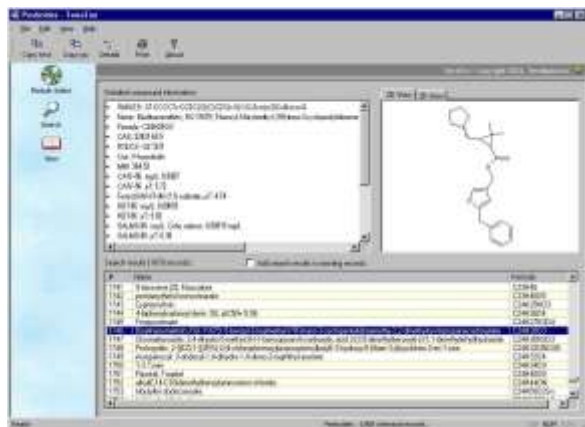


## TerraTox™ - Databases

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:

<b>Explorer</b>	99,200 chemicals, variety of data
<b>Antimalarials</b>	2,650 compounds w. antimal. act.
<b>AQUA</b>	6,500 compds. w. aquat. toxicity
<b>COX inhibitors</b>	680 compounds w. COX inh. act.
<b>Critical Data</b>	1,350 compounds w. critical data
<b>Drugs</b>	47,900 chemicals, variety of data
<b>Dyes</b>	1,880 chemicals, variety of data
<b>Fragrances</b>	2,760 chemicals, variety of data
<b>HBEE</b>	300 chemicals, honey bee data
<b>HIV-1</b>	6,900 chemicals with HIV-1 data
<b>Ionic Liquids</b>	1,290 chemicals, variety of data
<b>Natural Products</b>	13,600 chemicals, variety of data
<b>Pesticides</b>	5,500 pesticides, variety of data
<b>Skin</b>	3,300 chemicals w. skin & eye data
<b>Steroids</b>	4,900 chemicals with RBA data
<b>Surfs. &amp; Chelats.</b>	1,100 chemicals, variety of data
<b>Tetrahymena</b>	2,060 chemicals w. <i>T. pyriformis</i> data
<b>Vibrio fischeri</b>	3,200 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>

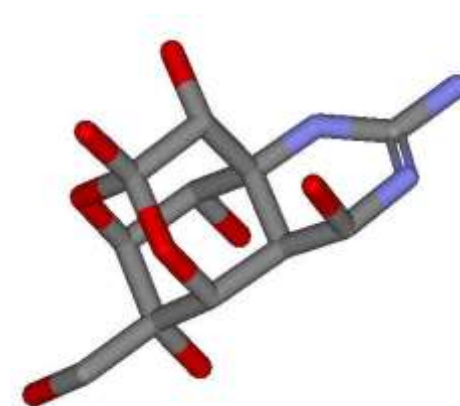


TerraBase Inc.

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 available

**TerraBase Inc.**  
**1063 King St. W., Suite 130**  
**Hamilton, Ontario L8S 4S3**  
**Canada**  
[mail@terrabase-inc.com](mailto:mail@terrabase-inc.com)

[www.terrabase-inc.com](http://www.terrabase-inc.com)

