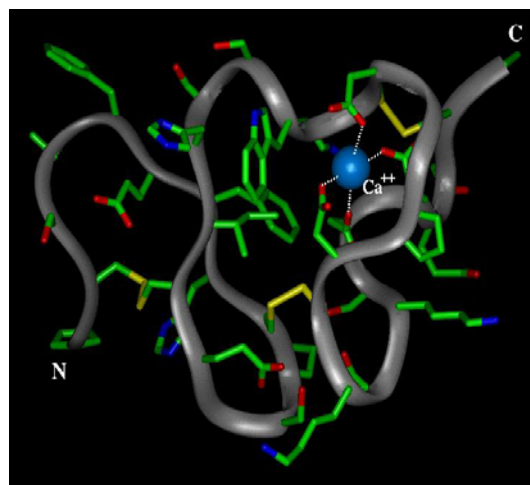


MedChem Database

MedChem Database consists of chemically diverse compounds/records, with Biological and Pharmacological Information. Data is extracted from all the articles published in standard Medicinal Chemistry Journals. MedChem Database is available in different user-friendly searchable formats such as ISIS/Base, SD-format, RD-format, ChemFinder, XML, Excel, MS-Access and Oracle Dump.

Each individual Record consists of

- **2D/3D** molecular structure
- **SMILES** notation and **IUPAC** Names
- **Title, Authors, Address and PubMed_ID** of the article
- **Bioassay** includes in-vitro studies like enzyme, protein, receptor/cell-based and in-vivo studies
- **Assay Type** (**B**inding, **B**inding with **M**utant, **F**unctional, **A**DME, **T**oxicity and **O**thers)
- **Implications/uses** in different indications
- **Quantitative activity** values and units

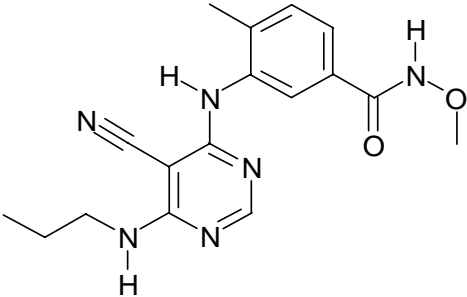


All biological activities reported in different articles for any one compound are included in one single record with details of **Assay method, Source-Name, Source-Code, Official gene name of protein, Locus_Id, Multiple Loci, Locus reference, values of the target, units of measurement and activity value**. The database can be further customized to suit any specific requirements or additional data.

This database is found to be very effective for the following applications:

- Query based on Structure, sub-structure, pharmacophore and molecular similarity is possible
- Easy export of the database or retrieved results to any format of interest is possible
- Pharmacophore hypothesis, analogue (3D-QSAR) or structure based drug design, enhanced potency
- Virtual Screening for improved potency and selectivity

Sample Record

Structure		Activity							
<p>Structure</p> 		*fmla_Structure C₁₇H₂₀N₆O₂							
		*mol.weight_Structure 340.3879							
		*go_to_compound 3-(5-Cyano-6-propylamino-pyrimidin-4-ylamino)-N-methyl-4-methyl-benzamide							
		*SMILES [H]N(CCC)C1=C(C#N)C(=NC=N1)N([H])C2=CC(=CC=C2C)C([O])N([H])OC							
		*Title 1) 5-Cyanopyrimidine Derivatives as a Novel Class of Potent, Selective, and Orally Active Inhibitors of p38alpha MAP Kinase							
Platform_Name MCD		Journal/Patent Journal		GVK_ID 3800547		REF_ID 39661		reference 1) J. Med. Chem., 2005, 48 (20), 6261-6270	
S_No	Journal	Year	Month	Day	Volume	Issue	Start_page	End_page	PubMed_Id
1	J. Med. Chem.	2005	4	15	48	20	6261	6270	16190753
bioassay 1) 5-cyanopyrimidine derivative as p38 alpha MAP kinase inhibitor : Useful in the treatment of inflammatory diseases									
Derivative 5-cyanopyrimidine		Target p38 alpha		Agonist/Antagonist/Inhibitor Inhibitor		Therapeutic_use Inflammatory diseases		Binding_Site	
remarks									
Final	Error_4	Reviewer_3	Error_3	Reviewer_2	Error_2	swappa_inp	Error_1	Curator	

Structure				Activity						
GVK_ID 3800547		reference 1) J. Med. Chem., 2005, 48 (20), 6261-6270			claim/example 1) Compound 14b					
protein\cell\anim	Source_name	Source_code	official_name	Locus_ID	MultipleLoci	Locus_Ref	assay_type	Assay_no	REFER	
p38 alpha	Escherichia coli	Human	MAPK14	1432			B	1	1	
	PBM cell line	Human					FI	2	1	
protein	Activity Type	Activity UOM	Activity Pre	Activity Value	Molar value	SD	enzyme/cell_assay		REFER	
p38 alpha	Ki	nM	=	0.97000000 00000000	0.000000 00097000 00		Binding affinity of the compound towards human p38 alpha kinase expressed in E. coli upon incubation for 21 hrs at RT in pH 7.4 using [gamma-33P]ATP as radioligand with compound dissolved in DMSO; n=4		1	
	IC50	uM	=	158.000000 0000000000	0.000158 00000000 00		Inhibitory concentration of the compound against LPS-induced TNFalpha production in human peripheral blood mononuclear cells; n=3		1	
Target_class	Family	Subfamily	Sub_subfamily	PDB_ID	Standard_nam	Alias	Other_names	P/S	REFER	
Kinase	Ser/Thr protein kinase family	MAP kinase subfamily		1A9U, 1BL6, 1BL7, 1BMK, 1DI9, 1IAN, 1KV1, 1KV2, 1M7Q, 1OLK	Mitogen-activated protein kinase 14	CSBP1, CSBP2, CSPB1, EXIP, Mxi2, PRKM14, PRKM15, RK, SAPK2A	p38alpha	P	1	
remarks										

Other Databases

Our other database products include:

- **TID** - Phosphatases, Kinases, Proteases and other Enzymes, Ion-Channel blockers, NHR and GPCR Agonist/Antagonist/ Inhibitors/Substrates data from Journals and Patents.
- **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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