SimulationsPlus

GastroPlus®

ADMET Predictor®

The ADMET Predictor Module uses enhanced pk_a models developed with greater accuracy. It uses the same QSPR models as our best-in-class ADMET Predictor standalone software.

What is the ADMET Predictor module?

The ADMET Predictor Module extends the capability of GastroPlus® by enabling you to obtain predictions from the compound structure of all physicochemical, pharmacokinetic, and CYP metabolism kinetic parameters required for the GastroPlus PBPK simulations.

You can now apply discovery PBPK modeling approaches to assist with lead selection and optimization activities!

This module automatically generates predictions for the following properties:

- ✓ Aqueous solubility
- ✓ Biorelevant solubility (*FaSSIF*, *FeSSIF*, and *FaSSGF*)
- ✓ pK_a(s)
- ✓ Diffusion Coefficient
- ✓ logP
- ✓ Human effective permeability
- ✓ CYP metabolism kinetics – V_{max}, K_m, and CL_{int}
- ✓ Transporter classification
- ✓ Human plasma protein binding
- ✓ Human blood-plasma concentration ratio
- ✓ Human volume of distribution
- ✓ Mouse plasma protein binding
- ✓ Mouse blood-plasma concentration ratio
- ✓ Mouse intrinsic clearance
- ✓ Rat plasma protein binding
- ✓ Rat blood-plasma concentration ratio
- ✓ Rat intrinsic clearance
- ✓ Tendency to supersaturate in water
- ✓ Blood:brain barrier permeation (classification)
- ✓ Mechanistic clearance classification (S+CL Mech)
- ✓ Extended Clearance Classification System (ECCS)

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Interested in collaborating?

Email us! info@simulations-plus.com

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