Resource Summary Report

Generated by NIF on Sep 13, 2026

ADMET Predictor

RRID:SCR_014903
Type: Tool

Proper Citation

ADMET Predictor (RRID:SCR_014903)

Resource Information

URL: http://www.simulations-plus.com/Products.aspx?pID=13

Proper Citation: ADMET Predictor (RRID:SCR_014903)

Description: Software program for advanced predictive modeling of Absorption, Distribution, Metabolism, Elimination, and Toxicity (ADMET) properties of chemical substances in the human body. ADMET Predictor can estimate a number of vital ADMET properties (listed below) from molecular structures and build predictive models of new properties from user's data.

Resource Type: software application, software resource

Keywords: admet, absorption, distribution, metabolism, elmininations, toxicity, chemical substances, human, prediction, model

Availability: Commercial

Resource Name: ADMET Predictor

Resource ID: SCR_014903

Record Creation Time: 20220129T080323+0000

Record Last Update: 20260912T200252+0000

Ratings and Alerts

No rating or validation information has been found for ADMET Predictor.

No alerts have been found for ADMET Predictor.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 15 mentions in open access literature.

Listed below are recent publications. The full list is available at NIF .

Noga M, et al. (2025) ADME of Bromo-DragonFLY as an example of a new psychoactive substance (NPS) - application of in Silico methods for prediction: absorption, distribution, metabolism and excretion. Scientific reports, 15(1), 22949.

Saif MZ, et al. (2024) Investigating the potential of 6-substituted 3-formyl chromone derivatives as anti-diabetic agents using in silico methods. Scientific reports, 14(1), 13221.

Ippolitov D, et al. (2024) Overcoming brain-derived therapeutic resistance in HER2+ breast cancer brain metastasis. bioRxiv : the preprint server for biology.

Ma Y, et al. (2024) Accurate prediction of Kp,uu,brain based on experimental measurement of Kp,brain and computed physicochemical properties of candidate compounds in CNS drug discovery. Heliyon, 10(2), e24304.

Kim MS, et al. (2023) Physiologically Based Pharmacokinetic Modelling to Predict Pharmacokinetics of Enavogliflozin, a Sodium-Dependent Glucose Transporter 2 Inhibitor, in Humans. Pharmaceutics, 15(3).

Fujioka K, et al. (2023) Preclinical assessment of drug-drug interaction of fb-PMT, a novel anti-cancer thyrointegrin ?v?3 antagonist. Clinical and translational science, 16(6), 987.

Scior T, et al. (2023) Targeting the Human Influenza a Virus: The Methods, Limitations, and Pitfalls of Virtual Screening for Drug-like Candidates Including Scaffold Hopping and Compound Profiling. Viruses, 15(5).

Punt A, et al. (2022) Predictive Performance of Next Generation Physiologically Based Kinetic (PBK) Model Predictions in Rats Based on In Vitro and In Silico Input Data. Toxicological sciences : an official journal of the Society of Toxicology, 186(1), 18.

Aminpour M, et al. (2021) Computational determination of toxicity risks associated with a selection of approved drugs having demonstrated activity against COVID-19. BMC pharmacology & toxicology, 22(1), 61.

Miyake T, et al. (2021) Quantitative prediction of P-glycoprotein-mediated drug-drug interactions and intestinal absorption using humanized mice. British journal of pharmacology, 178(21), 4335.

Shibuya K, et al. (2019) Brain Targeting of Acyl-CoA:Cholesterol O-Acyltransferase-1 Inhibitor K-604 via the Intranasal Route Using a Hydroxycarboxylic Acid Solution. ACS omega, 4(16), 16943.

Alskär LC, et al. (2018) Impact of Drug Physicochemical Properties on Lipolysis-Triggered Drug Supersaturation and Precipitation from Lipid-Based Formulations. Molecular

pharmaceutics, 15(10), 4733.

Gissi A, et al. (2015) Evaluation and comparison of benchmark QSAR models to predict a relevant REACH endpoint: The bioconcentration factor (BCF). Environmental research, 137, 398.

El-Saadi MW, et al. (2015) Use of in-silico assays to characterize the ADMET profile and identify potential therapeutic targets of fusarochromanone, a novel anti-cancer agent. In silico pharmacology, 3(1), 6.

Takaku T, et al. (2014) Metabolism and physiologically based pharmacokinetic modeling of flumioxazin in pregnant animals. Toxicology and applied pharmacology, 277(3), 242.