A CNS FOCUSED SCREENING COLLECTION

CNS-Set™ Library

Introduction

The CNS-Set Library from ChemBridge® is a selection of more than 50,000 druglike, small molecule compounds selected using physiochemical property filters and computational methods to identify compounds with increased probability of blood-brain barrier penetration and oral bioavailability. This CNS-directed library is designed for researchers focused on diseases of the central nervous system and provides a pre-selected collection with physiochemical properties aligned to blood-brain barrier penetration and to the requirements of orally available, leadlike, small molecule drugs. The CNS-Set Library is selected from compounds in ChemBridge's EXPRESS-Pick™ Collection, one of ChemBridge's two, non-overlapping stocks.

CNS-Set Filters

All EXPRESS-Pick Collection compounds are subject to ChemBridge's stringent druglike, chemical group, 2D similarity and other filters. EXPRESS-Pick Collection compounds are then passed through additional filters to create a subset suitable for CNS applications, with the properties listed below:

Property	CNS-Set Final Range	Lipinski Rules
Molecular Weight	≤ 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'hsa[4]	-1.5 to 1.2	

Formats

- Download and individually select from the 50,000+ CNS-Set Library (SDfile available).
- Compounds are available in mg or umol equivalent amounts undissolved (mostly powders, some oils) or dissolved in DMSO and plated to your requirements.
- Compounds dissolved in DMSO can be delivered in 96-well or 384-well format.

Please see reverse side for graphs and 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).

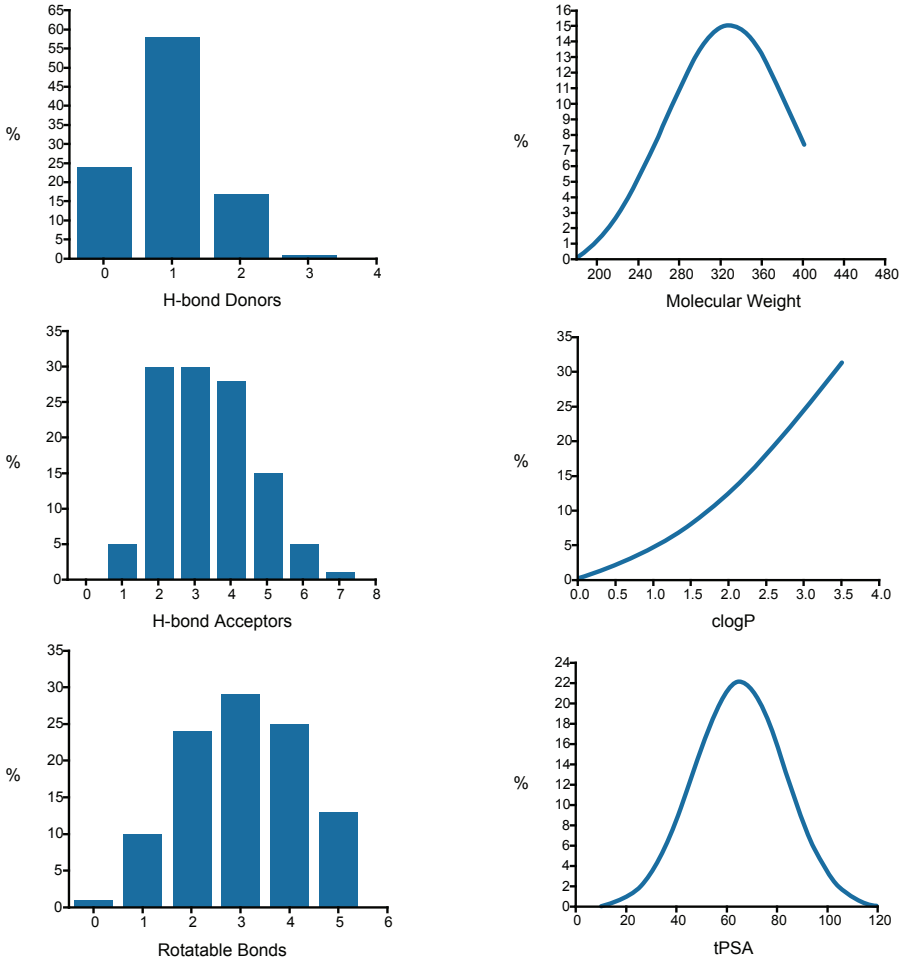
2 The Caco-2 value was calculated using QikProp as a measure of the predicted apparent Caco-2 permeability (nm/sec). Caco-2 cells are used as a model for the gut blood barrier. Determination as early as possible of whether a molecule is transported across the gut is vital in selecting lead compounds. 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.*

Physiochemical Property Distribution



ChemBridge Corporation
San Diego, CA, USA
Telephone: (858) 451-7400
sales@chembridge.com
www.chembridge.com

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