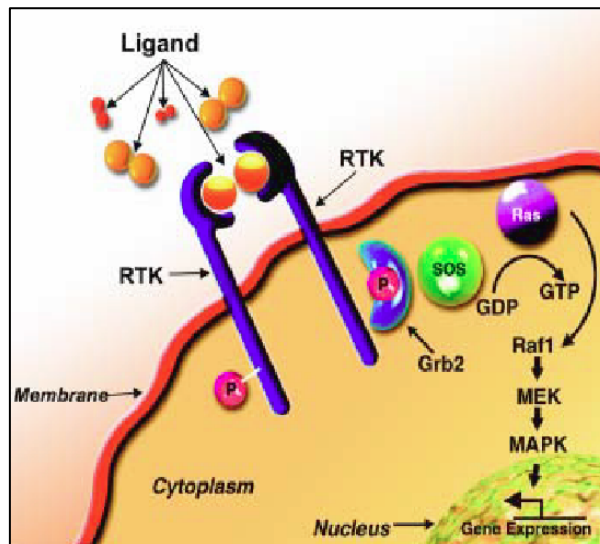


Kinase Inhibitor Databases

Chemical Biological and Pharmacological Information of Kinase 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 kinases. 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

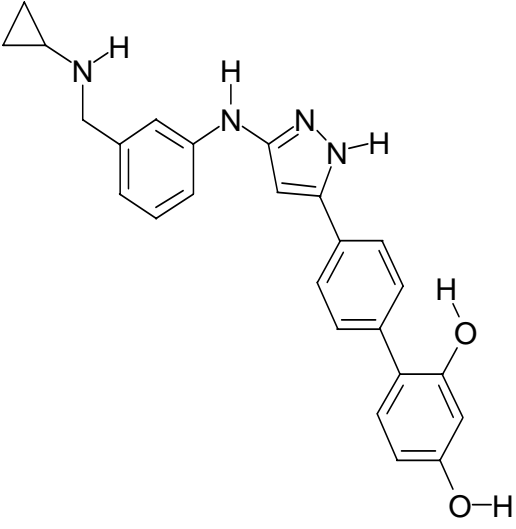


All structures listed in tables/text with activity data are generated from articles and patents have been curated to indicate the chemical space explored for each family of targets. Details of **Assay method**, **Source-Name**, **Source-Code**, **Official gene name of protein**, **Locus_Id**, **Multiple 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														
<p>Structure</p> 			*fmila_Structure C₂₅H₂₄N₄O₂														
			*mol.weight_Structure 412.4956														
			*iupac_name 4-((3-cyclopropylaminomethyl-phenylamino)-2,1,3-benzoxadiazol-5-yl)-biphenyl-2,4-diol														
			*smiles Oc1ccc(c(O)c1)-c2ccc(cc2)-c3cc(Nc4cccc(CNC5CC5)H)3														
			Title 1) AMINOPYRAZOLE COMPOUNDS AND USE AS INHIBITORS														
			Authors 1) JOHNSON, Michael, David; TENG, Min; ZHU, Jinj														
Platform_Name KINASE			Journal/Patent Patent		GVK_ID 1175075		REF_ID 3504		reference 1) WO 2005/009435 A1								
S_No			Journal		Year		Volume		Issue		Start_page		End_page		PubMed_Id		
1			WO 2005/009435 A1		2005												
bioassay 1) Aminopyrazole derivative as checkpoint kinase (CHK1) inhibitor : Useful to treat cell proliferative disorders																	
Derivative Aminopyrazole			Target CHK1			Agonist/Antagonist/Inhibitor Inhibitor			Therapeutic use Cell proliferative disorders, cancer			Binding_Site ATP binding site					
remarks																	
Final		Error_4		Reviewer_3		Error_3		Reviewer_2		Error_2		Reviewer_1		Error_1		Curator	

Structure			Activity						
GVK_ID 1175075		reference 1) WO 2005/009435 A1	claim/example 1) Example No. 3						
protein\cell\anima	Source_name	Source_code	official_name	Locus_ID	MultipleLoci	Locus_Ref	assay_type	Assay_no	REFER
CHK1	human	Hum	CHEK1	1111			B		1
CHK1	human	Hum	CHEK1	1111			B		1
protein	ActivityType	ActivityUOM	ActivityPrefix	ActivityValue	SD	Molarvalue	enzyme/cell_assay		REFERENCE
CHK1	Ki	nM	<	1.000000000000		0.0000000010000000	Inhibitory constant against human (CHK1) checkpoint kinase expressed in baculovirus/insect cell system		1
CHK1	EC50	nM	=	900.0000000000		0.0000009000000000	Inhibition of human (CHK1) checkpoint kinase expressed in baculovirus/insect cell system		1
Target_class	Family	Subfamily	Sub_subfamily	PDB_ID	Standard_name	Alias	Manning_name	P/S	REFERENCE
Kinase	Ser/Thr protein kinase family	NIM1 subfamily		1IA8, 1NVQ, 1NVR, 1NVS, 1ZLT, 2BR1, 2BRB, 2BRG, 2BRH, 2BRM	CHK1 checkpoint homolog (S. pombe)	CHK1, CHK1 (checkpoint, S.pombe) homolog; CHK1 checkpoint homolog	CHK1	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.

For further information contact: Sarma Jagarlapudi PhD, Sr. VP - Informatics, Email – sarma@gvkbio.com or Sreenivas Devidas, VP, Business development, Email – sreeni.devidas@gvkbio.com, GVK Biosciences Private Limited. Phone No. 914065180632 Fax No. 91 40 23721010; Website – www.gvkbio.com