

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: OATP1B3 inhibitor

OATP1B3 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

Experimental values	QSAR predictions		
	Non-inhibitor	Inhibitor	
Non-inhibitor	388	118	
Inhibitor	103	271	

Training set

Validation	set

Experimental values	QSAR predictions		
	Non-inhibitor	Inhibitor	
Non-inhibitor	99	57	
Inhibitor	69	70	

Parameters	Training	Validation		
Accuracy	0.75	0.57		
Sensitivity / recall	0.72	0.50		
Specificity	0.77	0.63		
Precision	0.70	0.55		
Negative predictive value	0.79	0.59		
F-score	0.71	0.53		
Matthews Correlation Coefficient	0.49	0.14		
Critical Success Index	0.55	0.36		
Area under the ROC	0.75	0.57		

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.

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