# **QSAR model for CYP450 2D6 substrate** (v1.0)



#### **ProtoADME**

ProtoADME is a computational (in silico) tool focused on the prediction of endpoints related with the ADME (Absorption, 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
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Experimental values	QSAR predictions		
	Non-substrate	Substrate	
Non-substrate	105	16	
Substrate	12	33	

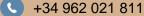
Parameters	Training	Validation
Accuracy	0.93	0.83
Sensitivity / recall	0.94	0.73
Specificity	0.92	0.87
Precision	0.83	0.67
Negative predictive value	0.97	0.90
F-score	0.88	0.70
Matthews Correlation Coefficient	0.83	0.59
Critical Success Index	0.79	0.54
Area under the ROC	0.93	0.80

ProtoADME is part of



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







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