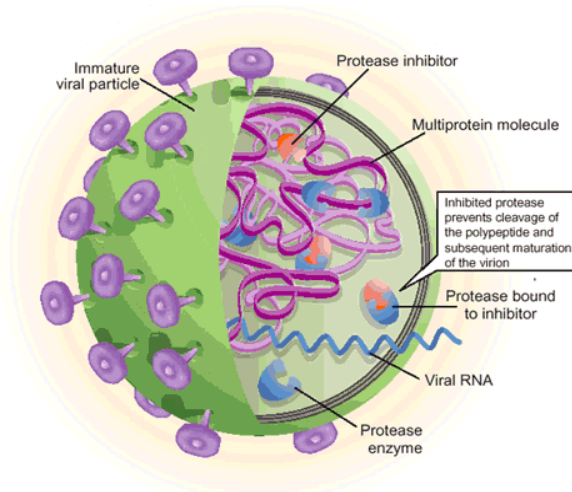


## Protease Inhibitor Database

Chemical Biological and Pharmacological Information of Protease 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 Nuclear Hormone 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



Structure			Activity						
GVK_ID 3675889		reference US 2003109517 A1				claim/example Example 10			
protein/cell/anim	Source_name	Source_code	official_name	Locus_ID	MultipleLoci	Locus_Ref	assay_type	Assay_no	REFER
Thrombin	human	Hum	F2	2147			B		
Factor Xa	human	Hum	F10	2159			B		
protein	Activity Type	Activity UC	Activity Prefix	Activity Value	SD	Molar value	enzyme/cell_assay		REFERENCE
Thrombin	Ki	uM	=	10.0000000000			In vitro inhibitory activity against human thrombin (0.5 nM) using N-succinyl-Ala-Ala-Pro-Arg-p-nitroanilide (32 mM) as substrate incubated for 15 min in pH 7.5 at 37 degree C with the compound dissolved in DMSO; Range is 0.70 - 10 uM		
Factor Xa	Ki	uM	=	10.0000000000			In vitro inhibitory activity against human factor Xa (10 nM) using N-benzoyl-Ile-Glu-Gly-Arg-p-nitroanilide hydrochloride (51 mM) as substrate incubated for		
Target_class	Family	Subfamily	Sub_subfamily	PDB_ID	Standard_name	Alias	Other_names	P/S	REFER
Protease	Serine-type peptidases			1A2C, 1A3B, 1A3E, 1A46, 1A4W, 1A5G, 1A61, 1ABI, 1ABI	coagulation factor II (thrombin)	PT, coagulation factor II; prothrombin; prothrombin B-chain; serine protease		P	
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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