

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: p-gp inhibitor.

P-glycoprotein (P-gp, also known as MDR1 or ABCB1) is a member of the superfamily of ABC transporters which transport various molecules across cellular membranes, and is highly expressed in the intestinal epithelium. P-gp is an energy-dependent efflux pump driven by ATP hydrolysis. Efflux by P-gp can be a major limitation for the oral delivery of a number of drugs.

Metrics

Training set

Experimental values	QSAR predictions	
	Non-inhibitor	Inhibitor
Non-inhibitor	378	37
Inhibitor	35	459

Validation set

Experimental values	QSAR predictions	
	Non-inhibitor	Inhibitor
Non-inhibitor	135	16
Inhibitor	20	136

Parameters	Training	Validation
Accuracy	0.92	0.88
Sensitivity / recall	0.93	0.87
Specificity	0.91	0.89
Precision	0.93	0.89
Negative predictive value	0.92	0.87
F-score	0.93	0.88
Matthews Correlation Coefficient	0.84	0.77
Critical Success Index	0.86	0.79
Area under the ROC	0.92	0.88

ProtoADME is part of



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

 +34 962 021 811

 protopred@protoqsar.com

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

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