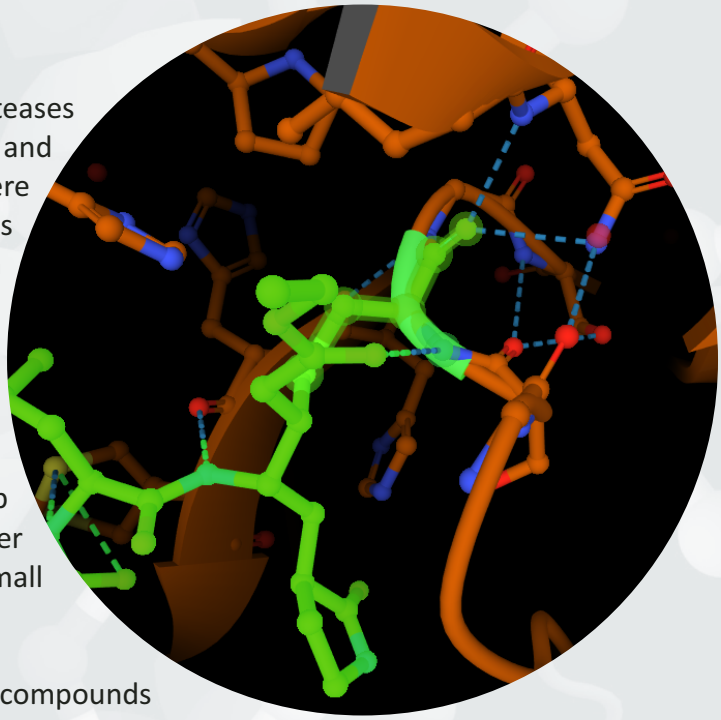
Reaxense

Covalent Inhibitors Library



Covalent inhibitors targeting enzymes such as kinases or proteases for a long time were set aside due to the high reactivity and potential toxicity. However, covalent kinase inhibitors were recently successfully introduced as cancer therapeutics agents. Thus, the benefits of irreversible kinase inhibition appeared to surpass the potential risks of such drugs. Traditionally, the most targeted residue in the protein kinase active site is cysteine. Due to the low abundance of this residue, drugs targeting cysteine appear to be more selective and have a lower chance of appearing to be toxic. All covalent enzyme inhibitors must contain specific reactive group (covalent "warhead"), and alternatively to cysteine, other amino acid residues were proposed as targets for reactive small molecules as well.

We designed our **Covalent Inhibitors Library** to comprise compounds with reactive covalent groups targeting Cys, Ser and Lys residues. There are **12,247 potentially biologically active molecules** in the library. For each molecule, the amino acid residue it targets is indicated.

Features:

- **12,247 compounds in total**
- **At least one covalent group targeting Cys, Ser, or Lys residues**
- **High diversity over the library**
- **Purity >90%; spectral data available**
- **Lipinski's rule of five compliant (one restriction can be violated)**

5000 Yonge Street, Suite 1901
Toronto, Ontario
M2N 7E9
CANADA

Email: rxinfo@reaxense.com
Phone: +1-855-745-5570
Fax: +1-866-608-0550
www.reaxense.com

