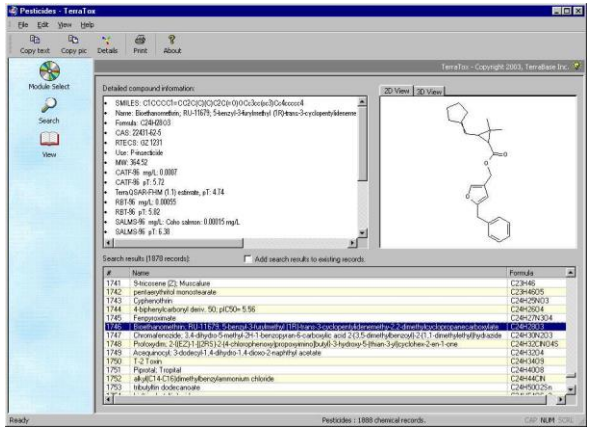
TerraTox™ - Databases

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	99,300 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	48,000 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	1,340 chemicals, variety of data
Natural Products	13,600 chemicals, variety of data
Pesticides	5,500 pesticidals, variety of data
Skin	3,300 chemicals w. skin & eye data
Steroids	4,900 chemicals with RBA data
Surfs. & Chelats.	1,1000 chemicals, variety of data
Tetrahymena	2,060 chemicals w. *T. pyrifor.* data
Vibrio fischeri	3,300 chemicals w. *V. fischeri* 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(IC50)
- 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 aggregration 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 inhhibition, 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 *Oncorhyncus 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

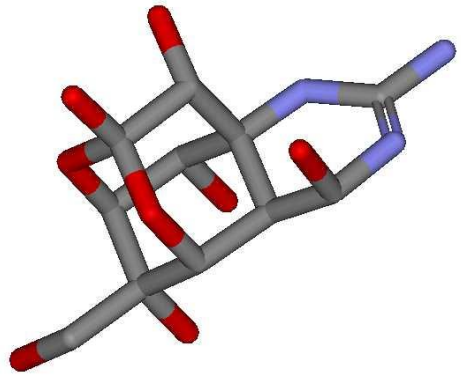
TerraTox data are carefully scrutinized for accuracy and consistency before acceptance.
For a complete list of organisms & effects, see:
http://www.terrabase-inc.com

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

www.terrabase-inc.com

 Jul. 2017

TerraQSAR™ - Programs

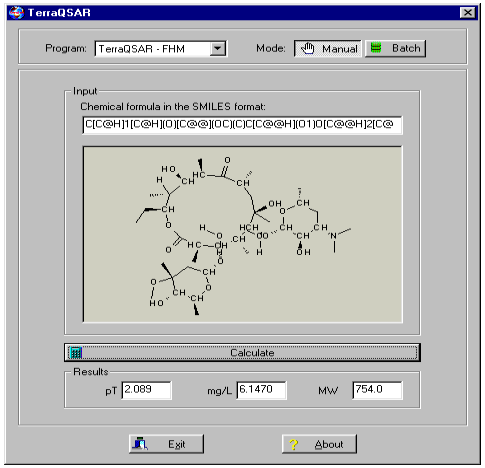
TerraQSAR™ computation programs are designed for the quick and reliable estimation of biological effects and physico-chemical properties of organic (carbon-containing) compounds using personal computers with a Windows® operating system.

Output: computed effect/property value in pT (log1/C) and mg/L (for RMIV: mg/kg b.w.), and mol. weight (MW).

Available TerraQSAR program modules:

- **CARC** carcinogenicity potential (in preparation)
- ***Daphnia*** 48-hr LC50 for *Daphnia magna* immobiliztn.
- **E2-RBA** estrogen receptor binding affinity (RBA), relative to 17*beta*-estradiol (E2)
- **FHM** 96-hr LC50 for fathead minnow (*Pimephales promelas*)
- **LOGP** octanol/water partition coefficient
- **OMAR** mouse & rat oral LD50
- **RMIV** rat & mouse *intravenous* LD50
- **SKIN** skin irritation % corrosion potential

