QSAR model for CYP450 3A4 inhibitor (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: CYP450 3A4 inhibitor

The microsomal cytochrome P450 (CYP) family 4 monooxygenases are the major fatty acid omega-hydroxylases. These enzymes remove excess free fatty acids to prevent lipotoxicity, catabolize leukotrienes and prostanoids, and also produce bioactive metabolites from arachidonic acid omega-hydroxylation. In addition to endogenous substrates, recent evidence indicates that CYP4 monooxygenases can also metabolize xenobiotics, including therapeutic drugs. If a compound is a CYP inhibitor may decrease the metabolism of comedicated drugs.

Metrics

Training set

Experimental values	QSAR predictions	
	Non-inhibitor	**Inhibitor**
Non-inhibitor	249	5
Inhibitor	30	203

Validation set

Experimental values	QSAR predictions	
	Non-inhibitor	**Inhibitor**
Non-inhibitor	64	30
Inhibitor	29	43

Parameters	Training	Validation
Accuracy	0.93	0.64
Sensitivity / recall	0.87	0.60
Specificity	0.98	0.68
Precision	0.98	0.59
Negative predictive value	0.89	0.69
F-score	0.92	0.59
Matthews Correlation Coefficient	0.86	0.28
Critical Success Index	0.85	0.42
Area under the ROC	0.93	0.64