



ADMET Predictor® 11

Proven algorithms. Premium data. Predictions you can rely on.

#1-ranked machine learning prediction software

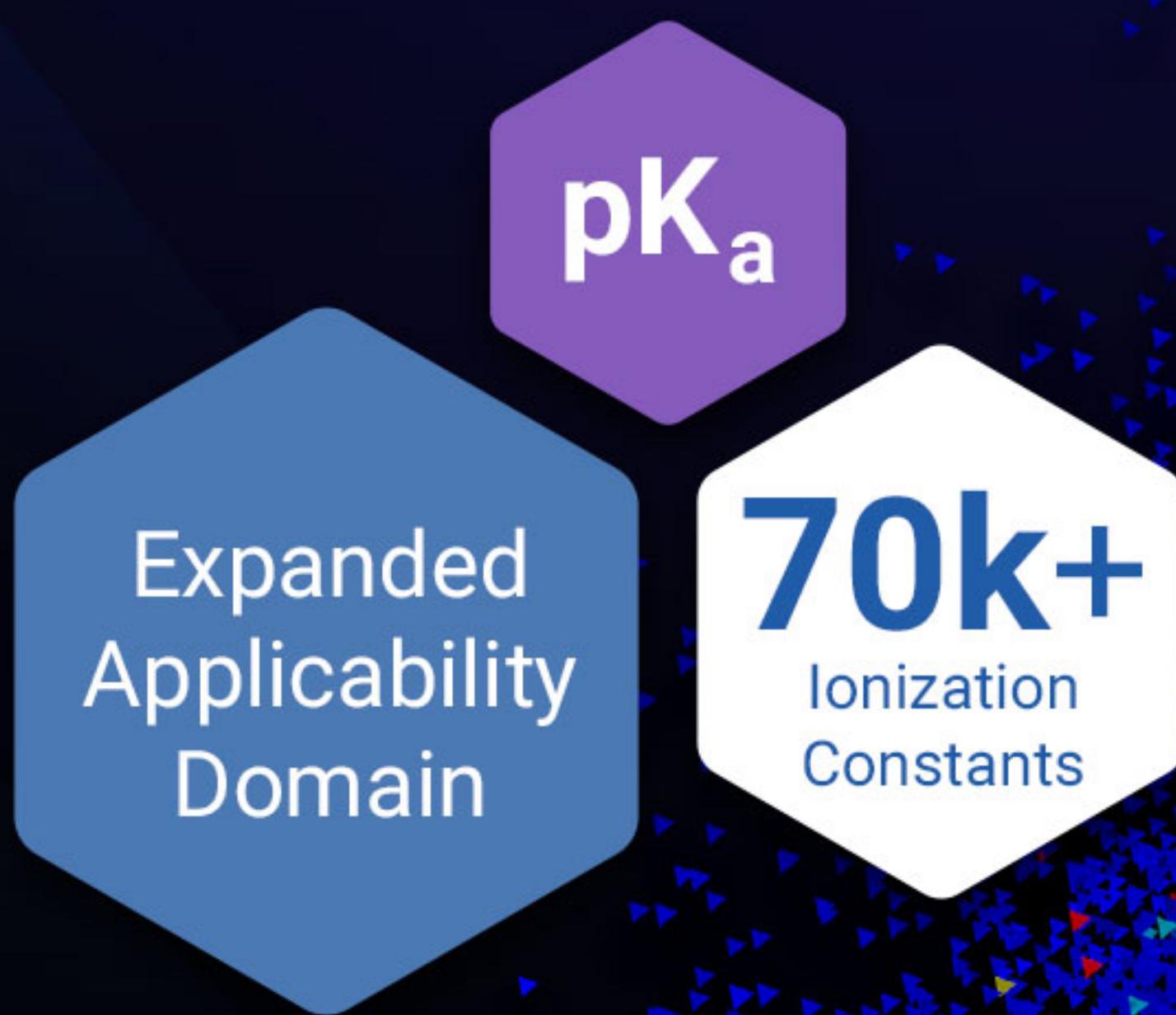
With ADMET Predictor, researchers like you can rapidly estimate absorption, distribution, metabolism, excretion and toxicity (ADMET) properties of new chemical entities simply from molecular structure.

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, pKa, sites of CYP metabolism, and Ames mutagenicity.

What's new in version 11?

- **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
- **NEW** functionality to perform 3D virtual screening based on shape and pharmacophore-feature similarity
- **NEW** CYP inhibition (Ki) models to allow for rapid DDI risk assessment

+ more!



Public | Bayer | Partner 1 | Partner 2 | Partner 3