QSAR model for CYP450 1A2 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: CYP450 1A2 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 it may decrease the metabolism of comedicated drugs.

Metrics

Training set

Experimental values	QSAR predictions	
	Non-inhibitor	**Inhibitor**
Non-inhibitor	7190	987
Inhibitor	716	7006

Validation set

Experimental values	QSAR predictions	
	Non-inhibitor	**Inhibitor**
Non-inhibitor	1575	470
Inhibitor	430	1501

Parameters	Training	Validation
Accuracy	0.89	0.77
Sensitivity / recall	0.91	0.78
Specificity	0.88	0.77
Precision	0.88	0.76
Negative predictive value	0.91	0.79
F-score	0.89	0.77
Matthews Correlation Coefficient	0.79	0.55
Critical Success Index	0.80	0.63
Area under the ROC	0.89	0.77