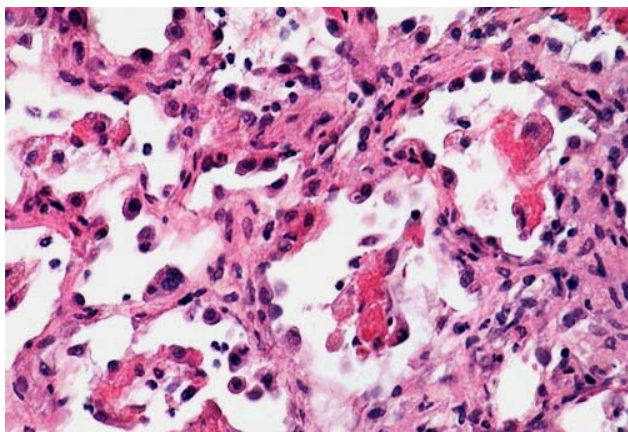


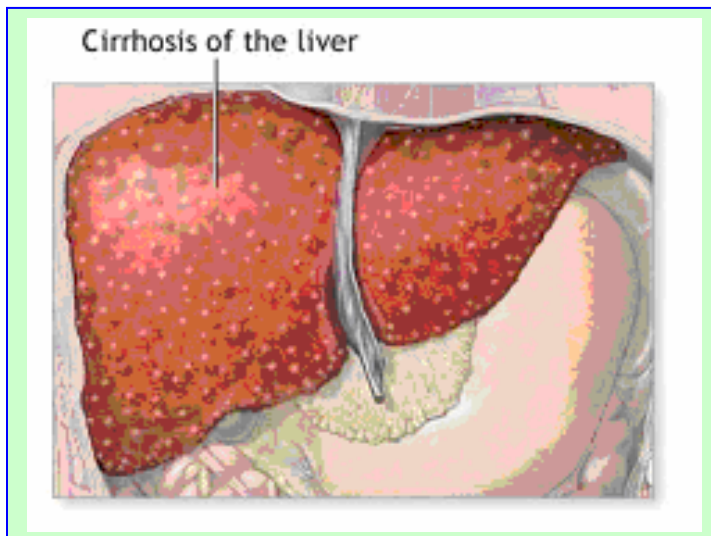
## Toxicity Database (TXD)

Toxicity Database contains the quantitative details of the different toxicities of compounds tested in various animal models. It contains details of in vivo and in vitro studies of toxicity, Neurotoxic dose, Cytotoxic dose, Hepatotoxicity, Neurotoxicity, Mortality, Lethality and Multiple dose effects etc.



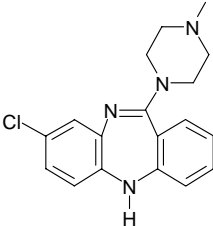
- Toxicity Database contains data mainly focused on Lethal Dose 50% (LD50), which causes death in 50% of the animals tested.
- A compound is registered in Toxicity database if acute toxicity or other in vivo toxicity is reported in any new-drug application sources like scientific literature, company source and etc.
- Compounds include synthetic compounds, drug-like substances, natural products and semi-synthetics etc.

- Type of Toxicities include:
  - Acute toxicity
  - Chronic toxicity
  - Sub-acute toxicity
  - Neurotoxicity
  - Hepatotoxicity
  - Nephrotoxicity
  - Ototoxicity
  - Cytotoxicity
  - Teratogenicity
  - Carcinogenicity
  - Mutagenicity
  - Dermatotoxicity
  - Genotoxicity
  - Embryotoxicity etc.



