

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: 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

ProtoADME is part of



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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