Know the Toxic Potential of Your Compounds Sooner

Tox Boxes

Predictions for a variety of common toxicological tests.

Advanced Chemistry Development

ACD/Labs

Pharma Algorithms

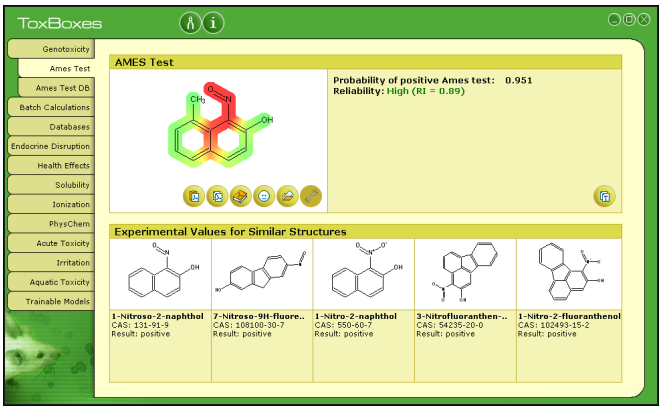
Visionary Software Advancing Research

Early toxicity screening with Tox Boxes can help reduce attrition rates, focus animal testing requirements, and provide information rapidly to help direct new compound synthesis. Using novel computational methods, Tox Boxes predicts probabilities for basic toxicity endpoints, and also allows for the assessment of prediction applicability and estimation of reliability that goes beyond abstract statistical modeling.

Customize Tox Boxes to Get the Results You Need

Modules are available for the prediction of:

- Acute Toxicity
- Genotoxicity
- Aquatic Toxicity
- Health Effects
- hERG Inhibition
- CYP3A4 Inhibition
- Endocrine System Disruption
- Eye/Skin Irritation

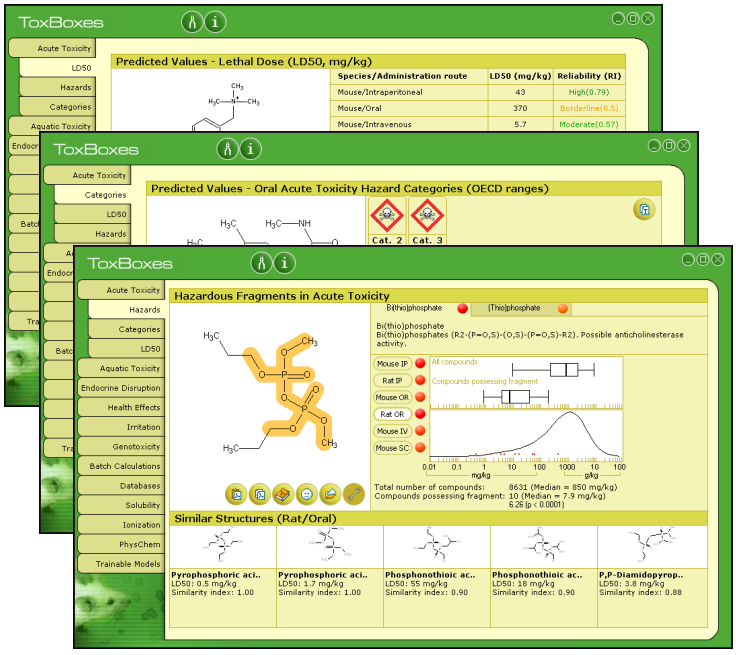


Visualize Toxic Elements

Structural fragments and toxicophores contributing to adverse effects are identified and highlighted with color-mapping, allowing you to easily visualize the problem areas.

Ensure the Quality of Your Predictions

For every predicted result, a Reliability Index (RI) indicates the 'applicability' of the prediction algorithm based on the structural similarities to compounds in the training set. Experimental values for the 5 most similar structures in the training set are displayed to help further understanding of the applicability domain of the model, ensuring high quality results.



Increase Applicability with Your Own Data

Expand the applicability and accuracy of certain models by incorporating proprietary structures with experimental data into the training sets, resulting in greater accuracy of predictions for the compounds in the chemical space of interest.

ACD/Labs and Pharma Algorithms, Inc., have joined forces, creating an opportunity for integrating the two companies' complementary physicochemical property and ADMET prediction products. The result will be the next-generation of *in silico* modeling tools for pharmaceutical and chemical research, assisting the research process to bring safe and effective novel compounds to market faster.

Prediction modules are based on large, validated databases, and robust Structure-Activity Relationship (C-SAR, QSAR) models in combination with expert knowledge of orgainic chemistry and toxicology.

Available Modules		DB size
hERG Inhibition Trainable	The hERG Inhibition module predicts the probability that a compound will exhibit cardiotoxicity associated with hERG channel inhibition at clinically relevant concentrations (Ki < 10 mM).	600 compounds
CYP3A4 Inhibition Trainable	CYP3A4 enzyme inhibition can lead to drug-drug interactions and adverse effects.	900+ compounds
Genotoxicity Trainable	Predicts the probability of compounds exhibiting a positive Ames test result, identifies well-known genotoxic alerts, and displays experimental confirmation of observed effects for different strains (with/without metabolic activation).	8500+ compounds
Acute Toxicity	Predict lethal dose (LD50) for 6 different animal systems: Rat–oral and intraperitoneal Mouse–oral, intraperitoneal, intravenous, subcutaneous The Acute Toxicity module also classifies compounds in OECD categories, and identifies 'toxicophores' and hazardous fragments that may be responsible for acute toxicity of compounds in rodents. Reliablity Index indicates whether compounds belong to the model's applicability domain.	100,000 compounds
Aquatic Toxicity	Predict LC50 (mg/L), the standard measure of aquatic toxicity based on experimental LC50 data for Fathead minnow (Pimephales promelas) and Water flea (Daphnia magna). Reliablity Index indicates whether compounds belong to the model's applicability domain.	900 compounds (P. promelas) 600 compounds (D. magna)
Health Effects	Predicts probabilities of adverse effect in different organ systems. Probabilistic models were based on data from long-term, organ specific toxicity studies incorporating data from chronic, subchronic, acute, and carcinogenicity studies encompassing various species and routes of administration.	
Irritation	The Irritation Module estimates the potential of a compound to cause eye or skin irritation in a standard Draize test on rabbits. Structural elements that may contribute to the adverse effect are highlighted using color-mapping.	2100+ compounds
Endocrine System Disruption	This module classifies compounds depending on the predicted ability to bind to ER (Strong, Weak, or No Binding) with probabilities given for Strong and Overall Binding.	1500 compounds
ADME Properties Requires ADME Boxes	Integration with ADME Boxes enables rapid property estimations of physicochemical properties including Log*P*, TPSA, No. of Rotatable Bonds, H-Bond Donors and H-Bond Acceptors, pK_a, Log*D*, and solubility in pure water values (LogSw).	