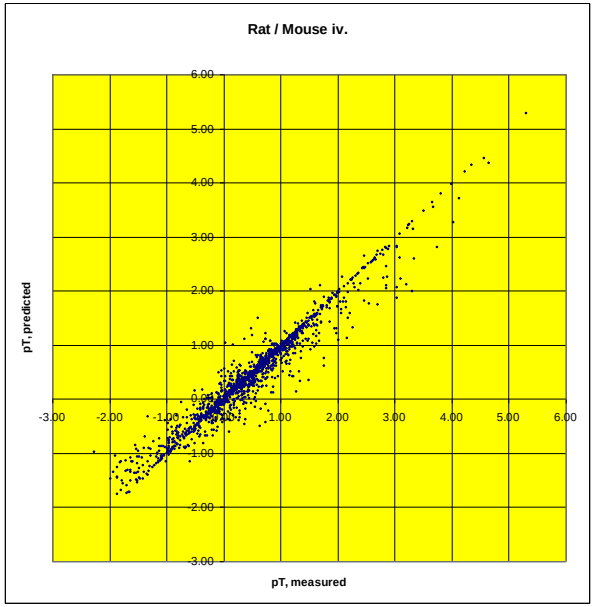
An example from TerraQSAR - FHM



The antibiotic compound **Erythromycin B**, CAS 527-75-3, (only part of the SMILES code is visible in the *Input* field) has a predicted fathead minnow 96-hr LC50 of 5.95 mg/L and a pT= log(1/LC50) of 2.08.

TerraQSAR software gives fast and reliable answers to your estimation requirements. Most computations take a few seconds only with seamless switching between the available program modules.

TerraQSAR – RMIV, measured *vs.* predicted



Above plot shows measured *vs*. predicted values of the 4000+ data in the TerraQSAR - RMIV training set. Leave-one-out cross-validation RMSE = 0.20.

Input

TerraQSAR programs use as input **SMILES** (Simplified Molecular Input Line Entry System) strings (2-D or 3-D). The built-in structure editor allows instant verification of each 2D or 3D string written. SMILES strings can also be copied form other sources, such as text or spreadsheet, or database files, and pasted into the TerraQSAR modules.

Methodology

TerraQSAR programs use the probabilistic neural network (PNN) methodology which is based on the **estimation of the conditional average**. Unlike most other neural network methodologies, the PNN training is 100% repeatable in every aspect of the training and application. Furthermore, and in contrast to entirely linear methodologies, such as regression methods, the PNN system uses both linear and non-linear relationships. Therefore, the PNN is particularly well suited for the computation of effects for compounds with unknown or multiple modes of action. Examples demonstrating the superiority of the PNN methodology are found at our website at www.terrabase-inc.com.

Fragments

Major fragments used in the TerraQSAR modules have been described in detail in several publications listed in the literature. An overview of the **types** of fragments used is given in Table 1 below.

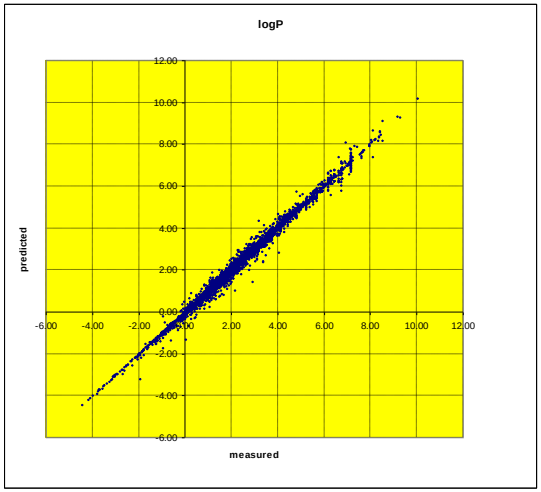
Table 1. Types of fragments used in **TerraQSAR**

Fragment type	Examples
Acidity fragment	C(=O)O, S(=O)(=O)O
Aliphatic ring fragment	C1CCCCC1, C1CC1
Aromatic ring fragment	c1ccccc1, c1ccccn1
Atom fragment	C, H, N, O
Bond fragment	C-C, C=C, C#C
Group fragment	C-O-H, C-O-C
Hydrophobicity fragmt.	C(C)(C)C, CCCC
Ionization fragment	[O-], [Na+]
Polarity fragment	O=N(=O)CC(O)
Reactivity fragment	C=CC=O
Stereo fragment	CC[C@H](C)N
Weight fragment	molecular weight

Manuals

All TerraQSAR programs come with built-in manuals in pdf format. They can also be downloaded from our web site.

TerraQSAR – LOGP, measured *vs.* predicted



Above plot shows measured *vs*. predicted values of the 4000+ data in the TerraQSAR - LOGP training set. Leave-one-out cross-validation RMSE = 0.11.