QSAR model for P-gp substrate (v1.0)

ProtoADME by ProtoQSAR

ProtoADME

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

Endpoint

Toxicokinetic: p-gp substrate

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-substrate	**Substrate**
Non-substrate	261	35
Substrate	53	261

Validation set

Experimental values	QSAR predictions	
	Non-substrate	**Substrate**
Non-substrate	72	31
Substrate	30	74

Parameters	Training	Validation
Accuracy	0.86	0.71
Sensitivity / recall	0.83	0.71
Specificity	0.88	0.70
Precision	0.88	0.70
Negative predictive value	0.83	0.71
F-score	0.86	0.71
Matthews Correlation Coefficient	0.71	0.41
Critical Success Index	0.75	0.55
Area under the ROC	0.86	0.71