ADMET Predictor® 12

Predict with confidence.

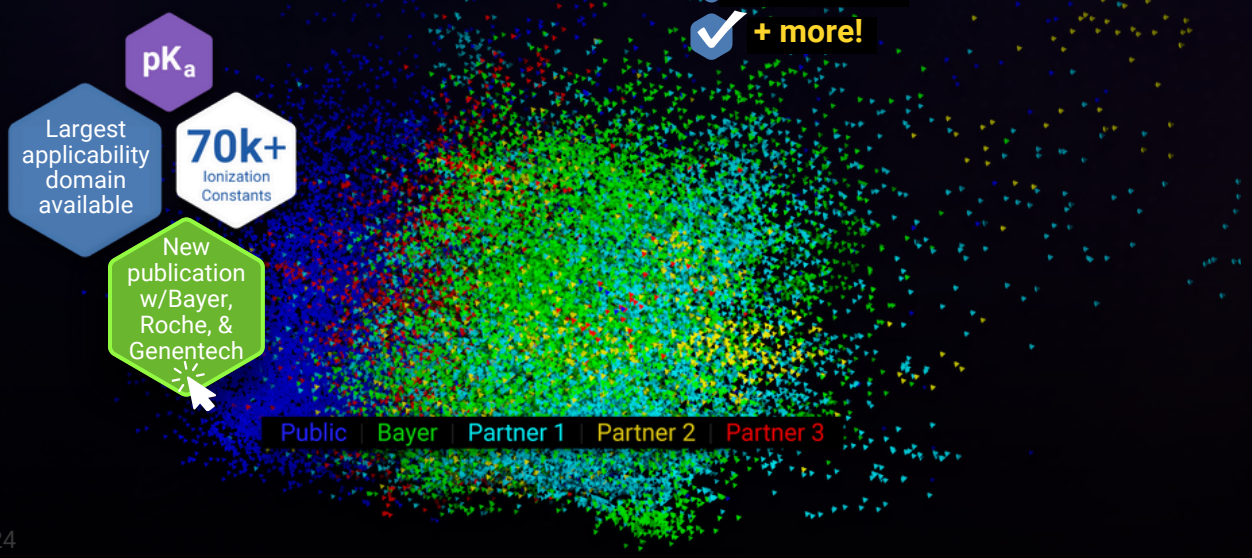
#1-ranked machine learning prediction

With ADMET Predictor, researchers like you can rapidly estimate absorption, distribution, metabolism, excretion and toxicity (ADMET) properties and animal/human systemic exposure of new chemical entities simply from molecular structure.

Medicinal chemistry and DMPK teams worldwide leverage ADMET Predictor for discovery PK assessment. It enables quick and accurate predictions of more than 175 properties, including solubility, logP, pK_a, sites of CYP metabolism, Ames mutagenicity, and major PK endpoints using integrated high-throughput GastroPlus® simulations.

What's NEW in version 12?

- **NEW** & improved models for predicting biorelevant solubility, clearance, permeability, CYP induction and more
- **ENHANCED** HT-PBPK capabilities including solution dosing and access to tissue GastroPlus K_p values
- **NEW** drug-induced liver injury (DILI) toxicity models to inform HT-DILIsym® simulations
- **EXPANDED** AI-driven drug design (AIDD) functions
- **BOOSTED** ANN regression models in ADMET Modeler™
- **IMPROVED** usability and informatics
- **+ more!**



Rev. 07/18/2024

simulations-plus.com/ap

Connect with us: