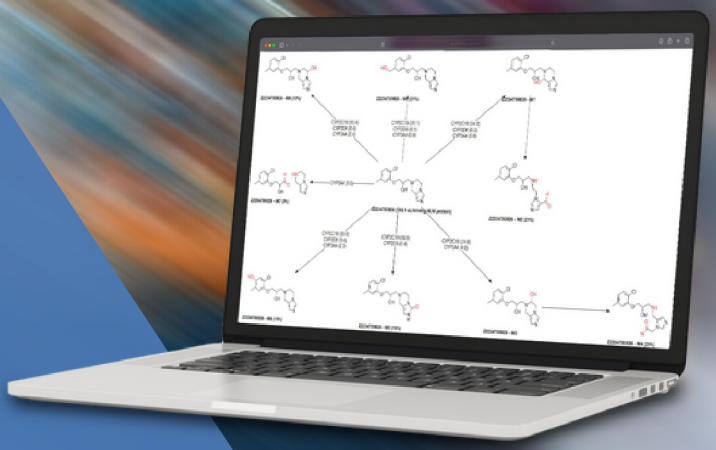
SimulationsPlus

ADMET Predictor

METABOLISM

Metabolism plays a critical role in the bioavailability of drugs, food additives, agrochemicals, and industrial chemicals. Knowledge of the specific metabolites resulting from these transformations is often important in understanding toxicities, efficacy (in the case of prodrugs), and clearance, along with many other key aspects of drug pharmacokinetics. Thus, models for metabolite prediction can be very useful in drug design and evaluation of toxicity.



Metabolite pathway for sample compound from the Enamine Discovery Diversity set. The pathway shows predicted metabolites with clearance contributions for the different CYP isoforms.

Human Cytochrome P450 Metabolism (CYP)

The cytochrome P450 metabolism models provide insight into:

- Prediction of substrate/non-substrate for supported isoforms
- Identification of metabolic hotspots (SOMs)
- Structure of predicted metabolites
- Kinetic parameters (K_m, V_{max} and CL_{int})

CYP Inhibition Models

The inhibitory potency of drugs against cytochrome P450 is important for the study of drug toxicities and drug-drug interactions. The ADMET Predictor™ CYP P450 inhibition classification package includes nine global inhibition models for CYP 1A2, 1A6, 2B6, 2C8, 2C9, 2C19, 2D6, 2E1, and 3A4.

UGT Metabolism

We have developed Artificial Neural Network Ensemble (ANNE) models from literature data for nine UGT isozymes that cause Phase II drug metabolism: UGT1A1, UGT1A3, UGT1A4, UGT1A6, UGT1A8, UGT1A9, UGT1A10, UGT2B7, and UGT2B15. The UGT models predict whether a compound will be metabolized by one or more of these enzymes.

Clearance Models

ADMET Predictor provides prediction of microsomal and hepatocyte intrinsic clearance. Supported physiologies are:

- Human
- Rat
- Mouse

Other Metabolism Models

- Aldehyde Oxydase (AOX)
- Esterase metabolites

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Interested in collaborating?

Email us! info@simulations-plus.com

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