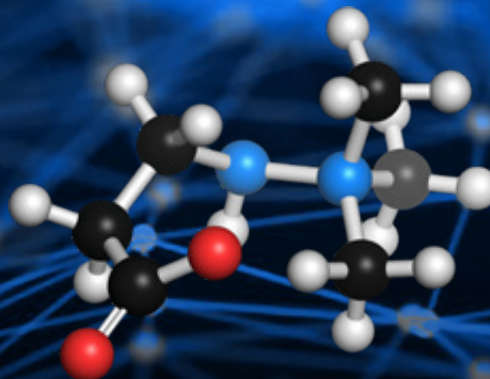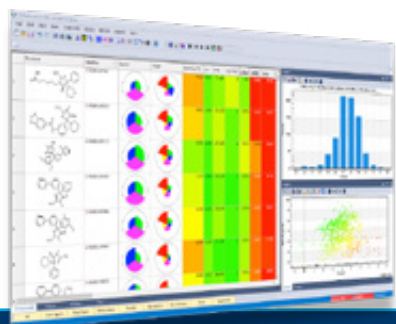# ADMET Predictor® 9.5

AI-Powered ADMET...

With the #1 ranked machine learning prediction software

ADMET Predictor® is a software package that quickly and accurately predicts over 140 absorption, distribution, metabolism, excretion, and toxicity (ADMET) properties. The graphical user interface is intuitive, easy to use, and contains stunning graphics that allows one to quickly assess ADMET properties. Cheminformatic features such as substructure and text queries, duplicate checking, structure standardization, and other tools are also included.

The HTPK Simulation™ Module - Now Available

This method can be used to filter compounds based on predicted exposure. Predict intestinal absorption (Fa%), oral bioavailability (F%), and the oral dose required to achieve a specified plasma concentration. The algorithm uses our Advanced Compartmental Absorption and Transit (ACAT™) and minimal PBPK models to simulate dissolution, absorption, and systemic exposure. Simulations can be performed using rat or human physiology. The liver clearance used in the algorithm can come from our *in silico* intrinsic clearance models or your *in vitro* experiments.

What else can it do?

• The MedChem Studio™ Module contains tools to cluster compounds containing the same scaffold, perform R-group deconvolution, matched molecular pair analysis (MMPA), and much more.

• The ADMET Modeler™ Module can be used to create highly accurate machine learning models from your in-house data sets.

• ADMET liabilities can be determined quickly using the ADMET Risk™ score that evaluates each molecule based on physicochemical, biopharmaceutical, metabolism, and toxicity properties. The property values are then compared to thresholds obtained by analysis of a subset of orally available compounds in the World Drug Index (WDI).

ADMET Predictor Modules

• Physicochemical and Biopharmaceutical
• Metabolism
• Toxicity
• MedChem Studio™
• ADMET Modeler™
• HTPK Simulation™

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