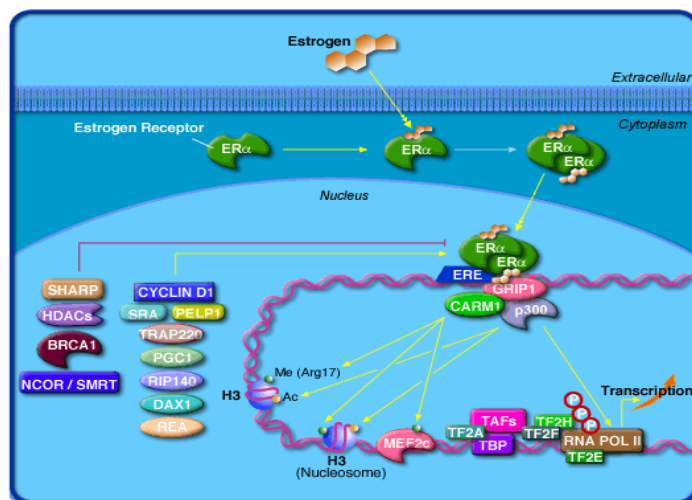


NHR Inhibitor Databases

Chemical Biological and Pharmacological Information of Nuclear Hormone Receptor (NHR) inhibitors from International Journals, US and International Patents have been curated and a unique database is now available in various formats like in ISIS/Base DB, SD, XML and Oracle. This database can also be made available for any set of Nuclear Hormone super families. The database will be licensed on a non-exclusive basis.

Each individual Record consists of:

- 2D/3D molecular structure with Mol. wt. & Formula, IUPAC and generic Name, SMILES
- Title, Authors, Company Address,
- Reference of the Patent or Journal,
- Compound number / Example number, GVK_ID
- Bioassay with details of units, quantitative biological activity, types of targets along with their isomeric or mutated forms,
- Cell specification if it is cell based assay.
- ADME parameters
- Any anomalies are observed

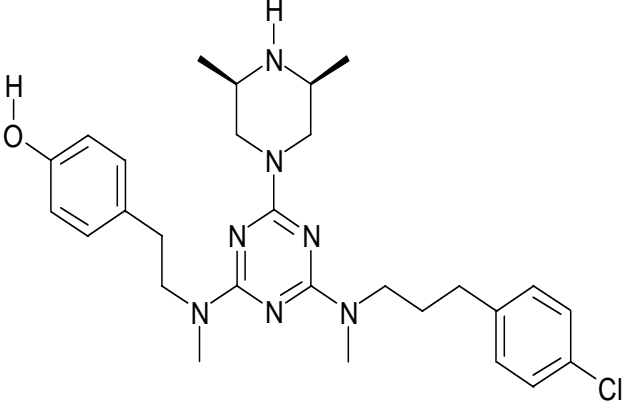


All structures listed in tables/text with activity data are generated from articles and patents have been curated to indicate the chemical space explored for each family of targets. Details of **Assay method**, **Source-Name**, **Source-Code**, **Official gene name of protein**, **Locus_Id**, **Multiple Loci**, **Locus reference**, **values of the target**, **units of measurement and activity value** are also curated. The database can be further customized to suit any specific requirements or additional data.

The databases could be effectively used:

- Easy query using any one or more number of fields or their logical combinations
- Structure, sub-structure, and similarity based query
- Easy export of the database or retrieved results to an SD or RD files, ChemFinder, excel sheet, MSAccess or Oracle databases
- Pharmacophore hypothesis, analogue (3D-QSAR) and structure based drug design and virtual screening

Sample Record

Structure		Activity	
		*fmla_Structure	C₂₈H₃₈ClN₇O
		*mol.weight_Structure	524.1144
		compound name	4-(2-((4-((3-(4-Chloro-phenyl)-propyl)-methyl-amino)-6-(4S)-3,5-dimethyl-piperazin-1-yl)-[1,3,5]triazin-2-yl)-methyl-amino)-ethyl)-phenol
		smiles	CCN(C)CCN(C)C1=NC2=C(N1)N=CN=C2C3=CC=C(C=C3)O
		title	PIPERAZINYL TRIAZINES AS ESTROGEN RECEPTOR MODULATORS
		inventor	Ronnie Lee Hale; Brad Richard Henke; Millard Hurst Lambert III; Amy Tsai Lu; Paul Kenneth Spearing; Philip Stewart Turnbull
		company address	DAVID J LEVY, CORPORATE, INTELLECTUAL PROPERTY, GLAXOSMITHKLINE, FIVE MOORE DR., PO BOX 13398, RESEARCH TRIANGLE PARK, NC 27709-3398 (US)
		claim/example	Example 16
Platform Name	Journal/Patent	GVK ID	REF_ID
NHR	Patent	7000056	
		reference	US 20040072829 A1
S_No	Journal	Year	Volume
1	US 20040072829 A1		
bioassay Piperazinyl triazine derivative as estrogen receptor modulator: Useful in the treatment of breast cancer, cardiovascular disease, dyslipidemia, uterine cancer, prostate cancer, prostate hyperplasia, urinary incontinence and atherosclerosis			
Derivative	Target	Agonist/Antagonist/Inhibitor	Therapeutic Use
Piperazinyl triazine	Estrogen receptor	Modulator	Breast cancer, Cardiovascular disease, Dyslipidemia, Uterine
Binding_Site remarks			
Final	Error_4	Reviewer_3	Error_3
			Reviewer_2
			Error_2
			Reviewer_1
			Error_1
			GVK
			SWAKUMAR

Structure				Activity					
GVK_ID 7000056		reference US 20040072829 A1			claim/example Example 16				
protein\cell\anim	Source_name	Source_code	official_name	Locus_ID	MultipleLoci	Locus_Ref	assay_type	Assay_no	REFER
Estrogen receptor alpha		Human	ESR1	2099			B		1
Estrogen receptor beta		Human	ESR2	2100			B		1
protein	Activity Type	Activity UOM	Activity Prefix	Activity Value	SD	enzyme/cell_assay			REFERENCE
Estrogen receptor alpha	pKi		=	6.6400000000		Binding affinity towards estrogen receptor alpha using [3H] estradiol (1 uM) as radioligand with the compound dissolved in DMSO			1
Estrogen receptor beta	pKi		=	7.9600000000		Binding affinity towards estrogen receptor beta using [3H] estradiol (1 uM) as radioligand with the compound dissolved in DMSO			1
Target_class	Family	Subfamily	Sub_subfamily	PDB_ID	Standard_name	Alias	Other_names	P/S	REFERENCE
NHR	NR3	NR3B		1A52, 1AKF, 1ERE, 1ERR, 1G50, 1GWQ, 1GWR, 1HCP	Estrogen Receptor Alpha	ER, ESR, ESRA, Era, NR3A1		P	1
remarks									

Other Databases

Our other database products include:

- **MCD** -Medchem Database consisting of biologically active compounds from journals.
- **CCD**—Compounds with pharmacokinetic, dynamic properties in various levels of clinical trials
- **DD** – Pharmacokinetic and dynamic properties of all the FDA approved drugs.
- **PCD** – Pre-clinical Pharmacokinetic, dynamic and Metabolite information of compounds.
- **MBT** - Proven or established mechanism of toxicity for 'drug like' compounds.
- **TXD** - Different Toxicities information of pharmacologically active compounds.
- **NPD** - Bio-active Natural Products and semi-synthetic compounds curated from Journals.