ADMET Predictor®

TRANSPORTERS

The new ADMET Predictor® Transporters Module contains models for P-gp, BCRP, OATP1B1, OATP1B3, OCT1, OCT2, OAT1, OAT3 and BSEP. For most transporters, we provide substrate/non-substrate and inhibitor/non-inhibitor classification models and K_m regression models.

Predict, Prioritize, and Reduce Experimental Costs

The ADMET Predictor Transporters Module enables data-driven decision-making by leveraging AI/machine learning (ML) models trained on premium experimental datasets. Optimized for performance, you can calculate outcomes for large virtual libraries in seconds. This module helps you:

- **Reduce Costs:** Avoid unnecessary *in vitro* screening expenses by prioritizing key transporters that are most relevant to your compound.
- **Align with FDA Guidance:** Our regression and classification models focus on the critical transporters outlined in the FDA's guidance for DDI studies, including P-gp, BCRP, OATP1B1, OATP1B3, OCT1, BSEP, and others.
- **Enhance Early-Stage Decision-Making:** Identify potential transporter liabilities, both from a victim and perpetrator perspective, before committing to costly wet-lab experiments, ensuring smarter resource allocation.
- **Improve Accuracy & Confidence:** Built on a foundation of carefully curated datasets, our predictive models offer high reliability and translatability to experimental outcomes.

Streamline Transporter Assessments in Drug Discovery

Transporters play a crucial role in drug absorption, distribution, and elimination. Regulatory agencies, including the FDA, emphasize the importance of evaluating key transporters for potential drug-drug interactions (DDIs) early in development. However, *in vitro* transporter assay experiments are costly and time-consuming, making it challenging to screen every compound efficiently during drug discovery.

Make Every Data Point Count

By integrating the ADMET Predictor Transporters Module into your workflow, you can streamline early-stage assessments, minimize costly late-stage failures, and accelerate your drug development pipeline.

Ready to leverage AI/ML models to optimize your *in vitro* costs? Contact us today to learn more!

Rev. 02/18/2025