QSAR model for blood-brain barrier (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: blood-brain barrier

Drugs that act in the CNS need to cross the blood–brain barrier (BBB) to reach their molecular target. By contrast, for drugs with a peripheral target, little or no BBB penetration might be required in order to avoid CNS side effects.

Metrics

Training set

Experimental values	QSAR predictions	
	Negative	**BBB+**
Negative	309	35
BBB+	58	1015

Validation set

Experimental values	QSAR predictions	
	Negative	**BBB+**
Negative	80	29
BBB+	32	335

Parameters	Training	Validation
Accuracy	0.93	0.87
Sensitivity / recall	0.95	0.91
Specificity	0.90	0.73
Precision	0.97	0.92
Negative predictive value	0.84	0.71
F-score	0.96	0.92
Matthews Correlation Coefficient	0.83	0.64
Critical Success Index	0.92	0.85
Area under the ROC	0.92	0.82