The ADMET Collection provides components that calculate predicted absorption, distribution, metabolism, excretion and toxicity (ADMET) properties for collections of molecules such as synthesis candidates, vendor libraries, and screening collections. Optimizing these properties during discovery efforts is critical for reducing problems in later development. The collection includes models for human intestinal absorption, aqueous solubility, blood brain barrier penetration, plasma protein binding, cytochrome P450 2D6 inhibition, and hepatotoxicity. With these components, you can create protocols that:

- Rapidly profile compound collections for ADMET property distributions
- Eliminate compounds with bad ADMET characteristics from further consideration
- Evaluate proposed refinements to compounds, designed to improve their ADMET properties, prior to synthesis
- Include ADMET properties together with experimental and other calculated properties in compound profiling reports
Predicts Human Intestinal Absorption (HIA) after oral administration and reports a classification of absorption level. The pattern recognition model underlying the method is based on calculations of logP and polar surface area and is derived from a training set of 199 well-absorbed molecules with actively transported molecules removed.


Predicts the solubility of each compound in water at 25°C and reports the predicted solubility and a ranking relative to the solubilities of a set of drug molecules. A genetic partial least squares method was used to derive the model using a training set of 784 compounds with experimentally measured solubilities.


Predicts the blood brain barrier penetration of a molecule, defined as the ratio of concentrations after oral administration, and reports the predicted penetration as well as a classification of penetration level. The model combines a confidence ellipse derived from over 800 compounds classified as CNS therapeutics with a robust regression model based on 120 compounds with measured penetration to predict penetration values for those molecules falling within the confidence ellipse.

Predicts whether or not a compound is likely to be highly bound to carrier proteins in the blood. Predictions are based on the similarity between the candidate molecule and two sets of marker molecules; one used to flag binding at a level of 90 percent or greater and the other at 95 percent or greater. Binding levels predicted by the marker similarities are modified according to conditions on calculated logP.


Predicts cytochrome P450 2D6 enzyme inhibition and reports whether or not a compound is likely to be an inhibitor, as well as a probability estimate for the prediction. Predictions are based on ensemble recursive partitioning model of a training set of 100 compounds with known CYP2D6 inhibitions.


Predicts the occurrence of dose-dependent human hepatotoxicity. Compounds are classified as either toxic or non-toxic, and a confidence level indicates the model’s likely accuracy. Predictions are based on an ensemble recursive partitioning model of 382 training compounds known to exhibit liver toxicity or to trigger dose-related elevated aminotransferase levels in more than 10 percent of the human population.