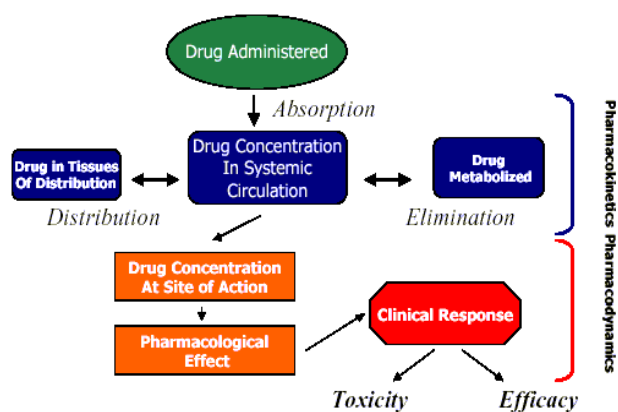


Drug Database

Many important Pharmacokinetic properties including the Metabolites information of nearly all the US-FDA approved and other drugs have been curated into a database. The data has been extracted from many standard books, online sources and various Pharmacological Journals. This unique and highly informative database can also be made available in various formats MS Access, SD-format, RD-format and Oracle upon request.

Pharmacodynamic vs. Pharmacokinetic



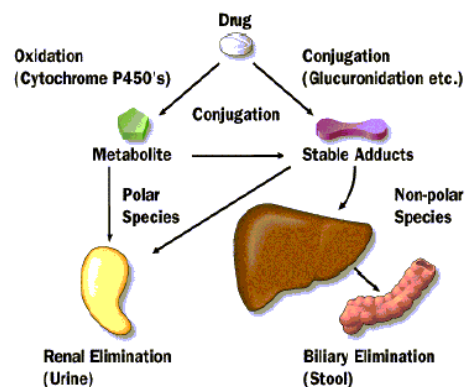
- The Database consists of drug records
- Each Individual record in the database consists of 2D molecular structures
- Usage against the disease, mode of action against enzyme, protein or Receptor.
- A list of important pharmacokinetic parameters such as pKa, solubility, Bioavailability, Excretion, % Plasma binding, Clearance, Volume of Distribution, Half-life, C_{max} , T_{max} , AUC, Drug interactions, Toxic Concentration, route of administration along with Clinical data.
- In vitro and In vivo biological activity of compounds in animals.

- LogP, number of Hydrogen bonding acceptors and donors and number of single bonds
- Useful Information on Drug Metabolism like Metabolites Structure and Name, converting enzyme and mode of conversion as well as references are also included. On the average, for each structure more than 6 metabolites information has been given as sub-records.
- All the text, numerical, structure and substructure fields are searchable and provides an opportunity for a very good correlation analysis with the help of many 2D and 3D molecular descriptors, fingerprints or molecular keys. Based on such a study, some of these important parameters can also be estimated for new compounds of interest.

This database offers the following possibilities:

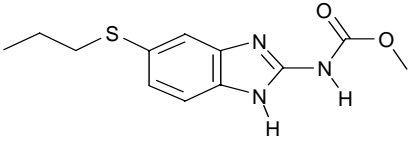
- Easy query using any one or more number of fields or their logical combinations involving text and numeric fields specified with limits structure.
- Structure, sub-structure, pharmacophore and molecular similarity based query.
- Easy export of the database or retrieved results to an SDF or RDF files, ChemFinder, Excel sheet, MS Access or Oracle databases.
- Easy query of Metabolite information like structure of Metabolite and Enzyme responsible for metabolism and Mode of conversion etc.
- The derived data can be used for modeling and alerts can be produced

Metabolic Pathway and Route of Elimination

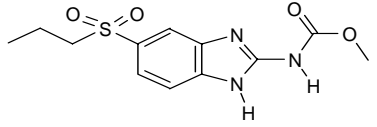
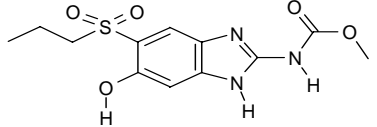
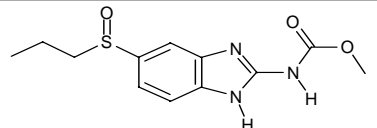


Sample Record

Drugs

	Drug_Name	ALBENDAZOLE							
	Category	Anthelmintic							
	Synonyms	Albenza(TM), SKF 62979, Valbazen							
	Use	Useful in treatment of neurocysticercosis, Hydatid disease							
	Smiles	O=C(OC)N([H])C1=NC(C=C2SCCC)=C(C=C2)N1[H]							
	IUPAC_Name	Methyl 5-(propylthio)-2-benzimidazolecarbamate							
GVK_ID		DD-26		CAS_No		54965-21-8			
Albendazole causes degenerative alterations in the tegument and intestinal cells of the worm by binding to the colchicine-sensitive site of tubulin, thus inhibiting its polymerization or assembly into microtubules.									
S_No	Title	Authors				Address			
3	Application of higher throughput screening (HTS) inhibition assays to evaluate the interaction of	Bapiro TE, Egnell AC, Hasler JA, Masimirembwa CM				Department of Biochemistry, University of Zimbabwe, Harare.			
S_No	Article	Year	Volume	Issue	Start_Page	End_Page	PubMed_ID	Compound_No	Parameter
1	GlaxoSmithKline, ALBENZA® (Albendazole) Tablets, Product Leaflet								Bioavailability, Plasma binding,
Binding Data		Functional Data		Clinical Data		Other Details		Bioavailability	
Plasma Binding		Distribution		Metabolites		Half Life		Tmax	
Toxicity		Cmax		AUC		Clearance		Excretion	
Remarks									

Drugs

Drug_Name		ALBENDAZOLE				GVK_ID		DD-26		Category		Anthelmintic	
No_of_Met	Metabolite_Structure		Metabolite_Smiles			Metabolite_Enzyme		Mode_of_Conversion		Metabolite_Name		Metab	
DD-26-M1			O=S(C(C=C2)=CC1=C2N([H])C(N([H])C(OC)=O)=N1)(CCC)=O			Hepatic biotransformation (Microsomal flavin-containing monooxygenases and CYP450)		Sulfur oxidation		Albendazole sulfoxide		2	
DD-26-M2			O=S(C(C(O[H])=C2)=CC1=C2N([H])C(N([H])C(OC)=O)=N1)(CCC)=O			Hepatic biotransformation (cytochromes P450)		Sulfur oxidation followed by hydroxylation		6-Hydroxyalbendazole sulfoxide		2	
DD-26-M3			O=C(OC)N([H])C1=NC(C=C2S(CCC)=O)=C(C=C2)N1[H]			Hepatic biotransformation		Sulfur oxidation		Albendazole sulfone		2	
Model	Vehicle	Dose	Activity_Type	Units	Value	Value_Desc	CYP Inhibition				Refe		
Human			Ki	uM		no inhibition	Inhibition of drug metabolizing CYP1A2 enzyme				3		
Human			Inhibition	%	8.0000	8.0000	Inhibition of drug metabolizing CYP1A2 enzyme				3		
Human			Ki	uM		no inhibition	Inhibition of drug metabolizing CYP2C9 enzyme				3		
Human			Inhibition	%	0.0000	0.0000	Inhibition of drug metabolizing CYP2C9 enzyme				3		
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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