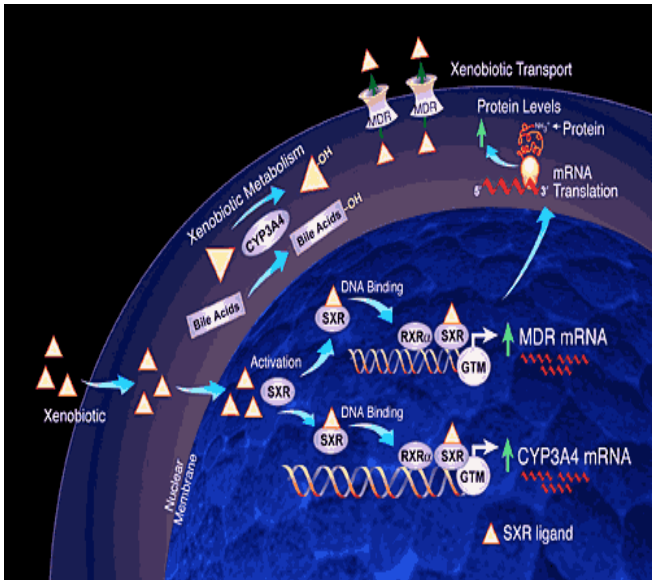
Mechanism Based Toxicity Database (MBT)

A database of compounds with its of Toxicity Mechanism and its Adverse or Side effects curated from Journals and other available sources. It contains the details of the compound and/or metabolites which induces toxicity and its significance, *In vivo* and *In vitro* details of Toxicity, Mutagenicity, skin and eye irritation, Tumorigenicity / Carcinogenicity, Reproductive effects and Multiple dose effects etc. Information from xenobiotic transformations and metabolism studies also reported apart from the toxicological data.

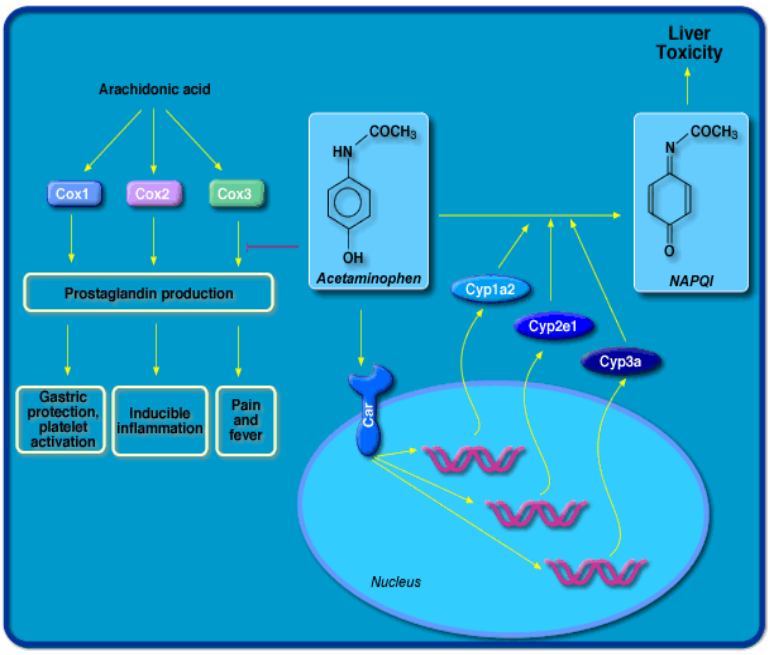


Some of the salient features are:

- Includes currently used and discontinued drugs, preclinical and clinical candidates, any other types of drug-like substances, natural products or semi-synthetics, and environmentally toxic substances like carcinogens, etc.
- Type of Toxicities includes: Neurotoxic, Hepatotoxic, Necrosis, Apoptosis, Nephrotoxic, Ototoxic, Cytotoxic, Teratogenic, Carcinogenic, Mutagenic, Dermatotoxic, Genotoxic, Embryotoxic, Acute toxicity etc.
- Includes the collection of metabolic schemes related to various toxicities.

