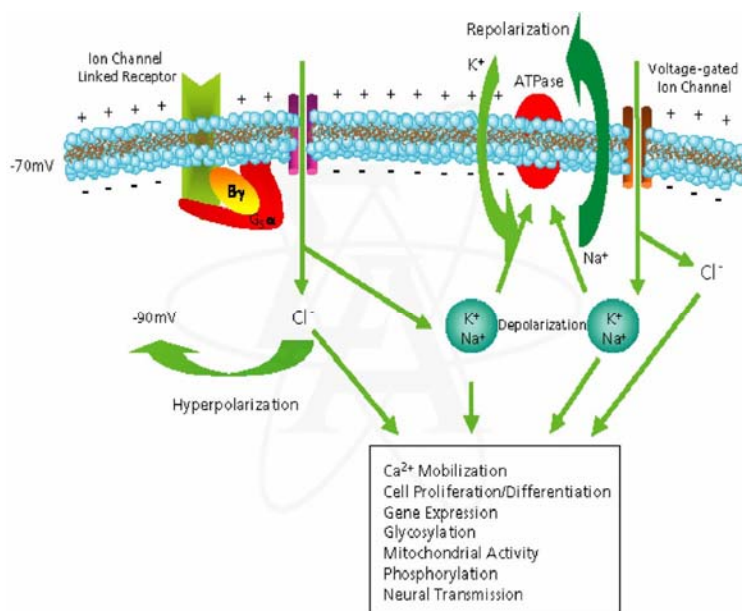


Ion-Channel Inhibitor Databases

Chemical Biological and Pharmacological Information of Ion-Channel (IC) 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 Ion-Channel 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

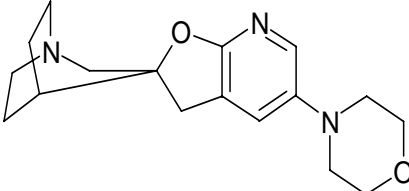


All structures listed in tables/text with activity data are generated from articles and patents have been curated to indicate the chemical space explored for each family of targets. Details of **Assay method**, **Source-Name**, **Source-Code**, **Official gene name of protein**, **Locus_Id**, **Multiple 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

GVK^{BIO} Sample Record

Structure		Activity						
Structure 		*fmla_Structure C₁₇H₂₃N₃O₂						
		*mol.weight_Structure 301.3918						
		*compound_name 5-(1,4-oxazinan-4-yl)spiro[4-azabicyclo[2.2.2]octane-2,2',3'-dihydrofuro[2,3-b]pyridine]						
		smiles O1C2(Cc3c1ncc(c3)N1CCOCC1)CN1CCC2CC1						
		Title NOVEL SPIROAZABICYCLIC HETEROCYCLIC COMPOUNDS						
		PHILLIPS, Eflion; MACK, Robert; MACOR, John; SEMUS, Simon						
company_address AstraZeneca AB, 151 85 Sodertalje (SE)		claim/example Example 15A(S)/15B(R)						
Platform_Name Ion Channel	Journal/Patent Patent	GVK_ID 2255286	REF_ID	reference EP 0996622 B1				
S_No	Journal	Year	Volume	Issue	Start_page	End_page	PubMed_Id	
1	EP 0996622 B1							
Spiroazabicyclic heterocyclic amine derivative as ligand for nicotinic cholinergic receptor: Useful in the treatment of schizophrenia, mania, anxiety, Alzheimer'a disease, memory loss, hyperactivity disorder, analgesic, Parkinson's disease, Huntington's disease, <input checked="" type="checkbox"/>								
Derivative Spiroazabicyclic heterocyclic amine	Target Nicotinic cholinergic receptor	Agonist/Antagonist/Inhibitor	Schizophrenia, Mania, Anxiety, Alzheimer'a disease, Memory loss. <input checked="" type="checkbox"/>		Binding_Site			
remarks								
Final	Error_4	Reviewer_3	Error_3	Reviewer_2	Error_2	Reviewer_1	Error_1	CSAT Savati RL

Structure			Activity						
GVK_ID 2255286		reference EP 0996622 B1				claim/example Example 15A(S)/15B(R)			
protein/cell/anim	Source_name	Source_code	official_name	Locus_ID	MultipleLoci	Locus_Ref	assay_type	Assay_no	REFER
Nicotinic cholinergic receptor alpha 7	Hippocampal membrane	Rat	Chrna7	25302			B		1
Nicotinic cholinergic receptor alpha 4	Brain	Rat	Chrna4	25590			B		1
protein	Activity Type	Activity UOM	Activity Prefix	Activity Value	SD	enzyme/cell_assay			REFERENCE
Nicotinic cholinergic receptor alpha 7	Ki	nM	<	1000.00000 00000		Binding affinity towards Nicotinic cholinergic receptor alpha 7 expressed in rat hippocampal membrane using [125I]alpha-Bungarotoxin (5nM) as radioligand done for 2 hrs at 21 degree C			1
Nicotinic cholinergic receptor alpha 4	Ki	nM	<	1000.00000 00000		Binding affinity towards rat Nicotinic cholinergic receptor alpha 4 using [3H]-(-)-nicotine (3nM) as radioligand done for 1 hr at 4 degree c			1
Target_class	Family	Subfamily	Sub_subfamily	PDB_ID	Standard_name	Alias	Other_names	P/S	REFERENCE
Ion Channel	Ligand-gated ion channel	TC 1.A.9			cholinergic receptor, nicotinic, alpha polypeptide 7	NACHRA7		P	1
Ion Channel	Ligand-gated ion channel	TC 1.A.9			cholinergic receptor, nicotinic	BFNC, EBN, EBN1, NACRA4		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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