REAXENSE

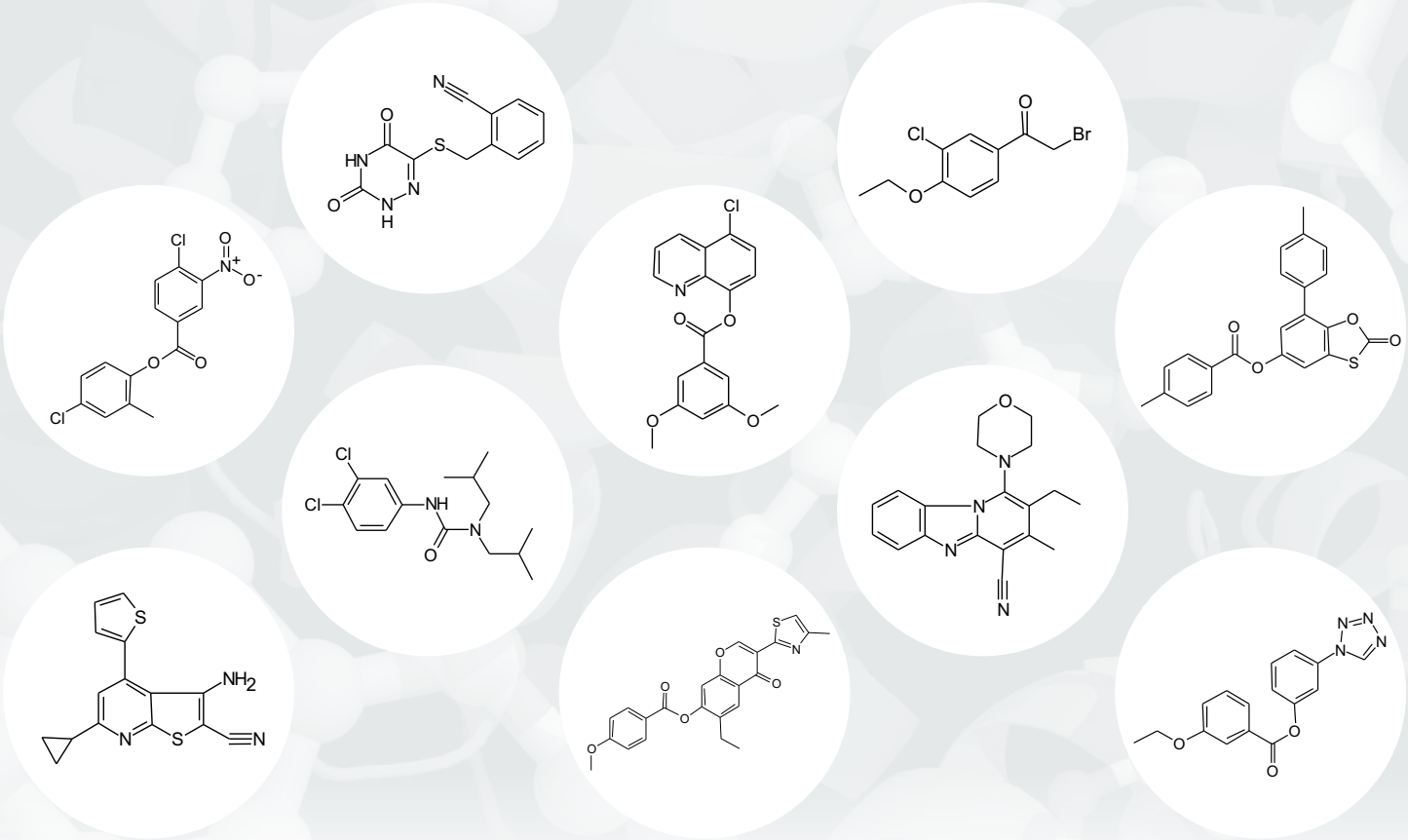
Selection Criteria:

Parameter	Value
Number of Hydrogen Bond Acceptors (HBA)*	≤ 10
Number of Hydrogen Bond Donors (HBD)*	≤ 5
Number of Rotatable Bonds (RB)	≤ 10
Topological Polar Surface Area (TPSA)	<140
Molecular Weight (MW)*	≤ 500
Octanol-water Partition Coefficient (cLogP)*	≤ 5

The library contains compounds with **acrylamide, phenyl nicotinate, aromatic nitrile, sulfonyl fluoride, carbamate** and other covalent groups.

*One of these criteria can be violated

Structure examples:



5000 Yonge Street, Suite 1901
Toronto, Ontario
M2N 7E9
CANADA

Email: rxinfo@reaxense.com
Phone: +1-855-745-5570
Fax: +1-866-608-0550
www.reaxense.com

REAXENSE