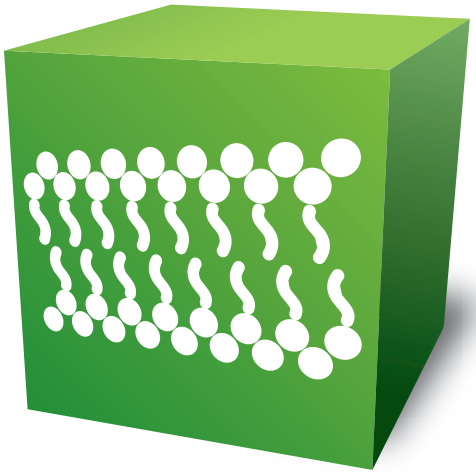
A Better Way to Turn Data into Decisions



ADME Boxes

In silico prediction of a variety of ADME–related properties.

Advanced Chemistry Development

ACD/Labs

Pharma Algorithms

Visionary Software Advancing Research

Reduce the need for expensive, labor intensive experimental testing and focus your efforts on compounds that exhibit those properties that meet certain physicochemical requirements. ADME Boxes helps by predicting a wide range of properties, complete with an assessment of prediction applicability and estimation of reliability that goes beyond abstract statistical modelling.

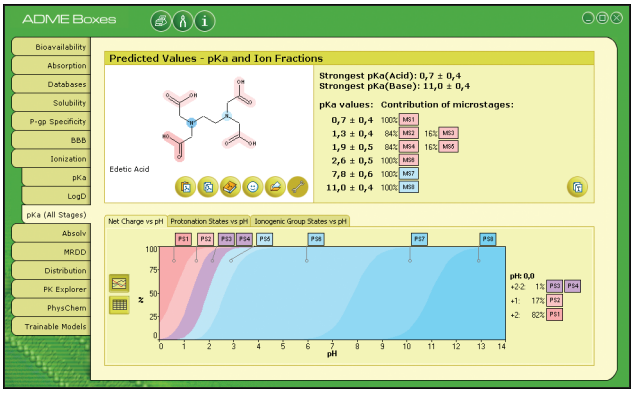
Customize ADME Boxes to Get the Results You Need

Modules are available for the prediction of :

- Oral Bioavailability
- BBB Permeation
- Passive Absorption
- Ionization
- P-gp Specificity
- Absolv (solvation parameters)
- Solubility and more

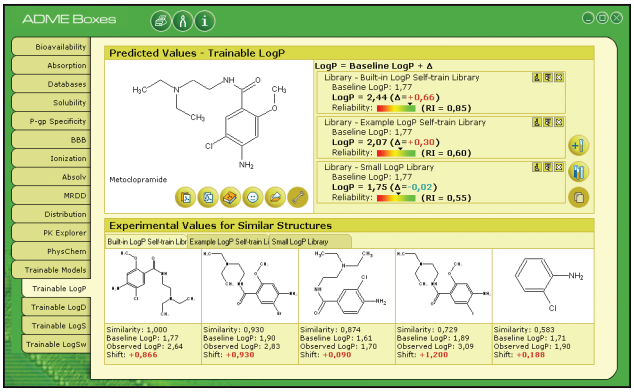
Visualization of Your Results

Structural elements contributing to a particular property are identified and highlighted with color-mapping, allowing you to easily visualize important molecular characteristics.



Ensure the Quality of Your Predictions

For most predicted results, 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 3 or 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 experimental or proprietary structures and data into the training sets, resulting in greater reliability for your compounds of interest.

Browse or Search Reference Databases

Access much of the data that constitutes the training sets of several ADME Boxes modules including:

- Oral Bioavailability Database (790 compounds)
- Solubility Database (5435 compounds)
- Human Intestinal Absorption Database (865 compounds)
- P-gp Specificity Database (2290 compounds)
- Absolv Database (5004 compounds)

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 scientific intuition.

Available Modules	
Passive Absorption	Makes accurate predictions of passive intestinal, Caco-2 permeability, and the extent of oral absorption based on models with the easily interpreted physicochemical parameters of lipophilicity and ionization.
Oral Bioavailability	As an extension of the absorption model, an evaluation of a series of factors that affect bioavailablity. Results are classified into one of three categories; Problematic, Suspect, and Acceptable. The influence of solubility, stability in acidic environment, passive absorption, first-pass metabolism, P-gp, efflux, and active transport are considered.
P-gp Specificity Trainable	Calculates the probability of a compound being a P-gp substrate or inhibitor–two properties that are important factors in pharmacokinetics of a drug, especially BBB permeation.
Solubility Module Trainable	Provides quantitative solubility predictions for pure water at 25°C and solubility-pH profile at various physiological pHs. Also has the capability to estimate qualitative solubility at four relevant thresholds.
Blood-Brain Barrier Permeation (LogPS)	Provides reliable and easily interpreted predictions of BBB permeability rate (expressed as LogPS constants) that allows ranking of compounds according to their passive BBB permeability. It may serve as an initial screen that could compete with, and at least partially replace, expensive LogPS determination in animals.
Ionization Trainable	Predicts acid and base pK_a values for complex polyelectrolytes as well as the distribution of ionic fractions at physiological pHs (all protonation states). Includes calculation of Log*D*.
Absolv	Developed with Prof M.H. Abraham, the Absolv module predicts Abraham solvation parameters such as H-binding acidity and basicity parameters (A, B, and B_o), gas phase–hexadecane partitioning coefficient (L), polarity/polarizability parameter (S), excessive molar refraction (E), McGowan volume (V), and contributions of each atom to the selected parameter.
Distribution *Trainable	This module can be used to predict plasma protein bound fraction*, equilibrium binding constant to blood serum albumin*, and the apparent volume of distribution for a compound.
PK Explorer	A tool for exploring the dependence of oral bioavailability, drug plasma levels on dose, and physicochemical and pharmacokinetic parameters of compounds. PK Explorer also simulates drug-plasma concentration versus time .
PhysChem *Trainable	This module provides a quick check of several useful physicochemical properties including Log*P**, total polar surface area (TPSA), number of rotatable bonds, H-Bond donors and H-Bond acceptors. The PhysChem module is included with all modules above.