![SimulationsPlus logo] **SimulationsPlus**
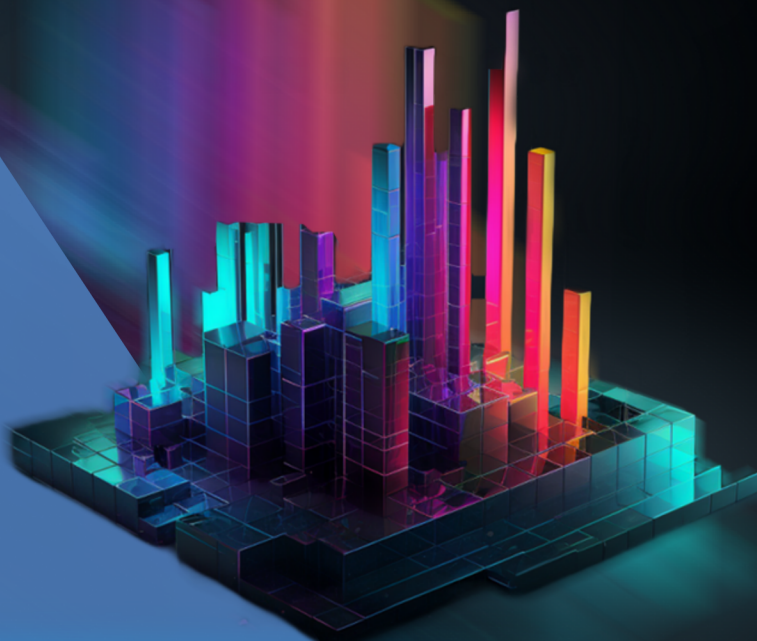
AP | ADMET Predictor

PCB

PHYSICOCHEMICAL AND BIOPHARMACEUTICAL (PCB)

ADMET Predictor's PCB Module contains models for physicochemical property prediction. Each model was built by Simulations Plus scientists using artificial neural network ensemble (ANNE) technology. The data sets were highly curated in order to generate high quality models.

Industry Validated pKa Model

- ✓ New data from three industrial partners more than doubles the number of ionization constants for enhanced predictive accuracy and wider applicability of our *S+pKa* model
- ✓ Multiprotic pKa model (*S+Acidic_pKa, S+Mixed_pKa, S+Basic_pKa*) – a thermodynamically accurate multiprotic model for multiple ionization sites based on atomic descriptors and neural networks – not a database lookup!

Permeability Models

- ✓ **Human effective permeability (*S+P$_{eff}$*)** – jejunal P_{eff}
- ✓ **MDCK apparent permeability (*S+MDCK*)** – *in vitro* P_{app}
- ✓ **Corneal permeability (*Perm_Cornea*)** – ocular permeability through rabbit cornea based on literature data obtained *in vitro*
- ✓ **Skin permeability (*Perm_Skin*)** – permeability through human skin of compounds dissolved in aqueous solution; based on literature data
- ✓ **Blood-brain barrier permeation** – there are two models, classification (*BBB_Filter*) and regression (*LogBB*)

Solubility Models

- ✓ *Aqueous*
- ✓ *FaSSGF*
- ✓ *FaSSIF*
- ✓ *FeSSIF*
- ✓ *Supersaturation*

Other Top-Ranking Models

- ✓ **logP (*S+logP, MlogP*)** – log of the octanol to water partition coefficient. There are two models, an artificial neural network ensemble (S+logP) and Moriguchi (MlogP) logD (S+logD) – estimation of octanol-water distribution coefficient at user-defined pH
- ✓ **Air-water partition (*logHLC*)** – estimation of air-water partition coefficient (Henry's Law constant) from US EPA data

Pharmacokinetic Models

- ✓ ***RBP*** - Blood to plasma concentration ratio in human
- ✓ ***RBP_rat*** - Blood to plasma concentration ratio in rat
- ✓ ***RBP_mou*** - Blood to plasma concentration ratio in mouse
- ✓ ***S+CL_Metab*** - Predicts whether or not clearance mechanism is metabolism.
- ✓ ***S+CL_Renal*** - Predicts whether or not clearance mechanism is renal
- ✓ ***S+CL_Uptake*** - Predicts whether or not clearance mechanism is hepatic uptake.
- ✓ ***S+CL_Mech*** - Predicts clearance mechanism as primarily metabolism, renal or hepatic uptake.
- ✓ ***S+fumic*** - Fraction unbound in human liver microsomes
- ✓ ***ECCS_Class*** - ECCS class describing major clearance mechanism
- ✓ ***Vd*** – Volume of distribution (L/kg) in human

simulations-plus.com/admetpredictor

Interested in collaborating?

Email us! info@simulations-plus.com

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