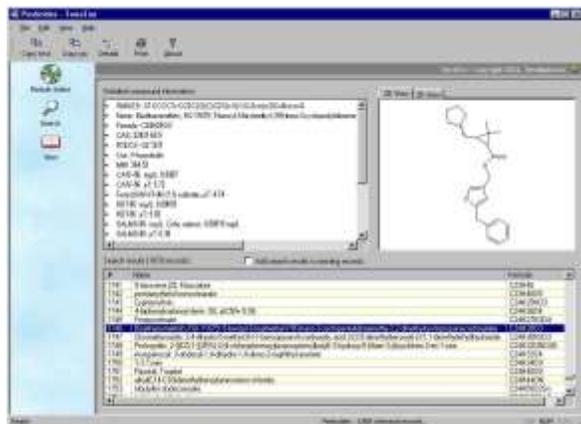


TerraTox™ - Databases

TerraTox™ databases provide for the quick search of compounds with structure/fragment-specific biological effects and properties. All modules include the superior TerraTox 3.0 search engine for the [simultaneous searching of all of the search types shown below](#):

Structure: 2D or 3D structure fragment
Name: both present and absent text fragments
Formula: exact or partial chemical formula
CAS: complete or partial CAS registry number
Property: choose 2 from available parameter list
Value: choose range(s) or specific value(s)

An example from TerraTox - Pesticides



Available TerraTox database modules:

Explorer	100,000+ chemicals, variety of data
Antimalarials	2,650 compounds w. antimal. act.
AQUA	6,500 compds. w. aquat. toxicity
COX inhibitors	680 compounds w. COX inh. act.
Critical Data	1,350 compounds w. critical data
Drugs	48,300 chemicals, variety of data
Dyes	1,880 chemicals, variety of data
Fragrances	2,760 chemicals, variety of data
HBEE	300 chemicals, honey bee data
HIV-1	6,900 chemicals with HIV-1 data
Ionic Liquids	1,400 chemicals, variety of data
Natural Products	13,700 chemicals, variety of data
Pesticides	5,530 pesticidals, variety of data
Skin	3,300 chemicals w. skin & eye data
Steroids	4,900 chemicals with RBA data
Surfs. & Chelats.	1,110 chemicals, variety of data
Tetrahymena	2,060 chemicals w. <i>T. pyriformis</i> data
Vibrio fischeri	3,540 chemicals w. <i>V. fischeri</i> data

Data notations & compatibility

Most TerraTox databases have data notations both in mg/L or mg/kg and also in a normalized notation (pT) as log(L/mmol) or log(kg [b.w.]/mmol) values for most toxicity endpoints.

Examples of parameters in TerraTox modules:

Receptor effects (partial list):

Adrenoreceptor (beta3) agonist activity, EC50 [microM]
Anti-malarial activity, (*Plasmodium falciparum*), log(1/C50)
Calcium channel blocking activity, log(1/IC50) [M]
Cyclooxygenase-2 inhibition, log(1/IC50)
Diazepam binding inhibition, IC50 [nanoM]
Dopamine beta-hydroxylase inhibition, log(1/IC50) [M]
Endothelin antagonist activity, IC50 [nanoM]
Histamine H2 agonist activity, pD2
Lipase inhibition (*Pseudomonas* sp.) [microM]
Norepinephrine inhibition, log (1/IC50) [M]
Octopaminergic activity, pKi
Platelet aggregation inhib. (rabbit plasma), log(1/IC50)
Protein tyrosine p56lck kinase inhibition, log(1/IC50)
Protox assay, IC50, [microM]
Relative sweetness, log(RSI)
Retinoid receptor binding, Kd-alpha [nanoM]
Serotonin (5-HT) inhibition, log (1/IC50) [M]
Tetracycline efflux antiport prot. inhib., log(1/C) [microM]
Tubuline polymerization inhibition, IC50 [microM]
Tumor growth inhibition, log(% tumor weight inhib.)

Organism effects (partial list):

ARTEM, 24-hr LC50 for shrimp *Artemia salina*
BGILL, 96-hr LC50, bluegill sunfish *Lepomis macrochirus*
CEROD, 48-hr LC50 (mg/L) for *Cerodaphnia dubia*
CHLORV, 96-hr LC50 for green algae *Chlorella vulgaris*
DM, 48-hr LC50 for *Daphnia magna*
FHM, 96-hr LC50 for fathead minnow *Pimephales prom.*
GOLDF, 96-hr LC50 for the goldfish *Carassius auratus*
GUPPY, 96-hr LC50 for the guppy *Poecilia reticulata*
IPMOUS, *i.p.* LD50 for the mouse *Mus musculus*
IVMOUS, *i.v.* LD50 for the mouse *Mus musculus*
MTOX-15, 15-min EC50 for *Vibrio fischeri*
MUSCAd, 24-hr topical LD50 for fly *Musca domestica*
MYSID, 96-hr LC50 for *Mysidopsis bahia*
OMOUS, LD50 for the mouse *Mus musculus*
RBT, 96-hr LC50 for rainbow trout *Oncorhynchus mykiss*
RKF, 96-hr LC50 for the red killifish *Oryzias latipes*
SELEc, 96-hr LC50 for algae *Selenastrum capricornutum*
TEHY, 48-hr LC50 for the ciliate *Tetrahymena pyriformis*
WSUCK, 96-hr LC50 for sucker *Catostomus comm.*
ZEBF, 96-hr LC50 for the zebrafish *Brachydanio rerio*

Other data & effects (partial list):

BIODEG, ready & inherent biodegradability, (%)
CARCIN, carcinogenicity information
SOL, the aqueous solubility of the compound (measured)
LOGBCF, bioconcentration factor (measured)
Use / Effect, the major use and/or effect(s) of chemical

TerraTox data are carefully scrutinized for accuracy and consistency before acceptance.

For a complete list of organisms & effects, see:

<http://www.terrabase-inc.com>

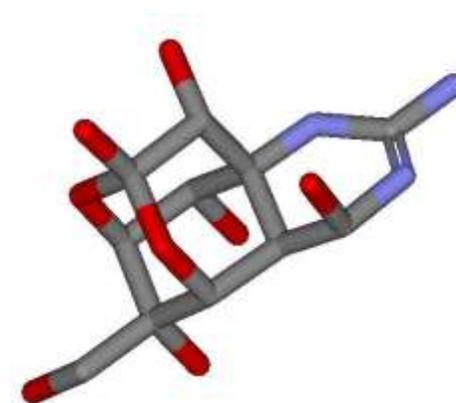


TerraBase Inc.

TerraTox™ - Databases

TerraQSAR™ - Programs

Services



tetrodotoxin (pufferfish toxin), CAS 4368-28-9, *i.v.* mouse LD50: 0.007 mg/kg b.w. (pT = 4.64), TerraQSAR-RMIV: 4.64, TerraQSAR-LOGP: -1.01

DEMO CDs pro tem. unavailable

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