Reaxense

CNS Compound Library

Fundamental physico-chemical features required for optimal brain exposure of successful CNS drugs have been extensively studied in an attempt to define the attributes related to their ability to penetrate the blood-brain barrier (BBB) and exhibit CNS activity. On the other hand, BBB penetration may be a liability for many of the non-CNS drug targets, and a clear understanding of the physicochemical and structural differences between CNS and non-CNS drugs may assist both research areas.

Reaxense has designed its **CNS Compound Library** **(6,492 molecules)** applying both the hard cutoffs crucial for CNS-related drugs as well as prospective alignment of drug-like attributes such as high permeability, low P-gp efflux liability, low metabolic clearance, and high safety for each molecule.

Features:

- **6,492 drug-like molecules with predicted BBB permeability**
- **Each compound has high CNS Multiparameter Optimization score**
- **No pan-assay interference (PAINS) compounds**
- **Compounds with reactive and toxic groups filtered out**
- **High diversity over the library**
- **Purity >90%; spectral data available**

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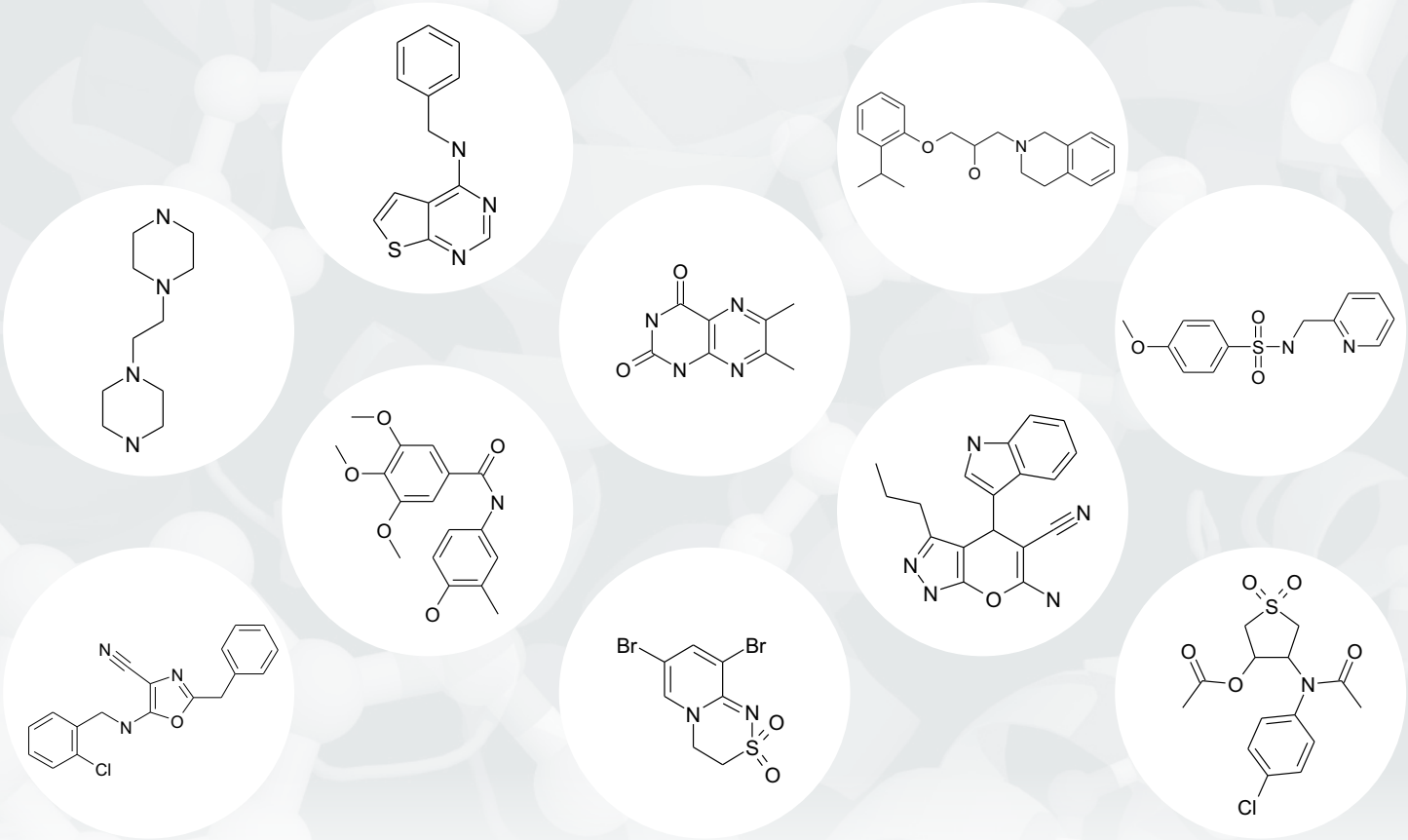
REAXENSE

Selection Criteria:

Parameter	Value
Number of Sulphur (S) Atoms	≤ 1
Number of Amide Groups	≤ 1
Number of Hydrogen Bond Acceptors (HBA)	≤ 6
Number of Rotatable Bonds (RB)	≤ 8
Number of COOH Groups	0
CNS Multiparameter Optimization (CNS MPO)*	≥ 4

*Using a set of six physicochemical parameters (ClogP, ClogD, MW, TPSA, HBD, pK_a), the novel CNS MPO algorithm showed that 74% of marketed CNS drugs displayed a high CNS MPO score (MPO desirability score ≥ 4, using a scale of 0-6) (*ACS Chem. Neurosci.* **2010,** 1, 6, 435-449)

Structure examples:



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