Cheminformatics

Understand Your Compound

Whether your work focuses on drug design, library screening, agrochemical discovery or toxicology, you need to be able to predict the ADMET properties of the compounds you're working on and how they will impact a variety of populations and environments.

The ADMET Predictor® platform allows you to accurately and rapidly predict more than 175 absorption, distribution, metabolism, excretion and toxicity (ADMET) properties, including…

- pKa and ionization-related descriptors
- Aqueous and biorelevant solubility
- LogD vs. pH
- Species-specific protein binding, blood:plasma ratio, and intrinsic clearances
- Sites of CYP metabolism
- Ames mutagenicity
- + more

Our Experts Can Support You In...

- Leveraging AI/ML technology to access industry-best ADMET and HTPK predictions for your drug discovery and design
- Filtering candidate molecules for novelty, rapid commercial availability, and IP position
- Identifying existing therapies and molecules for your target that you'll be competing against
- Reviewing the literature to inform the direction of your compound development