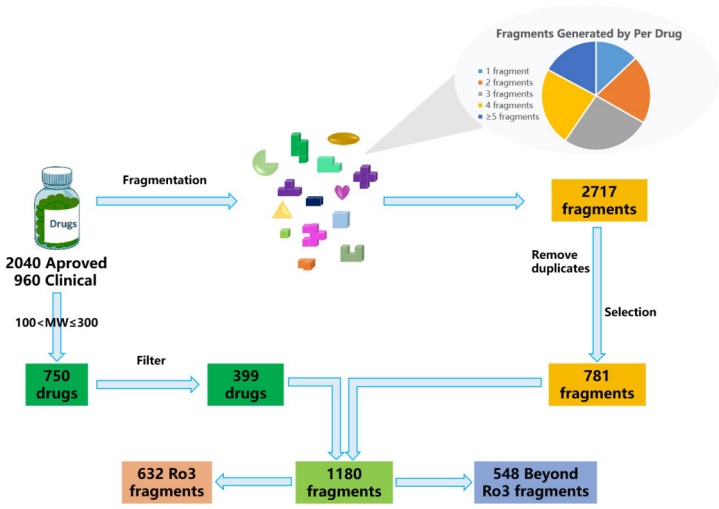
Principles of Drug Fragmentation

All fragments must follow these principles:

1. Can bind to a target;
2. Can be chemically synthesized;
3. Have chemical structures that can be extended.



Designing a Drug-Fragment Library



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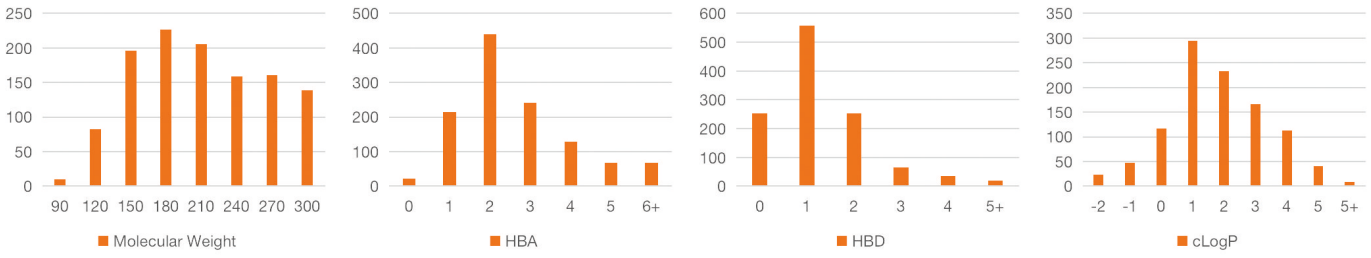
III Physicochemical Properties

The Drug-Fragment Library has good physicochemical properties, reasonable distribution of molecular weight and cLogP. More than 53% of the compounds are fully compliant with the Ro3 principle.

The compounds that do not fully comply with the Ro3 guidelines provided a greater diversity of drug-fragment structures for researchers, increasing the probability of successful drug screenings.



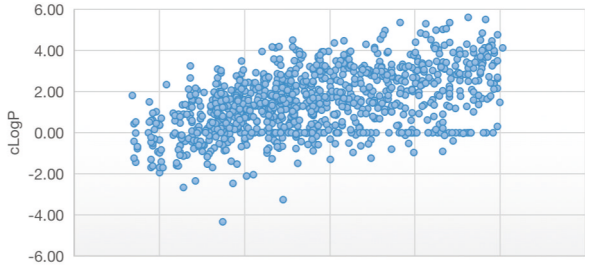
Parameter	Range	Average
MW	84—301	195
HBA	0—10	2.6
HBD	0—7	1.3
cLogP	-4.3—5.6	1.2
Rot. Bond	0—10	2.1
PSA	0—172	48.6

Ro3 Fragments

Parameter	Range	Average
MW	84—298	164.7
HBA	0—3	2.0
HBD	0—3	1.0
cLogP	-4.3—3	1.0
Rot. Bond	0—3	1.1
PSA	0—93	37.9

Beyond Ro3 Fragments

Parameter	Range	Average
MW	110—301	230
HBA	0—10	3.4
HBD	0—7	1.6
cLogP	-3.5—5.6	1.4
Rot. Bond	0—10	3.3
PSA	0—172	61



IV Summary

Through structural analysis and screening of 2342 marketed drugs and 1487 clinical phase drugs, TargetMol® has constructed a Drug-Fragment Library consisting of 1159 fragments.

V Product Features

- Quantity: 1159 drug fragments, which are essential tools for new drug screening by FBDD method.
- Pharmacochemical properties: more than 53% of the fragments meet the Ro3 principle, and all the fragments can be identified with corresponding drugs and have a better potential for drug discovery.
- Quality assurance: NMR, HPLC/LCMS, and other detection techniques to ensure correct structure and high purity.
- Versatility: Suitable for SPR, NMR, Single crystal X-ray diffraction and other assays in drug development.

Targetmol Chemicals Inc.

— Drug Screening Expert (Inhibitors, Natural Products, Compound Libraries)