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

Drugs that act in the Central Neural System (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**

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

### Training set

Val	lidation	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, using proprietary (Q)SAR models.

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