



A CNS FOCUSED SCREENING COLLECTION

CNS-Set™

Introduction

ChemBridge's CNS-Set™ is a collection of 50,000+ druglike, small molecule compounds selected using medicinal chemistry expertise. Computational methods have been applied to select compounds with increased probability of oral bioavailability and blood brain barrier penetration. This collection is designed for researchers focused on diseases of the central nervous system and provides a pre-selected set with physiochemical properties adapted to the requirements of orally available, leadlike, CNS small molecule drugs. The CNS-Set™ is derived from ChemBridge's main stock collection, the EXPRESS-Pick™ Collection of 450,000+ handcrafted compounds.

CNS-Set™ Filters

All compounds are subject to ChemBridge's stringent druglike, chemical group, 2D similarity and other filters. The CNS-Set™ is further filtered to create a subset suitable for CNS applications, with the properties listed below:

Property	CNS-Set™ Final Range	Lipinski Rules
MW	≤ 400	≤ 500
cLogP	≤ 3.6	≤ 5
H-Bond Acceptors	≤ 8	≤ 10
H-Bond Donors	≤ 5	≤ 5
tPSA	≤ 120	
Rotatable Bonds	≤ 5	
LogBB ¹	-3.0 to 1.0	
Caco-2 ²	≥ 25	
MDCK ³	≥ 25	
LogK ^h _{sa} ⁴	-1.5 to 1.2	

Formats

- Download and individually select from the 50,000+ CNS-Set™ library (SDfile and ISIS db files available). Individually selected compounds are available in powder form or dissolved in DMSO.
- Pre-plated DMSO library sets from 10,000 to 20,000 compounds are available.
- CNS-Set™ compounds can be expanded with additional EXPRESS-Pick™ Collections (DIVERSet™, KINASet, Ion Channel Set, MicroFormats™) or in-house diversity libraries such as the NOVACore Library.

Please see reverse side for specific footnotes ►

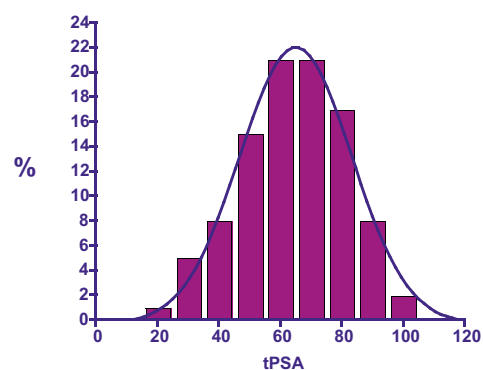
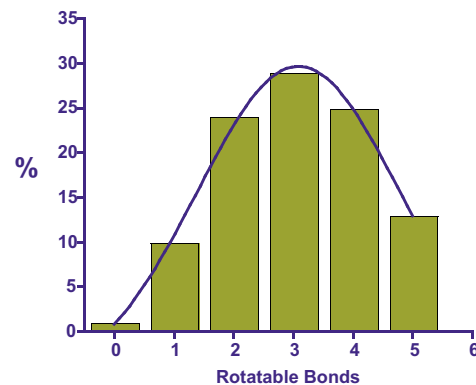
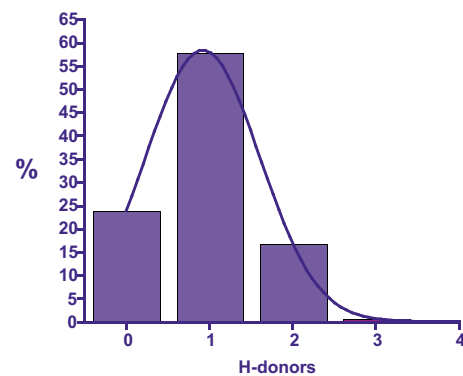
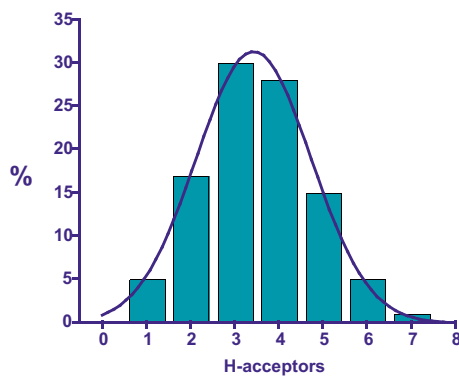
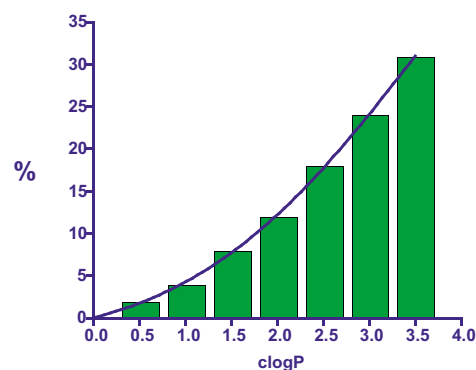
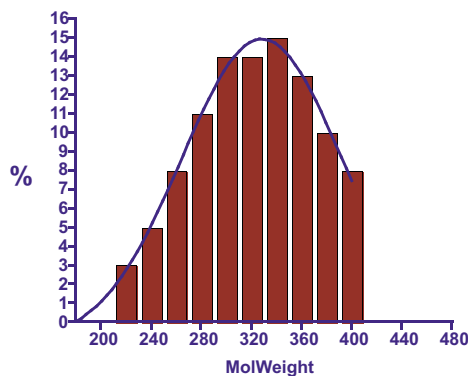
Notes

1. The log [brain]/[blood] (partition coefficient) value was calculated using QikProp* as a predictor of a compound's ability to cross the blood brain barrier (note that QikProp predictions are for orally delivered drugs).
2. The Caco-2 value was calculated using QikProp as a measure of the predicted apparent Caco-2 permeability (nm/sec). Caco-2 cells are used as a model for the gut blood barrier. Determination as early as possible of whether a molecule is transported across the gut is vital in selecting lead compounds. Use of Caco-2 cell monolayers is widely used as *in vivo* human absorption surrogate for transport across the gut blood barrier based on its correlation with human bioavailability data. Acceptable range is values >25, with values > 500 being excellent (note that QikProp predictions are for non-active transport).
3. Predicted MDCK cell permeability in nm/sec calculated using QikProp. MDCK cells are considered to be a good model for transport across the blood brain barrier (note that QikProp predictions are for non-active transport). Acceptable range is values >25, with values > 500 being excellent.
4. The logK_{hsa} is a prediction of binding to human serum albumin and was calculated using QikProp. Binding affinity of molecules to serum protein albumin is an important ADME property. Binding to serum proteins in human plasma is a major determinant of the pharmacodynamic and pharmacokinetic properties of the molecule and can affect systemic distribution of a drug.

* QikProp, version 2.1, Schrödinger, LLC, New York, NY, 2005.

Properties

CNS-SET™ PHYSIOCHEMICAL PROPERTY DISTRIBUTION



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