



ADMET Predictor® X.3

Drug Design... Meet PBPK

#1-ranked Machine Learning prediction software

ADMET Predictor 10.3 (APX.3) 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 in APX.3?

- **NEW** capabilities in the Artificial Intelligence-driven Drug Design (AIDD) Module to incorporate calculations from any 3rd-party program for use in compound optimization
- **MAJOR UPDATE** to CYP metabolism models with new knowledge-base that significantly expands the addressable chemical space coverage
- **ACCESS** to MedChem Studio™ extended to **all users** to provide high-quality data visualization, compound clustering, R-group analysis, subset selection, activity cliff detection and more
- **NEW** REST API for deployment via Web services



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