

ProtoADME

ProtoADME is a computational (*in silico*) tool focused on the prediction of endpoints related with the ADME (Absorption, Distribution, Metabolism and Excretion) of chemical substances.

Endpoint

Toxicokinetic: CYP450 3A4 substrate

The microsomal cytochrome P450 (CYP) family 4 monooxygenases are the major fatty acid omega-hydroxylases. These enzymes remove excess free fatty acids to prevent lipotoxicity, catabolize leukotrienes and prostanoids, and also produce bioactive metabolites from arachidonic acid omega-hydroxylation. In addition to endogenous substrates, recent evidence indicates that CYP4 monooxygenases can also metabolize xenobiotics, including therapeutic drugs. If a compound is a CYP substrate means that the compound will be subjected to metabolic clearance.

Metrics

Training set

Experimental values	QSAR predictions	
	Non-substrate	Substrate
Non-substrate	197	32
Substrate	46	206

Validation set

Experimental values	QSAR predictions	
	Non-substrate	Substrate
Non-substrate	49	23
Substrate	28	66

Parameters	Training	Validation
Accuracy	0.84	0.69
Sensitivity / recall	0.82	0.70
Specificity	0.86	0.68
Precision	0.87	0.74
Negative predictive value	0.81	0.64
F-score	0.84	0.72
Matthews Correlation Coefficient	0.68	0.38
Critical Success Index	0.73	0.56
Area under the ROC	0.84	0.69

ProtoADME is part of



ProtoPRED platform allows the easy, fast and user-friendly prediction of different properties of chemical compounds, by proprietary (Q)SAR models.

 +34 962 021 811

 protopred@protoqsar.com

<https://protopred.protoqsar.com/>

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