QSAR model for CYP450 2C9 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: CYP450 2C9 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	228	28
Inhibitor	35	202

Validation set

Experimental values	QSAR predictions	
	Non-inhibitor	**Inhibitor**
Non-inhibitor	63	31
Inhibitor	26	46

Parameters	Training	Validation
Accuracy	0.87	0.66
Sensitivity / recall	0.85	0.64
Specificity	0.89	0.67
Precision	0.88	0.60
Negative predictive value	0.87	0.71
F-score	0.87	0.62
Matthews Correlation Coefficient	0.74	0.31
Critical Success Index	0.76	0.45
Area under the ROC	0.87	0.65