QSAR model for CYP450 1A2 substrate (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 1A2 substrate

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 substrate means that the compound will be subjected to metabolic clearance.

Metrics

Training set

Experimental values	QSAR predictions	
	Non-substrate	**Substrate**
Non-substrate	207	20
Substrate	15	243

Validation set

Experimental values	QSAR predictions	
	Non-substrate	**Substrate**
Non-substrate	50	29
Substrate	25	62

Parameters	Training	Validation
Accuracy	0.93	0.67
Sensitivity / recall	0.94	0.71
Specificity	0.91	0.63
Precision	0.92	0.68
Negative predictive value	0.93	0.67
F-score	0.93	0.70
Matthews Correlation Coefficient	0.86	0.35
Critical Success Index	0.87	0.53
Area under the ROC	0.93	0.67