QSAR model for OATP1B3 inhibitor (v2.0)

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: OATP1B31 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	173	22
Inhibitor	6	111

Validation set

Experimental values	QSAR predictions	
	Non-inhibitor	**Inhibitor**
Non-inhibitor	45	20
Inhibitor	13	26

Parameters	Training	Validation
Accuracy	0.91	0.68
Sensitivity / recall	0.95	0.67
Specificity	0.89	0.69
Precision	0.83	0.57
Negative predictive value	0.97	0.78
F-score	0.89	0.61
Matthews Correlation Coefficient	0.82	0.35
Critical Success Index	0.80	0.44
Area under the ROC	0.92	0.68