- The database also contains other biological activities that the compound has been tested for along with the toxicity data
- The data can be queried with any one or combination of many of the available fields and the structure can be queried with substructure search.
- Each record in the database consists of Chemical substance structure, IUPAC Name, Smiles, Authors, Literature reference, Toxicity General with its Mechanistic Terms, In vivo and In vitro Toxicity and other Biological activity data,

## Sample Record

Structure		*fmwla_Structure <b>C<sub>18</sub>H<sub>19</sub>ClN<sub>4</sub></b>	*mol.weight_Structure <b>326.8319</b>	GVK_ID <b>TXD-23965</b>	Platform_Name <b>TOXICITY</b>								
		compound_name <b>8-Chloro-11-(4-methyl-piperazin-1-yl)-5H-dibenzo[b,e][1,4]diazepine</b>											
		smiles <b>C1c1cc2c(cc1)Nc1c(ccc1)C(=N2)N1CCN(CC1)C</b>											
		Title			Ref.No								
		Prediction of hERG Potassium Channel Affinity by Traditional and Hologram QSAR Methods			1								
		5-Piperazinylalkyl-2(3H)-oxazolones with neuroleptic activity			2								
		Authors			Ref.No								
		Gyorgy M. Keseru			1								
		company_address			Ref.No								
		Computer Assisted Drug Discovery, Gedeon Richter Ltd., PO Box 27, H-1475 Budapest, Hungary			1								
		claim/example			Ref.No								
		Clozapine			1								
		reference											
		1) Bioorg. Med. Chem. Lett., 2003, 13 (16), 2773-2775											
		2) J. Med. Chem. 1989, 32 (10), 2241-2247			<input checked="" type="checkbox"/>								
S_No	Journal	Year	Volume	Issue	Start_page	End_page	PubMed_id						
1	Bioorg. Med. Chem. Lett.	2003	13	16	2773	2775	12873512						
<b>Toxicity_General</b>		<b>Mechanistic_Terms</b>		Ref.No									
Cardiotoxic		Inhibition of HERG channel		1	1) hERG potassium channel affinity								
QT interval prolongation				1	2) 5-Piperazinylalkyl-2(3H)-oxazolone derivative with Neuroleptic activity								
Torsades de pointes				1	3) 4-Piperazinyl-10H-thieno[2,3-b][1,5]benzodiazepine as potential Neuroleptic agent								
Acute toxicity				2	4) Benzodiazepine analogue with neuroleptic activity								
					5) Antipsychotic Agent								
					6) Antagonist of dopamine receptors useful as antipsychotic agent.								
<b>Toxicity in vivo Assay</b>													
Vehicle	Dose	ActivityType	Units	prefix	Value	Assay	Assay_type	REFEREN					
Mouse		LD50	mg/Kg	=	100.0000	Lethal dose in mice after intraperitoneal administration	T	2					
Mouse		LD50	mg/Kg	=	150.0000	Lethal dose in mice after peroral administration	T	3					
Mice		LD50	mg/Kg	=	150.0000	Lethal dose in mice after peroral administration	T	4					
<b>Toxicity in vitro Assay</b>													
protein	Source_Nam	Source_Coc	official_na	Locus_ID	MultipleL	Locus_ref	ActivityTy	ActivityU	Activity	ActivityValue	enzyme/cell_assay	Assay_type	REFERE
hERG potassium channel	human	Hum	KCNH2	3757			IC50	nM	=	6.4900	Inhibition of hERG potassium channel expressed in mammalian cells (HEK, CHO, COS, neuroblastoma cells)	B	1
<b>Biological_data</b>													
protein	Source_name	Source_coc	official_name	Locus_ID	MultipleL	Locus_ref	ActivityTy	ActivityU	ActivityP	ActivityValue	enzyme/cell_assay	Assay_type	REFERE
Mouse	mouse	Mouse					ED50	mg/Kg	=	4.2000	Inhibition of spontaneous motor activity in mouse, by administering perorally	F	2
Mouse	mouse	Mouse					ED50	mg/Kg	=	4.5000	Antagonistic activity against amphetamine-induced hyperactivity in mouse by administering perorally	F	2

## Other Databases

### Our other database products include:

- **TID** - Phosphatases, Kinases, Proteases and other Enzymes, Ion-Channel blockers, NHR and GPCR Agonist/Antagonist/ Inhibitors/Substrates data from Journals and Patents.
- **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.

For further information contact: Sarma Jagarlapudi PhD, Sr. VP - Informatics, Email – sarma@gvkbio.com or Sreenivas Devidas, VP, Business development, Email – sreeni.devidas@gvkbio.com, GVK Biosciences Private Limited. Phone No. 914065180632 Fax No. 91 40 23721010; Website – www.gvkbio.com