ADMET Predictor

Flagship AI/ML platform for fast and accurate prediction of over 175 ADMET properties for drug discovery and chemical risk assessment.

https://www.simulations-plus.com/software/admetpredictor/

Overview

ADMET Predictor is the flagship artificial intelligence/machine learning (AI/ML) platform developed by Simulations Plus for predicting Absorption, Distribution, Metabolism, Excretion, and Toxicity (ADMET) properties of chemical compounds. It is an essential tool for drug discovery and chemical risk assessment scientists, enabling them to quickly screen large compound libraries and prioritize molecules with optimal pharmacokinetic and safety profiles.

Key Benefits and Capabilities:

High-Throughput Prediction: Quickly and accurately predicts over 175 properties, including aqueous and biorelevant solubility, logD vs. pH curves, pKa, CYP and UGT metabolism outcomes, and key toxicity endpoints (e.g., Ames mutagenicity, Drug-Induced Liver Injury - DILI).
AI-Driven Drug Design (AIDD): Features an upgraded AIDD engine that combines AI/ML with mechanistic High-Throughput PBPK (HT-PBPK) simulations, powered by the integrated GastroPlus® software, for faster and smarter decision-making at the intersection of chemistry and pharmacokinetics.
Custom Model Building: The ADMET Modeler™ module allows researchers to build their own high-quality QSAR/QSPR models using state-of-the-art machine learning algorithms and ADMET Predictor's extensive set of molecular descriptors.
Enterprise Automation: Offers enterprise-ready automation via a REST API, Python scripting support, and components for third-party informatics platforms like KNIME and BIOVIA Pipeline Pilot, allowing seamless deployment into existing R&D workflows.

Visualization and Analysis: Includes customizable visualization tools like star plots, distribution and 2D/3D scatter plots, and the integrated MedChem Studio™ module for advanced cheminformatics features like R-group analysis, clustering, and compound selection.
ADMET Predictor models are built on premium datasets and have been consistently ranked as highly accurate in independent published comparisons, making it a reliable and powerful platform for optimizing lead compounds and reducing the risk of late-stage drug failure.

Key Features

- Prediction of over 175 ADMET properties
- AI-Driven Drug Design (AIDD)
- High-Throughput PBPK (HT-PBPK) Simulation
- ADMET Modeler™ for custom QSAR/QSPR model building
- MedChem Studio™ for cheminformatics analysis
- CYP and UGT metabolism prediction
- Toxicity prediction (e.g., DILI, Ames mutagenicity)
- REST API and Python wrappers for enterprise automation

Pricing

Model: enterprise

Commercial software licensed to pharmaceutical, biotechnology, and chemical companies. Pricing is not publicly disclosed and is typically based on a license agreement for specific modules and user count. Special programs are available for biotech and pharma incubator companies.

Target Company Size: medium, enterprise

Integrations

GastroPlus®, Certara D360, Schrödinger LiveDesign®, BIOVIA Pipeline Pilot, KNIME

Compliance & Certifications

FDA 21 CFR Part 11 (Implied by industry use)