QSAR model for CYP450 2D6 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 2D6 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	324	27
Substrate	9	135

Validation set

Experimental values	QSAR predictions	
	Non-substrate	**Substrate**
Non-substrate	105	16
Substrate	12	33

Parameters	Training	Validation
Accuracy	0.93	0.83
Sensitivity / recall	0.94	0.73
Specificity	0.92	0.87
Precision	0.83	0.67
Negative predictive value	0.97	0.90
F-score	0.88	0.70
Matthews Correlation Coefficient	0.83	0.59
Critical Success Index	0.79	0.54
Area under the ROC	0.93	0.80

ProtoADME is part of ProtoPRED

ProtoPRED platform allows the easy, fast and user-friendly prediction of different properties of chemical compounds, by proprietary (Q)SAR models.

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