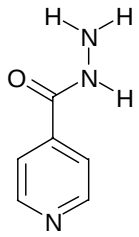
Fields available in the database:

- Each record in the database consists of Structure, Toxicity Metabolism Scheme, Structure of Toxic Metabolite/Substance, IUPAC Name, Smiles, CAS No., Species, Toxicity General, Organ Toxicity and its Indications, Mechanistic terms and its Effects, Toxicity data of Compound and its Metabolite, Literature Reference,
- The data can be queried with any one or combination of many of the available fields except the Scheme, however the metabolites can be queried with substructure or similarity search.
- Easy export of the database or retrieved results to an sdf or rdf files, ChemFinder, excel sheet, MSAccess or Oracle databases.

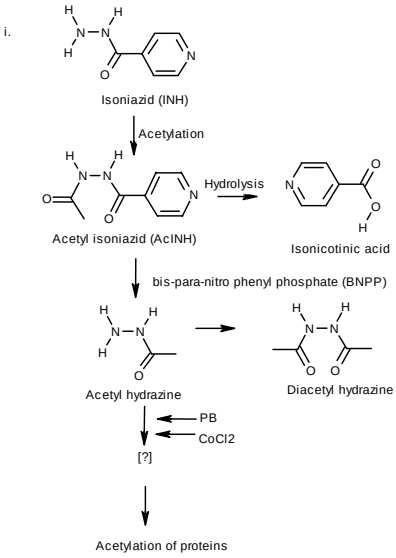


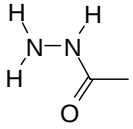
Sample Record

Structure



Metabolism



Compound Name	Toxic_Compound
Isoniazid	
Chemical/Therapeutic Category: Antituberculosis	
Toxic/Compound Metabolite Nam: Acetyl hydrazine	
Mechanism Hypothesis/Proof: Proven	TCD_ID: MBT-5083-TCD-1

*fmla_Structure	*mol.weight_Structure	GVK_ID	CAS. NO
$C_6H_7N_3O$	137.1422	MBT-5083	54-85-3

Metabolism	Species	Ref_No
i	Human	1

IUPAC Name: **Isonicotinic acid hydrazide**

Smiles: **O=C(c1ccncc1)NN**

Mechanism	Species	Ref
Isoniazid on acetylation produces acetylisoniazid which further produces acetylhydrazine undergoes phase I type oxidation and	Human	1

S. No	Journal	Year	Volume	Issue	Start Page	End Page	PubMed_ID
1	Toxicology, Edited by Hans Marquardt, Siegfried G. Schafer, Roger McClellan and Frank Welsch,	1999			273	296	

Toxicity General	Species	Ref	Organ Specific	Indications	Species	Ref	Mechanistic Terms	Species	Ref	Effects	Species	Ref
Hepatotoxic	Human	1	Liver	Jaundice	Human	3	Reactive metabolite	Human	1	Hepatic necrosis	Human	1
Neurotoxic	Human	2	Neural	Seizures	Human	3	Covalent binding	Human	1			

Toxicity Data

Species	Route	Value	Exposure Time	Units	End Point	Assay Description	Assay_Method	Ref_No
Salmonella typhimurium		0.0000		revertants/plate	Mutagenicity	Mutagenicity of the compound in S. typhimurium TA1537 was determined using ames reversion test; No increase of revertants	AMES	5
Salmonella		0.0004		revertan	Mutagenicity	Mutagenic potency of the compound was	AMES	5

Metabolite Toxicity Data

Metabolite Nam	Species	Route	Value	Exposure Tim	Units	End Point	Assay Description	Assay_Method	Ref_N
Acetyl hydrazine	Dog	Oral	50.0000		mg/kg	LD50	Oral lethal dose in dog	Acute toxicity	2
Acetyl	Mouse	Intraveno	149.0000		mg/kg	LD50	Intravenous lethal dose in mouse	Acute toxicity	2

Other Databases

Our other database products include:

- **MCD** - Medchem Database consisting of biologically active compounds.
- **TID** - Kinases, Phosphatases, Proteases and other Enzymes, NHRs, Ion-Channel blockers, Transporters and GPCR Agonist/Antagonist/ Inhibitors data from Journals and Patents.

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