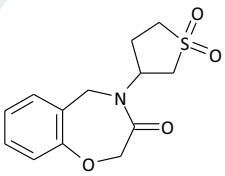
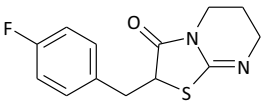
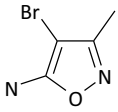
Reaxense

Broad Spectrum Fragment Library



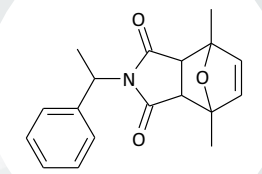


In the past decade, fragment based drug design (FBDD) has risen as a new and effective approach to identify lead compounds and continues to show great promise in drug discovery. It requires the use of sensitive techniques such as X-ray crystallography to identify hits among low molecular weight fragment compounds that have a weak binding affinity to a drug target. The hit fragments could be then structurally optimized to lead compounds with high affinity and specificity.

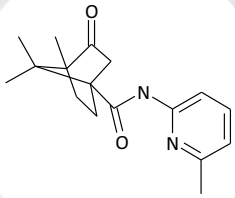


Reaxense's Broad Spectrum Fragment Library is a product of choice for FBDD project of any level. The library contains **1,226 high-quality fragments** selected to meet top industry requirements. It provides an optimal, diverse set of compounds to be included in your next fragment screen.

Features:



- **1,226 small molecule fragments**
- **No pan-assay interference (PAINS) compounds**
- **Compounds with reactive and toxic groups filtered out**
- **High predicted water solubility (LogS > -5)**
- **High diversity over the library**
- **Each fragment contains at least 1 aromatic or aliphatic ring**
- **Purity >90%; spectral data available**



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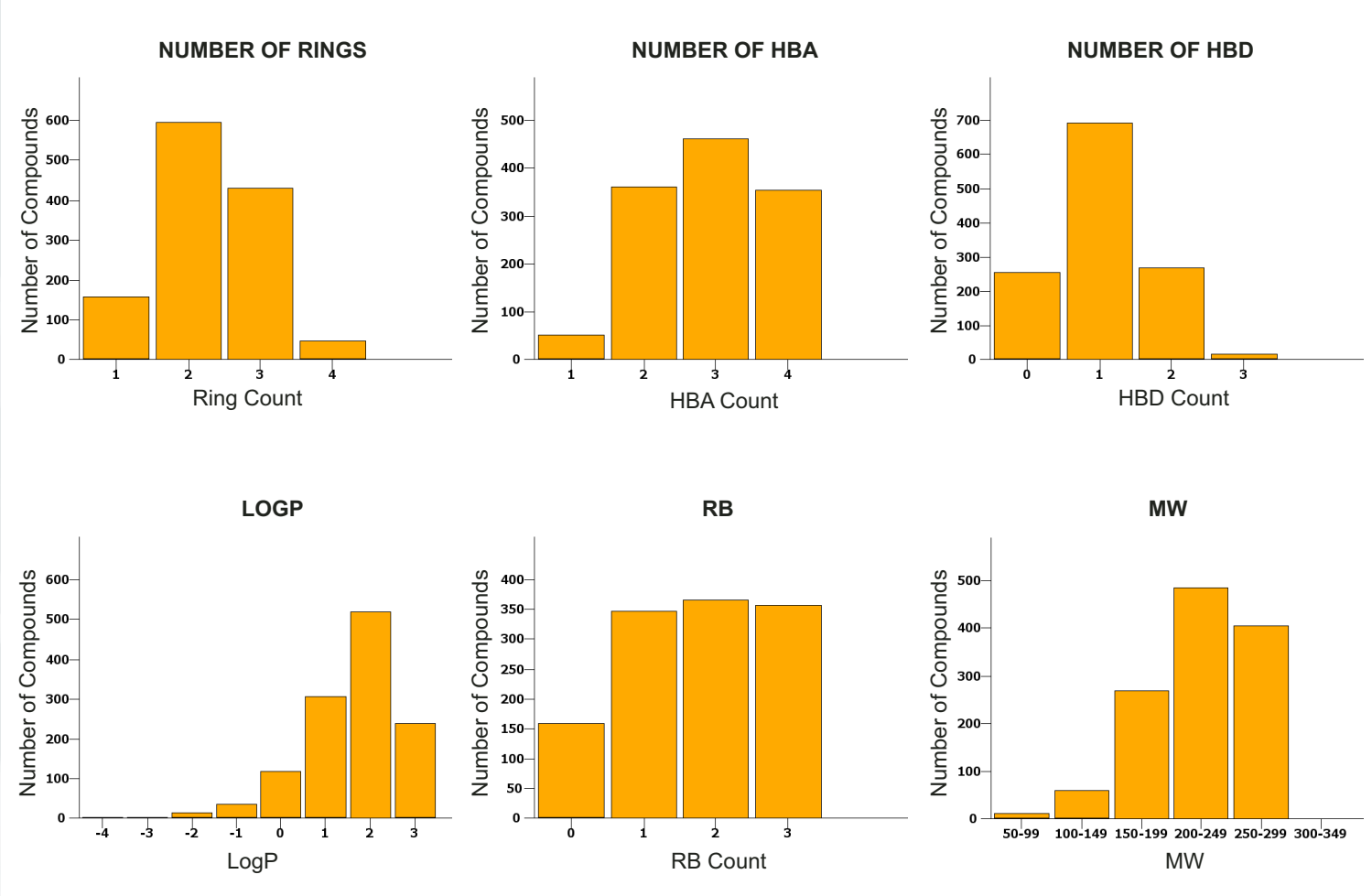
REAXENSE

Selection Criteria:

Parameter	Value
Molecular Weight (MW)	≤ 300
Number of Hydrogen Bond Donors (HBD)	≤ 3
Number of Hydrogen Bond Acceptors (HBA)	≤ 4
Octanol/Water Partition Coefficient (LogP)	≤ 3
Number of Rotatable Bonds (RB)	≤ 3
Topological Polar Surface Area (TPSA)	≤ 80 Å^2
Predicted Water Solubility (LogS)	> -5
Number of Rings	1 - 4
Sum of Halogen Atoms	≤ 4

Properties Distribution:



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