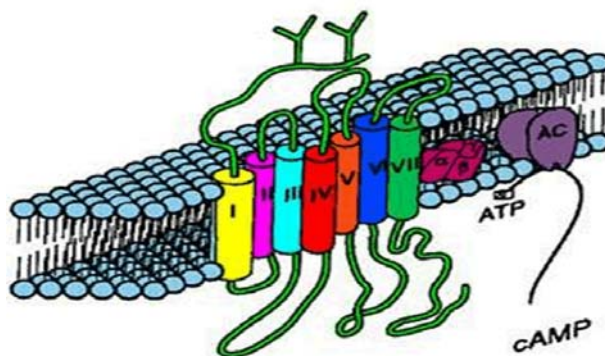


GPCR Inhibitor Databases

Chemical Biological and Pharmacological Information of G protein-coupled receptors (GPCR) 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. 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

GVK^{BIO} Sample Record

Structure		Activity						
<div style="text-align: center;"> </div>		*fmia_Structure C₂₄H₃₄N₂O₂						
		*mol.weight_Structure 382.5508						
		*compound_Name 1-(4-(1,1-Dimethyl-heptyl)-2'-hydroxy-biphenyl-2-yl]-urea						
		*inchi [H]OC1=C(C=CC(=C1)C(C)(C)CCCCC)C2=C(C=CC=C2)C(=O)N([H])CC						
		Title 1) PHENYL DERIVATIVES AND METHODS OF USE						
		Authors 1) Roland E. Dolle; Karin Worm; Q. Jean Zhou						
Platform_Name GPCR		Journal/Patent Patent		GVK_ID 4113462		REF_ID 18892		reference 1) US 20060074086 A1
S_No	Journal		Year	Volume	Issue	Start_page	End_page	PubMed_Id
1	US 20060074086 A1		2006					
bioassay 1) Phenyl derivative as cannabinoid receptor agonist: Useful for the treatment of pain, gastro intestinal disorders, gen disorders, inflammation, glaucoma, autoimmune diseases, ischemic conditions, immune related disorders and neurode								
Derivative Phenyl		Target Cannabinoid recepto		Agonist/Antagonist/Inhibitor Agonist		Therapeutic Use Pain, Gastro intestinal disorders, Genitourinar disorders, Inflammatio		Binding_Site
remarks								
Final	Error_4	Reviewer_3	Error_3	Reviewer_2	Error_2	Reviewer_1	Error_1	Curator

Structure				Activity						
GVK_ID 4113462		reference 1) US 20060074086 A1			claim/example 1) Compound 1					
protein/cell/animal	Source_name	Source_code	official_name	Locus_ID	MultipleLoci	Locus_Ref	assay_type	Assay_no	REFERE	
Cannabinoid receptor 1	human	Hum	CNR1	1268			B		1	
Cannabinoid receptor 2	human	Hum	CNR2	1269			B		1	
protein	ActivityType	ActivityUOM	ActivityPrefix	ActivityValue	SD	Molarvalue	enzyme/cell_assay		REFERENCE	
Cannabinoid receptor 1	Ki	nM	=	5000.0000000000		0.0000050000000000	Binding affinity towards human cloned Cannabinoid receptor 1 expressed in CHO-K1 cells using [3H]CP55940 (0.2-0.6 nM) as radioligand upon incubation with tris buffer, pH 7.0 at 30 degree C for 120 minutes		1	
Cannabinoid receptor 2	Ki	nM	=	5000.0000000000		0.0000050000000000	Binding affinity towards human cloned Cannabinoid receptor 2 expressed in CHO-K1 cells using [3H]CP55940 (0.2-0.6 nM) as radioligand upon incubation with tris buffer, pH 7.0 at RT for 60 minutes		1	
Target_class	Family	Subfamily	Sub_subfamily	PDB_ID	Standard_name	Alias	Other_names	P/S	REFERENCE	
GPCR	Family 1 Rhodopsin like receptors	Cannabinoid receptors	Cannabinoid receptors	1LVQ, 1LVR	Cannabinoid receptor 1 (brain)	RP1-23D17.1, CANN6, CB-R, CB1, CB1A, CB1K5, CNR, central cannabinoid		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.