A NUCLEAR RECEPTOR DIRECTED LIBRARY

NHRCore Library

Highlights

- High quality, ChemBridge® proprietary compounds with potential activity against nuclear receptors
- Custom select compounds to meet your requirements
- Structural analogs available for SAR studies

Introduction

The NHRCore™ Library is a computationally selected library of more than 1,500 lead-like small molecules. NHRCore compounds are part of ChemBridge's CORE Library Stock and were selected for synthesis based on similarity to 3D pharmacophore fingerprints generated from published compounds with activity against nuclear hormone receptor targets. More than 180 synthetic schemes and more than 1,000 unique Bemis-Murcko scaffolds (atomic frameworks)[1] are represented.

Selection

Compounds showing activity against nuclear hormone receptor targets were extracted from public, scientific databases. 3D conformers were generated for each agonist or antagonist compound, and 3D pharmacophore fingerprints were generated from the 3D conformers. These fingerprints were then compared to the 3D pharmacophore fingerprints generated for virtual compounds based on novel scaffolds designed by ChemBridge. Virtual compounds with a high similarity to a published active fingerprint were synthesized and included in the NHRCore Library selection.

Potential Targets

The published actives used to generate the 3D pharmacophore fingerprints showed activity against the following nuclear receptors:

Androgen Receptor
Estrogen Receptor
Farnesoid X Receptor
Glucocorticoid Receptor
Liver X Receptor alpha
Liver X Receptor beta
Peroxisome Proliferator-Activated Receptor (PPAR) alpha
Peroxisome Proliferator-Activated Receptor (PPAR) gamma
Peroxisome Proliferator-Activated Receptor (PPAR) delta
Progesterone Receptor
Retinoic Acid Receptor (RAR) alpha
Retinoic Acid Receptor (RAR) beta
Retinoic Acid Receptor (RAR) gamma
Thyroid Hormone Receptor
Vitamin D Receptor

Properties

NHRCore Library compounds are lead-like and drug-like and have the following physiochemical and calculated property averages:

Molecular Weight Average = 345.2

Fsp3 Average = 0.5

clogP Average = 2.0

TPSA Average = 60.3

H-bond Donor Count Average = 0.4

H-bond Acceptor Count Average = 3.6

Rotatable Bond Count Average = 4.2

Format

- Custom select from more than 1,500 NHRCore Library compounds
- Available in 384-well and 96-well formats including 384-well acoustic qualified plates
- Amounts as low as 0.25 micromole (25ul of 10mM DMSO solution) available
- Available as DMSO solutions or dry in micromole or mg amounts

Structure File

For a file of structures, please email sales@chembridge.com

Reference

1. Bemis GW et al. The properties of known drugs. 1. Molecular frameworks. J. Med. Chem. 1996 39(15), 2887-93

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Rev. 20240906