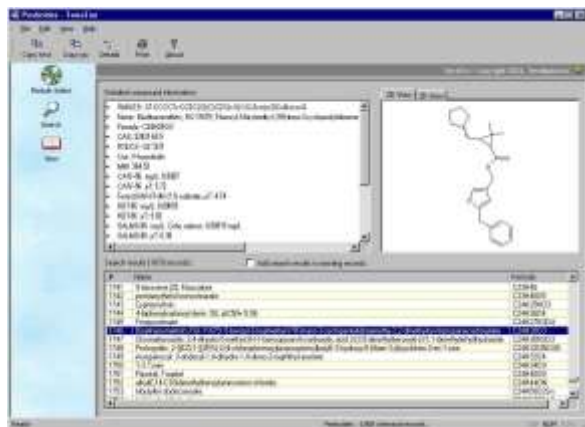


TerraTox™ - Databases

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. pyrifer</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>

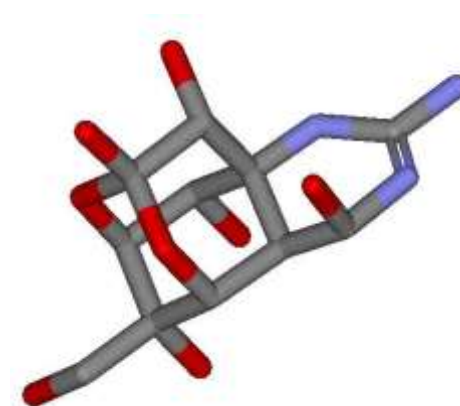


TerraBase Inc.

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

TerraBase Inc.
1063 King St. W., Suite 130
Hamilton, Ontario L8S 4S3
Canada
mail@terrabase-inc.com

www.terrabase-inc.com

