

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: OATP1B1 inhibitor

OATP1B1 is an uptake transporter exclusively expressed on the sinusoidal side of hepatocytes. It is responsible for the hepatic uptake of drugs and endogenous compounds from the blood. Inhibition of OATPs may be responsible for enhanced plasma concentration of OATP substrates and may influence drug efficacy and toxicity.

Metrics

Training set

Experimental values	QSAR predictions	
	Non-inhibitor	Inhibitor
Non-inhibitor	333	75
Inhibitor	62	383

Validation set

Experimental values	QSAR predictions	
	Non-inhibitor	Inhibitor
Non-inhibitor	99	84
Inhibitor	61	137

Parameters	Training	Validation
Accuracy	0.84	0.62
Sensitivity / recall	0.86	0.69
Specificity	0.82	0.54
Precision	0.84	0.62
Negative predictive value	0.84	0.62
F-score	0.85	0.65
Matthews Correlation Coefficient	0.68	0.24
Critical Success Index	0.74	0.49
Area under the ROC	0.84	0.62

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/>

© 2022 ProtoQSAR, S.L.