QSAR model for CYP450 2D6 inhibitor (v1.0)

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 2D6 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	116	16
Inhibitor	45	268

Validation set

Experimental values	QSAR predictions	
	Non-inhibitor	**Inhibitor**
Non-inhibitor	38	17
Inhibitor	37	107

Parameters	Training	Validation
Accuracy	0.86	0.73
Sensitivity / recall	0.86	0.74
Specificity	0.88	0.69
Precision	0.94	0.86
Negative predictive value	0.72	0.51
F-score	0.90	0.80
Matthews Correlation Coefficient	0.70	0.40
Critical Success Index	0.81	0.66
Area under the ROC	0.87	0.72