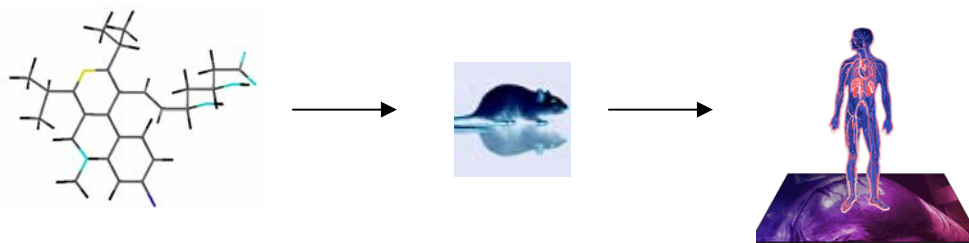


## Clinical Candidate Database (CCD)

Clinical Candidate Database consists of chemically diverse compounds/records with Biological, Pharmacological, Clinical pharmacokinetic Information which are in various stages of drug development. Besides it also includes drugs, which have been approved by FDA, failed drugs and discontinued drugs. Data is extracted from the articles published in various standard journals covering clinical development of new drugs and also from patents. Clinical Candidate Database is available in different user-friendly searchable formats such as ISIS/Base, SD-format, RD-format and Oracle Dump.



### Characteristics of the available fields:

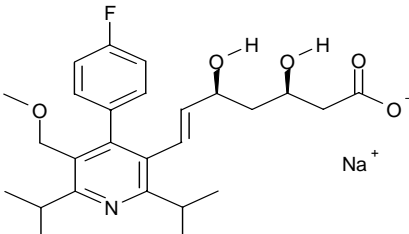
- Each individual record in the database consists of 2D structure of the compound.
- In vitro and In vivo biological activity of compounds in animals.
- Contains important pharmacokinetic parameters like Oral bioavailability, Excretion, Clearance, Plasma Binding, Volume of Distribution, Half-life, Effective Concentration, Tmax, AUC, Toxicity data obtained from pre-clinical and clinical trials.
- Metabolites information are given along with the mode of conversion.
- Besides these the synonyms, category of drug and the company developing the drug are also included.
- All the text, numerical, structure and substructure fields are searchable.

### This database offers the following utilities:

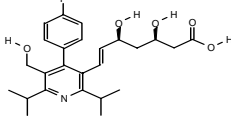
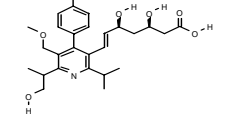
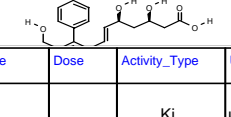
- Easy query using any one or more number of fields or their logical combinations involving text and numeric fields specified with limits structure
- Structure, sub-structure, pharmacophore and molecular similarity based query
- A number of PK and PD parameters, Toxicity can be modeled effectively to produce alerts in the Drug Discovery Pipelines and one could find out early the failed compounds
- Gives over view of Drug discovery pipelines over the last 20 years.

## Sample Record

### Clinical Candidate

Structure		1071		Drug_Name Cerivastatin Sodium															
		Category HMG-CoA reductase inhibitor		S.No BAYW 6228, Baycol®, Certal®, Cervastat®, Cholstat®, Lipobay®, Liposterol®, Rivastatin, Selta®, Staltor®, Stativa, Vaslip®, Zenas Micro®															
		Use Treatment of lipoprotein disorders, Hypercholesterolaemia, Hyperlipidaemia, Hyperlipoproteinaemia		Smiles <chem>O[C@H](C=Cc1c(nc(c1c1ccc(cc1)F)COC)C(C)C)C[C@H](CC(=O)[O-])[O].[Na+]</chem>															
		IUPAC_Name Sodium; (E)-(3R,5S)-7-[4-(4-fluoro-phenyl)-2,6-diisopropyl-5-methoxymethyl-pyridin-3-yl]-3,5-dihydroxy-hept-6-enoate		GVK_ID <b>CCD-279</b>		CAS_No 145599-86-6													
		Mode_Of_Action HMG-CoA reductase inhibitor		S.No   Title   Authors   Address															
1		Absolute and relative bioavailability of the HMG-CoA		Muck W, Ritter W, Ochmann K		Bayer Bayer AG, Wuppertal, Germany													
S.No		Article		Year		Volume		Issue		Start_Page		End_Page		PubMed_ID		Compound_No		Parameter	
1		International Journal of Clinical Pharmacology and Therapeutics		1997		35		6		255		260						Cmax, Tmax, Half Life, AUC, Bioavailability.	
Binding Data		Functional Data		Clinical Data		Other Details		Bioavailability											
Plasma Binding		Distribution		Metabolites		Half Life		Tmax											
Toxicity		Cmax		AUC		Clearance		Excretion											
Remarks																			

### Clinical Candidate

Drug_Name Cerivastatin Sodium		S.No BAYW 6228, Baycol®, Certal®, Cervastat®, Cholstat®, Lipobay®, Liposterol®, Rivastatin, Selta®, Staltor®,							
Category HMG-CoA reductase inhibitor		GVK_ID <b>CCD-279</b>		Use Treatment of lipoprotein disorders, Hypercholesterolaemia, Hyperlipidaemia.					
No. of Meta	Metabolite_Structure	Metabolite_Smiles		Metabolite_Name	Metabolite_Enzyme	Mode_of_Conversion	Metabolite		
CCD-279-M1		<chem>O=C(O[H])C[C@H](O[H])C[C@H](O[H])/C=C/C1=C(C(C)C)N=C(C(CO[H])=C1C(C=C2)=CC=C2F)C(C)C</chem>		M1	Cytochrome P450 (CYP) 2C8 and CYP3A4	Demethylation of the benzylic methylether	6		
CCD-279-M2		<chem>O=C(O[H])C[C@H](O[H])C[C@H](O[H])/C=C/C1=C(C(C)C)N=C(C(COC)=C1C(C=C2)=CC=C2F)C(C)CO[H]</chem>		M23	Cytochrome P450 2C8	Hydroxylation of a methyl group in the 6'-isopropyl moiety	6		
CCD-279-M3		<chem>O=C(O[H])C[C@H](O[H])C[C@H](O[H])/C=C/C1=C(C(C)C)N=C(C(CO[H])=C1C(C=C2)=CC=C2F)C(C)CO[H]</chem>		M24	Cytochrome P450 (CYP) 2C8 and CYP3A4	Demethylation of the benzylic methylether	6		
Model	Vehicle	Dose	Activity_Type	Units	Value	Value_Desc	CYP Inhibition	Refere	
CYP3A4			Ki	µM/L	290.0000	290	Ki value of the drug on CYP3A4-mediated biotransformation reaction as determined by in vitro enzyme affinity investigations	6	
CYP3A4			Ki	µM/L	150.0000	150	Ki value of the metabolite M1 on CYP3A4-mediated biotransformation reaction as determined by in vitro enzyme	6	
Binding Data		Functional Data		Clinical Data		Other Details		Bioavailability	
Plasma Binding		Distribution		Metabolites		Half Life		Tmax	
Toxicity		Cmax		AUC		Clearance		Excretion	
Remarks									

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