TARGETED & FOCUSED Libraries

Overview

ChemBridge offers small molecule sets targeted or focused towards specific targets or applications. These include kinase, GPCR, ion channel and nuclear receptor targeted sets, macrocycles for protein-protein interaction inhibition and other difficult targets, and CNS focused sets enhanced for higher probability of penetrating the blood brain barrier. Clients can custom select/cherry-pick compounds from any of the sets.

Macrocycles

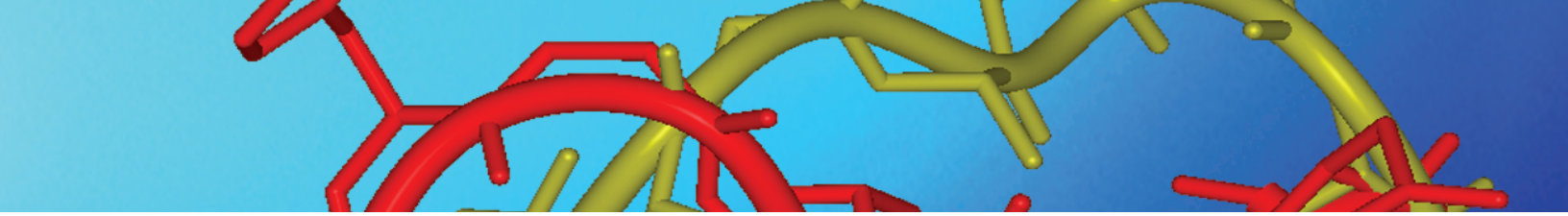
The **Macrocycle Library** is a new library of more than 6,000 macrocyclic compounds. The use of synthetic macrocycles is becoming a well-recognized approach for low druggability targets such as antimicrobial, antiviral, and protein-protein interaction inhibition. ChemBridge chemists have produced a diverse collection of novel synthetic macrocycle scaffolds, some based on natural products. To date we have developed over 70 core macrocyclic scaffolds. Primary ring sizes range from 11 to 27 atoms and MW weight up to 800. Researchers can custom select compounds from the Macrocycle Library or purchase the full set.

CNS

The **CNS-MPO Library** represents high quality, PAINS-free, small molecule compounds for CNS drug discovery. CNS MPO analysis was applied to identify compounds with high probability of blood-brain barrier (BBB) penetration and improved clearance and safety profiles. Custom select from more than 250,000 structures to meet your specific requirements. Structurally diverse hit-finding and lead-like subsets available.

The **CNS-Set Library** is a biased set of more than 50,000 druglike small molecules selected from the EXPRESS-Pick Collection stock using physicochemical property filters including the Lipinski Rules of Five, PSA (polar surface area) and other filters that increase probability of BBB (blood-brain barrier) penetration and bioavailability.

The **Macrocycle CNS Subset** represents approximately 4,000 macrocycles from the Macrocycle Library with potential application for CNS drug discovery. Extensive conformational analysis was performed to identify low energy macrocyclic conformations with internal hydrogen bonds and adjusted CNS MPO scores were calculated. Macrocycles with CNS MPO 4.0 or higher are included in the subset.



Kinase

The **KINACore™ Library** is a computationally selected library of more than 12,000 small molecules from ChemBridge's CORE Library stock. The KINACore Library is composed of compounds selected using pharmacophores generated from known kinase actives. More than 420 core scaffolds are represented in the KINACore Library.

The **KINASet™ Library** is a computationally selected group of more than 10,000 small molecules from our EXPRESS-Pick Collection stock chosen using a ligand-based pharmacophore search query based on pharmacophores generated from the adenosine portion of ATP. KINASet compounds also exhibit other pharmacophores which may contribute to selectivity towards more specific kinases.

GPCR

The **GPCR Library** contains more than 9,000 scaffold-based compounds designed using a series of GPCR-relevant scaffolds that mimic the beta-turn motif of endogenous peptide ligands. A random selection taken from the entire GPCR Library has been validated against GPCR targets with both agonists and antagonists being identified. GPCR Library compounds are part of ChemBridge's CORE Library stock.

Ion Channel

The **IONCore Library™** is a computationally selected library of more than 6,000 small molecules selected from ChemBridge's CORE Library stock. Compounds were selected using pharmacophores generated from known ion channel actives. More than 320 core scaffolds are represented in the IONCore Library.

The **IONSet Library™** is a computationally selected group of more than 6,000 small molecules selected from our EXPRESS-Pick Collection stock. It contains compounds biased towards ligand-gated (5HT3, GABA, glycine, nAChR and PCP receptors) and voltage-gated (sodium, potassium and calcium) ion-channels. Compounds were selected using published pharmacophore data for active compounds.

Nuclear Receptor

The **NHRCore Library** is a computationally selected library of more than 3,000 small molecules selected from ChemBridge's CORE Library stock. Compounds were selected using pharmacophores generated from known nuclear hormone receptor actives. More than 250 core scaffolds are represented in the NHRCore Library.

 Rev. 20171108