QSAR model for CYP450 2C19 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 2C19 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	316	31
Substrate	29	113

Validation set

Experimental values	QSAR predictions	
	Non-substrate	**Substrate**
Non-substrate	103	18
Substrate	13	32

Parameters	Training	Validation
Accuracy	0.88	0.81
Sensitivity / recall	0.80	0.71
Specificity	0.91	0.85
Precision	0.78	0.64
Negative predictive value	0.92	0.89
F-score	0.79	0.67
Matthews Correlation Coefficient	0.70	0.54
Critical Success Index	0.65	0.51
Area under the ROC	0.85	0.78