Reaxense

Natural Fragment Library

Natural products have contributed to the development of many drugs for diverse indications and they continue to be an important source of leads for new medicines, despite reduced interest from large pharmaceutical companies. The development of new technologies including fragment-based drug discovery (FBDD) has revolutionized the screening of natural products as potential therapeutic agents.

We designed our **Natural Fragment Library** to fulfill the need of natural compound-like fragments in FBDD. The library includes **250 small molecule fragments** which are based on chemical scaffolds similar to those found in natural compounds.

Features:

- **250 natural compound-like fragments**
- **Each fragment is a synthetic derivative of a natural chemical scaffold**
- **No pan-assay interference (PAINS) compounds**
- **Compounds with reactive and toxic groups filtered out**
- **Each fragment contains at least 1 aromatic or aliphatic ring**
- **High diversity over the library**
- **Purity >90%; spectral data available**

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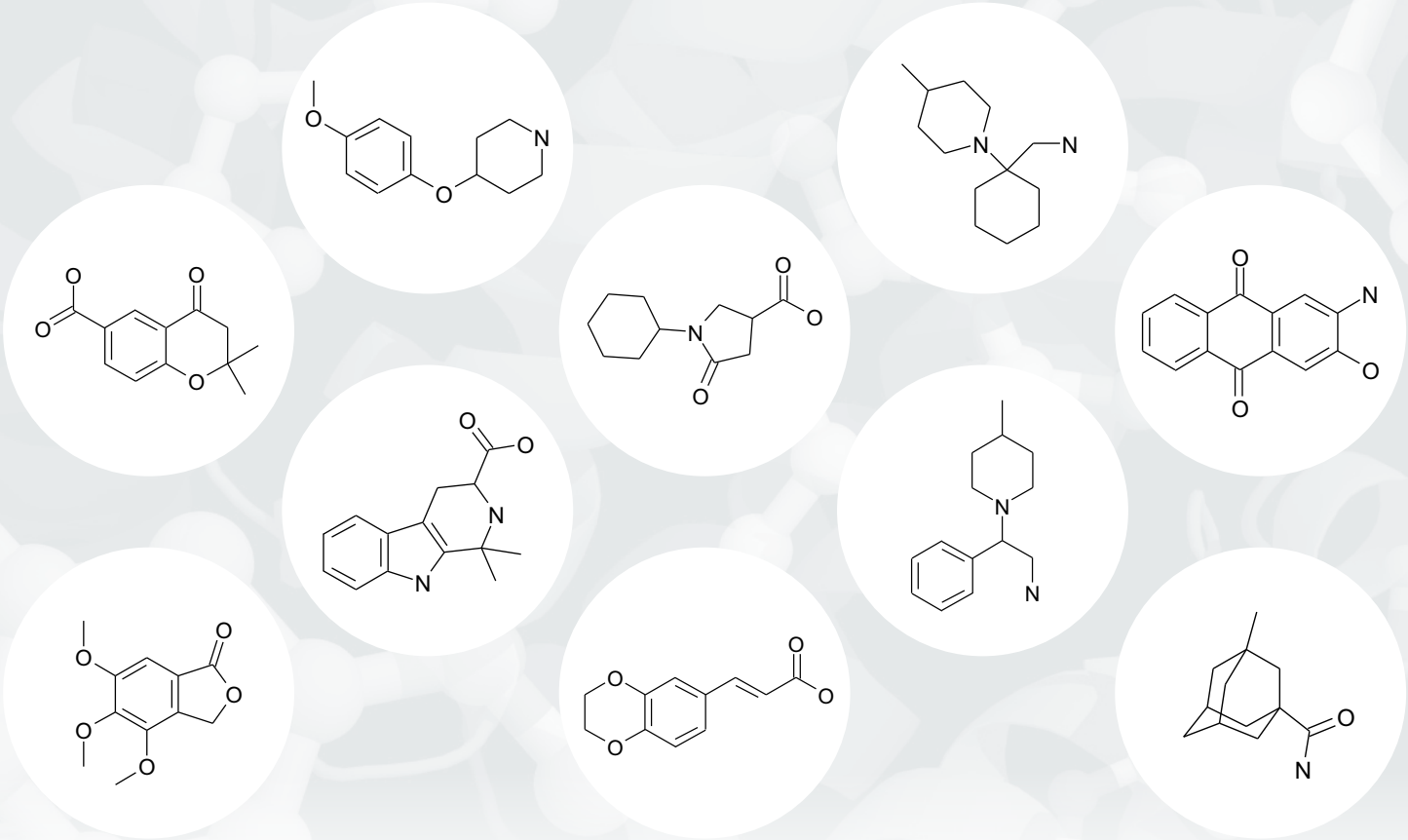
Selection Criteria:

Parameter	Value
Number of Heavy Atoms	5 - 18
Number of Hydrogen Bond Donors (HBD)	≤ 3
Number of Hydrogen Bond Acceptors (HBA)	≤ 6
Octanol/Water Partition Coefficient (LogP)	≤ 2.5
Number of Rotatable Bonds (RB)	≤ 3
Topological Polar Surface Area (TPSA)	≤ 90 $Å^2$
Distribution Coefficient at pH = 7.4 (logD)	≤ 2.5
Number of Rings	≤ 3

Structure examples:



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