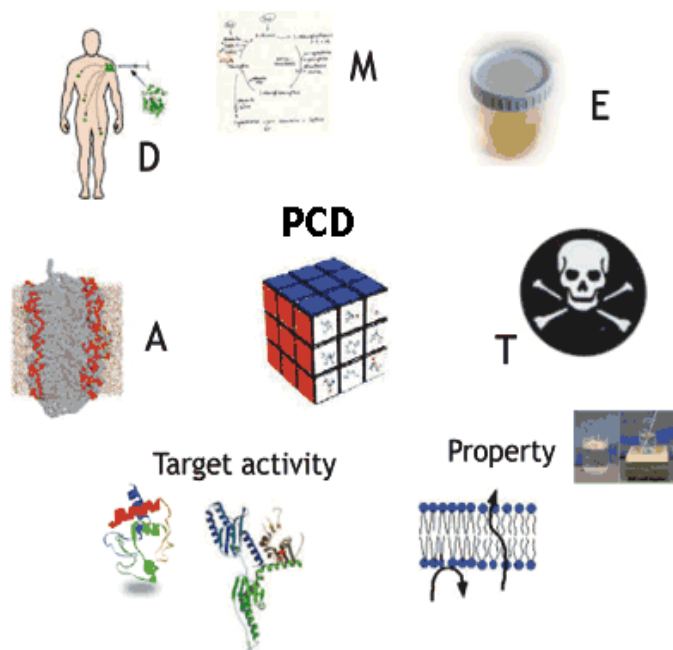


Pre-Clinical Candidate Database (PCD)

Pharmacokinetic, Pharmacodynamic and CYP inhibition data along with target Protein binding data of about 20,470 Compounds and their Metabolites reported in a number of Pharmacology and Metabolism journals have been curated into the PCD database. This database would be available in various formats like ISIS/Base, SD-format, RD-format and Oracle dump on request.

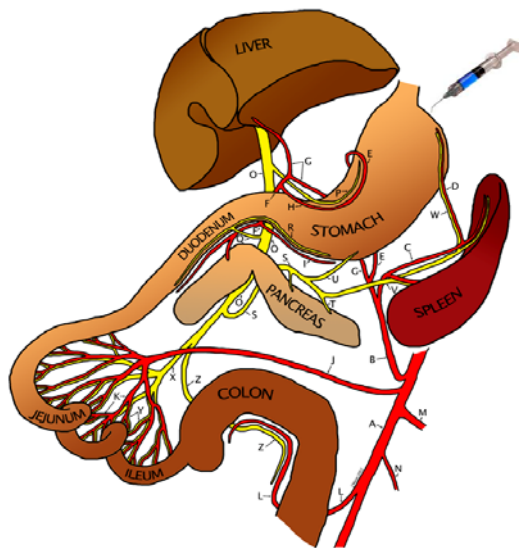


Characteristics of the available fields:

- Each Individual record in the database consists of 2D, Binding Data, Functional Data, CYP inhibition data
- A list of important pharmacokinetic parameters like Bioavailability, Excretion, Clearance, Volume of Distribution, Half-life, Plasma binding, Tmax, Cmax, AUC, Toxicity data as well as Vehicle, dose and route of administration are given
- Metabolites Structure and Name, converting/involved enzyme
- Metabolite that carries pharmacological information is curated as a separate record.
- All the text, numerical, structure and substructure fields are searchable.

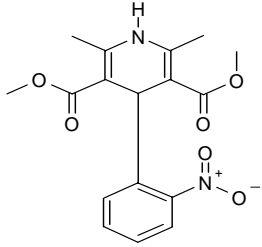
This database offers the following utilities:

- Easy query using a combination of one or more fields with logical combinations.
- Structure, sub-structure, pharmacophore and molecular similarity based query
- A number of PK and PD parameters
- Biological activities in terms of protein target and functional activities
- Each Record consists of a number of references indicating the parameter bibliographic details and pubmed ids.
- Easy query of Metabolite information like structure of Metabolite and Enzyme responsible for metabolism and Mode of conversion etc.

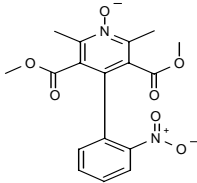
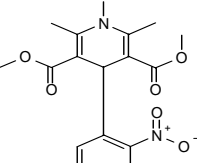


Sample Record

Pre-Clinical Candidate

Structure		Drug_Name							
		Category							
		Synonyms							
		Use							
		Smiles [O-][N+](=O)c1c(cccc1)C1C(=C(NC(=C1C(=O)OC)C)C(=O)OC							
		IUPAC_Name 2,6-Dimethyl-4-(2-nitro-phenyl)-1,4-dihydro-pyridine-3,5-dicarboxylic acid dimethyl ester							
GVK_ID PCD-1688		CAS_No							
Mode_Of_Action									
S_No	Title	Authors	Address						
1	Characterization of the Serotonin Receptor Mediating Contraction in the Mouse Thoracic Aorta and Signal Pathway Coupling	C. M. MCKUNE; S. W. WATTS	Department of Pharmacology and Toxicology, Michigan State University, East Lansing, Michigan						
S_No	Article	Year	Volume	Issue	Start Page	End Page	PubMed ID	Compound No	Parameter
1	J. Pharmacol. Exp. Ther.	2001	297	1	88	95	11259531	Nifedipine	Functional Data
Binding Data		Functional Data		Clinical Data		Other Details		Bioavailability	
Plasma Binding		Distribution		Metabolites		Half Life		Tmax	
Toxicity		Cmax		AUC		Clearance		Excretion	
Remarks				PCD-28873					

Pre-Clinical Candidate

Drug_Name		Category		GVK_ID PCD-1688					
No. of_Metabolites	Metabolite_Structure	Metabolite_Name	Metabolite_Smiles	Metabolite_Enzyme	Metabolite_Reference				
PCD-168 8-M1		Oxidized Nifedipine	[O-]N1=C(C)C(C(OC)=O)=C(C(C(OC)=O)=C1C)C(C=CC=C2)=C2[N+]([O-])=O	Cytochrome P450 enzymes	13, 16				
PCD-168 8-M2		1,2,6-Trimethyl-4-(2-nitro-phenyl)-1,4-dihydro-pyridine-3,5-dicarboxylic acid dimethyl ester	[O-][N+](C2=C(C=CC=C2)C1C(C(OC)=O)=C(C)N(C)C(C)=C1C(OC)=O)=O	Cytochrome P450 enzymes	65				
Model	Vehicle	Dose	Activity_Type	Units	Value	Value_Desc	CYP Inhibition	Reference	
Human			IC50	uM	23.0000	23	Inhibition of CYP3A activity in human liver microsome in presence of testosterone 6beta-hydroxylase for 30 min without NADPH	5	
Human			IC50	uM	27.0000	27	Inhibition of CYP3A activity in human liver microsome in presence of testosterone 6beta-hydroxylase for 30 min	5	
Binding Data		Functional Data		Clinical Data		Other Details		Bioavailability	
Plasma Binding		Distribution		Metabolites		Half Life		Tmax	
Toxicity		Cmax		AUC		Clearance		Excretion	
Remarks				PCD-28873					

See other leaflets for products such as **Medichem, Target Inhibitor, Pharmacokinetic, Toxicity** and **Natural Product Databases**.

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