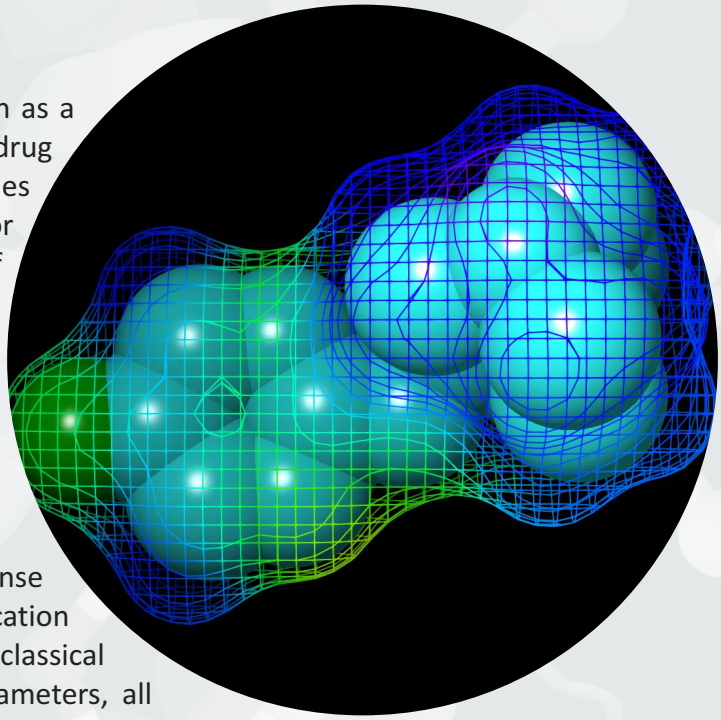
Reaxense

Halogen-Enriched Fragment Library



Recently, halogen bonds have gained increased recognition as a useful molecular interaction in the life sciences and drug discovery. However, despite the potential of halogen moieties to positively affect ligand binding, standard libraries for fragment-based screening display very low number of compounds containing heavy halides. Halogen-enriched fragment libraries (HEFLibs) consist of chemical probes that allow to identify halogen bonds as one of the main features of the protein-ligand binding mode. Besides that, these fragment libraries provide smart starting points for hit-to-lead evolution.

Halogen-Enriched Fragment Library available from Reaxense consists of **2,659 fragment molecules** facilitating the identification of favourable halogen bonds by sharing the advantages of classical fragment-based screening. Selected by modified Ro3 parameters, all compounds in this library contain at least one atom of halogen.

Features:

- **2,659 halogen-containing fragments**
- **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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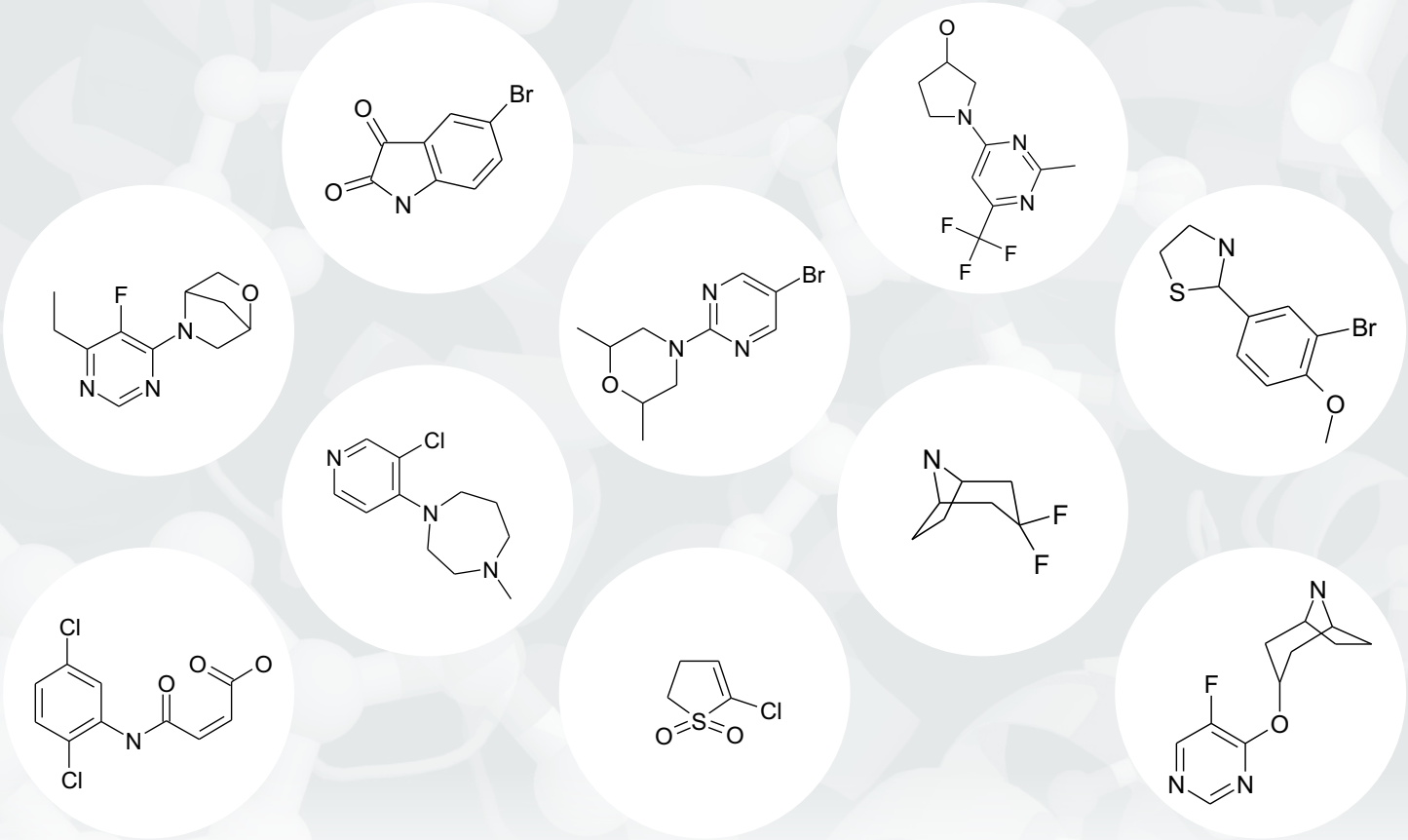
Selection Criteria:

Parameter	Value
Heavy Atom Count (HAC)	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	1 - 3
Number of Halogen Atoms	> 0

Structure examples:



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