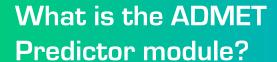
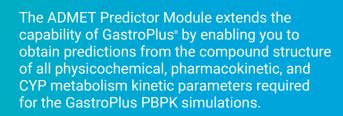




ADMET Predictor®

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





GastroPlus

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:

- Agueous solubility
- Biorelevant solubility (FaSSIF, FeSSIF, and FaSSGF)
- \vee 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)



Interested in collaborating?



Email us! info@simulations-plus.com



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