QSAR model for human intestinal absorption (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: human intestinal absorption

The human intestinal absorption of an oral drug is the essential prerequisite for its apparent efficacy. What's more, the close relationship between oral bioavailability and intestinal absorption has also been proven and HIA can be seen an alternative indicator for oral bioavailability to some extent.

Metrics

Training set

Experimental values	QSAR predictions	
	Negative	**Positive**
Negative	130	17
Positive	25	755

Validation set

Experimental values	QSAR predictions	
	Negative	**Positive**
Negative	39	11
Positive	10	252

Parameters	Training	Validation
Accuracy	0.95	0.93
Sensitivity / recall	0.97	0.96
Specificity	0.88	0.78
Precision	0.98	0.96
Negative predictive value	0.84	0.80
F-score	0.97	0.96
Matthews Correlation Coefficient	0.83	0.75
Critical Success Index	0.95	0.92
Area under the ROC	0.93	0.87