

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: bioavailability20.

Bioavailability describes the passage of a substance from the site of absorption into the blood of the general circulation. Bioavailability is not necessarily equivalent to the amount of a substance absorbed, because in some cases parts of that amount may be excreted or metabolized before reaching the systemic circulation. This may occur, for instance, for substances metabolized in the gut after oral exposure before any absorption has taken place. Substances absorbed from the intestine can be partly eliminated by the liver at their first passage through that organ.

Metrics

Training set

Experimental values	QSAR predictions	
	Negative	Positive
Negative	173	10
Positive	108	448

Validation set

Experimental values	QSAR predictions	
	Negative	Positive
Negative	45	27
Positive	50	127

Parameters	Training	Validation
Accuracy	0.84	0.69
Sensitivity / recall	0.81	0.72
Specificity	0.95	0.62
Precision	0.98	0.82
Negative predictive value	0.62	0.47
F-score	0.88	0.77
Matthews Correlation Coefficient	0.67	0.32
Critical Success Index	0.79	0.62
Area under the ROC	0.88	0.67

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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