

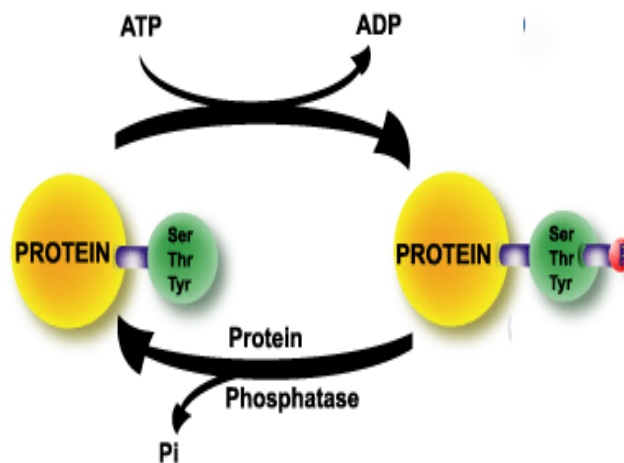
GVK^{BIO}

Phosphatase Inhibitor Database

Chemical Biological and Pharmacological Information of Phosphatase 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 Phosphatase 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 C₁₆H₁₄F₃N₃O₈S				
				*mol.weight_Structure 465.3645				
				*compound_name (4-Nitrophenylamino)-3-(2-nitro-4-trifluoromethyl-phenoxy)-propan-2-ol				
				SMILES S(=O)(=O)(c1cc(c(cc1)OCC(CNc1ccc(cc1)[N+](=O)[O-])C(F)(F)F)				
				Title PHOSPHATE MIMICS AND METHODS OF TREAT USING PHOSPHATASE INHIBITORS				
Authors HUANG, Ping; WEI, Chung, Chen; TANG, Peng, Cho LIANG, Chris; RAMPHAL, John; JALLAL, Bahija; BIL John; LI, Sharon; MATTSON, Matthew, Neil; MCMANUS, John								
Company address Viering, Hans-Martin et al, Patentanwälte, Viering, Jäger & Partner, Postfach 22 14 43, 80504 Munchen (DE)								
claim/example Example 56								
Platform_Name Phosphatase	Journal/Patent Patent	GVK_ID 730127	REF_ID 273	reference EP 1212296 B1				
S_No	Journal	Year	Volume	Issue	Start_page	End_page	PubMed_Id	
1	EP 1212296 B1	2005						
bioassay Trifluoromethyl sulfonamide derivative as protein tyrosine phosphatase inhibitor: Useful in the treatment of diabetes, rheumatoid arthritis, neurodegenerative diseases, cancer								
Derivative Trifluoromethyl sulfonamide	Target Protein tyrosine phosphatase	Agonist/Antagonist/Inhibitor Inhibitor	Theophylline Diabetes mellitus, Rheumatoid arthritis, Neurodegenerative	Binding_Site				
remarks								
Final	Error_4	Reviewer_3	Error_3	Reviewer_2	Error_2	Reviewer_1	Error_1	Curator

Structure				Activity					
GVK_ID 730127		reference EP 1212296 B1				claim/example Example 56			
protein\cellname	Source_name	Source_code	official_name	Locus_ID	MultipleLoci	Locus_Ref	assay_type	Assay_no	REFER
Protein tyrosine phosphatase 1B	human	Hum	PTPN1	5770			B		1
Protein tyrosine phosphatase MEG2	human	Hum	PTPN9	5780			B		1
Protein	human	Hum	PTPRA	5786			B		1
protein	ActivityType	ActivityUOM	ActivityPrefix	ActivityValue	SD	Molarvalue	enzyme/cell_assay		REFERENCE
Protein tyrosine phosphatase 1B	IC50	uM	=	4.800000000		0.0000480000000000	In vitro inhibitory concentration against Protein tyrosine phosphatase 1B with the compound dissolved in DMSO upon incubation at 25 degree C for 15 minutes using DiFMUP as substrate		1
Protein tyrosine phosphatase MEG2	IC50	uM	=	16.200000000		0.0001620000000000	In vitro inhibitory concentration against Protein tyrosine phosphatase MEG2 with the compound dissolved in DMSO upon incubation at 25 degree C for 15 minutes using DiFMUP as substrate		1
Protein tyrosine	IC50	uM	=	50.900000000		0.0005090000000000	In vitro inhibitory concentration against Protein tyrosine phosphatase Alpha with the compound		1
Target_class	Family	Subfamily	Sub_subfamily	PDB_ID	Standard_name	Alias	Other_names	P/S	REFERENCE
Phosphatase	Protein-tyrosine phosphatase family	Non-receptor class 1 subfamily		1A5Y, 1AAX, 1BZC, 1BZH, 1BZJ, 1C83, 1C84, 1C85, 1C86, 1C87, 1C88, 1ECV	protein tyrosine phosphatase, non-receptor type 1	PTP1B, non-receptor tyrosine phosphatase 1; protein tyrosine phosphatase 1B: protein		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.

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