SimulationsPlus

ADMET Predictor®

HTPK

HIGH-THROUGHPUT PHARMACOKINETIC (HTPK) SIMULATION

The HTPK Simulation Module is the preferred methodology for discovery PBPK simulations and integrates the industry's **#1-ranked mechanistic absorption/PBPK models** with **#1-ranked machine learning ADME property predictions.**

HTPK predicts the following properties:

- Fraction absorbed (*%Fa*)
- Oral bioavailability (*%Fb*)
- Volume of distribution (*Vd*)
- Maximum plasma concentration (*Cmax*)
- Time at which maximum plasma concentration is reached (*Tmax*)
- Area under the concentration-time curve (*AUC*)
- *in-vivo* half-life in rat and human (T1/2)

The HTPK technology is fast enough for large-scale PK profiling of datasets

Support for 3 key physiologies:

- Rat
- Human
- Mouse

Combine models & experimental data:

You can immediately integrate your experimental values into the simulation routines to increase the accuracy of the predictions. Advanced setup capabilities allow the combined use of experimental (preferred) and calculated (fallback) values within the same run.

Calculation and Optimization

Optimal dose predictions can be quickly calculated within the virtual rat, mouse, or human PBPK models and factored into compound prioritization decisions at the discovery stage.

Scientifically rooted in the GastroPlus ACAT™ model

The algorithm uses our top-rated Advanced Compartmental Absorption and Transit (ACAT™) model from GastroPlus to simulate dissolution, transit, and absorption in the GI tract. The rapid dose optimization capabilities provide flexible options to compute the estimated dose (D) needed to reach different types of user-specified concentrations:

- Average plasma concentration (*Cave*)
- Minimum plasma concentration (*Cmin*)
- Maximum plasma concentration (*Cmax*)

simulations-plus.com/admetpredictor

Interested in collaborating?

Email us! info@simulations-plus.com

Rev. 12/06/2023