



A NUCLEAR RECEPTOR DIRECTED LIBRARY

NHRCore Library

Introduction

The NHRCore™ Library is a computationally selected library of more than 3,000 leadlike 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 250 novel scaffolds are represented in the NHRCore Library, and in-stock analogs are available for any compound identified as a hit. Clients can purchase the full NHRCore Library or custom-select a subset of compounds.

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

Properties

NHRCore Library compounds are leadlike and have the following physicochemical property ranges and averages:

	Range	Average
Molecular Weight	200 – 415	331.0
H-bond Donors	0 – 3	0.6
H-bond Acceptors	1 – 7	3.4
cLogP	-2 – 5	2.5
Rotatable Bonds	1 – 13	4.6
tPSA	3 – 116	53.0

Format

- Download structures and custom select NHRCore Library compounds
- Compounds can be provided in 96-well or 384-well format
- Compounds are available as DMSO solutions or dry films