# ADMET Predictor® X.4

## Drug Design... Meet PBPK

### #1-ranked Machine Learning prediction software

ADMET Predictor 10.4 (APX.4) enhances the already industry-leading capabilities within the ADMET Predictor AIDD Module and establishes the program as the premier environment for AI-driven drug discovery. Leveraging the outputs from 3rd-party programs, such as those from 3D molecular docking applications or advanced statistical packages such as R, complements the novel physiologically based pharmacokinetic (PBPK) modeling methods embedded within the module and unlocks the completely unique ability to optimize molecules based on combinations of activity and systemic exposure. This differentiates ADMET Predictor from other companies and opens new doors for the AI-driven drug design community.

"The **AIDD Module** integrates ADMET Predictor's top-ranked machine learning models with new **generative chemistry**, **evolutionary algorithms**, and **#1-rated PBPK capabilities** - drug design... meet PBPK"

### What's NEW! in APX.4?

- **NEW** 3D conformer generation functionality to easily predict properties using advanced 3D molecular and atomic descriptors
- **NEW** mouse species models added to the HTPK Simulation Module to complement the rat and human options for novel lead selection activities
- **NEW** transform rules added to the AIDD Module to boost the virtual design space
- **REBUILT** Ames mutagenicity property models which significantly expand the chemical coverage space and improve prediction reliability
- **IMPROVEMENTS** to the API and command line features for flexible deployment and workflow option

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