

ActiTarg-N library of 1040 analogs is selected from a compound pool with cumulative structural features that are inherent across some 90 known nuclear receptors ligands.

Nuclear Receptors ligands analogs compound pool started with “de-fragmented” active molecules. TimTec stock was scanned to identify molecules with the same fragments, which re-assembled themselves in new chemical possibilities. Additional computational manipulations drew in more compounds with overall structural similarity to known nuclear receptors ligands. Further filtering ensured structural diversity in the final selection.

ActiTarg-N being a part of TimTec ActiTarg Series reflects preferred “focused diversity” library design approach providing structurally versatile chemical material relevant to a certain target .

Compounds are available for cherry-picking and/or as an entire collection of 1040 compounds in 96, 384-well plates and in vials.

[Contact us](#) for structural info, formatting options and pricing.

Nuclear Receptors target pool:

ER , estrogen receptor and estrogen related receptor **AR**, androgen receptor **GRR**, glucocorticoid receptor

RAR
, retinoic acid receptor

THR
, thyroid hormone receptor

VDR
, vitamin D receptor

FXR
, Farnesoid X Receptor

PPAR α / γ

, Peroxisome proliferator-activated receptors

LXR

, liver X receptor

CCR5

, C-C chemokine receptor type 5

MRR

, mineralocorticoid

PR

, progesterone receptor

CAR

, Constitutive androstane receptor

and others

About nuclear receptors

Nuclear receptors are inside-cell proteins that regulate gene transcription and affect wide range of biological functions throughout organism normal and pathological development. These are the superfamily of 48 structurally related transcription factors that can be regulated by small molecules.

Selected Reference:

Betz B.F., et. al. Determination of the Binding Mode of Thienopyrimidinedione Antagonists to the Human Gonadotropin Releasing Hormone Receptor Using Structure–Activity Relationships, Site-Directed Mutagenesis, and Homology Modeling. *J. Med. Chem.*, 2006, 49 (21), pp 6170–6176

Lund B.W., et.al. Discovery of a Potent, Orally Available, and Isoform-Selective Retinoic Acid β 2 Receptor Agonist. J. Med. Chem., 2005, 48 (24), pp 7517–7519

Zuercher, W.J., et. al. Identification and Structure–Activity Relationship of Phenolic Acyl Hydrazones as Selective Agonists for the Estrogen-Related Orphan Nuclear Receptors ERR β and ERR γ . J. Med. Chem., 2005, 48 (9), pp 3107-3109

Zhou H-B, et.al. Structure-Guided Optimization of Estrogen Receptor Binding Affinity and Antagonist Potency of Pyrazolopyrimidines with Basic Side Chains. J. Med. Chem., 2007, 50 (2), pp 399–403

Prante O., et. al. Synthesis, Radiofluorination, and In Vitro Evaluation of Pyrazolo[1,5-a]pyridine-Based Dopamine D4 Receptor Ligands: Discovery of an Inverse Agonist Radioligand for PET. J. Med. Chem., 2008, 51 (6), pp 1800–1810

Azadeh M., et al. 7-Hydroxy-benzopyran-4-one Derivatives: A Novel Pharmacophore of Peroxisome Proliferator-Activated Receptor α and γ (PPAR α and γ) Dual Agonists. J. Med. Chem., 2009, 52 (21), pp 6835–6850

Repo, S., et.al. Ligand Specificity of Constitutive Androstane Receptor as Probed by Induced-Fit Docking and Mutagenesis. J. Med. Chem., 2008, 51 (22), pp 7119–7131

Related Products

ActiTarg-N is one of TimTec targeted libraries. Other targeted screening collections of interest are:

[ActiTarg-G](#) GPCR Ligands
[ActiTarg-K](#) Kinase Modulators
[ActiTarg-P](#) Protease Inhibitors
[ActiTarg-S](#) Serpins Inhibitors
[ActiTarg-I](#) Potassium Channel Modulators
[ActiTarg-H](#) HDAC Inhibitor [ActiTarg-CNS](#) Central Nervous System Receptors Modulators Library