QSAR model for BSEP inhibitor (v1.0)

ProtoADME by ProtoQSAR

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: BSEP inhibitor

The bile salt export pump (BSEP) actively transports conjugated monovalent bile acids from the hepatocytes into the bile. This facilitates the formation of micelles and promotes digestion and absorption of dietary fat. Inhibition of BSEP leads to decreased bile flow and accumulation of cytotoxic bile salts in the liver.

Metrics

Training set

Experimental values	QSAR predictions	
	Non-inhibitor	**Inhibitor**
Non-inhibitor	256	43
Inhibitor	12	133

Validation set

Experimental values	QSAR predictions	
	Non-inhibitor	**Inhibitor**
Non-inhibitor	84	16
Inhibitor	8	43

Parameters	Training	Validation
Accuracy	0.88	0.84
Sensitivity / recall	0.92	0.84
Specificity	0.86	0.84
Precision	0.76	0.73
Negative predictive value	0.96	0.91
F-score	0.83	0.78
Matthews Correlation Coefficient	0.74	0.66
Critical Success Index	0.71	0.64
Area under the ROC	0.89	0.84