QSAR model for bioavailability 30% (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: Bioavailability 30%

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 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. The original values were retrieved as %F and then transformed to categorical value, being considered positive if the value is bigger than 30.

Metrics

Training set

Experimental values	QSAR predictions	
	Negative	**Positive**
Negative	224	20
Positive	60	435

Validation set

Experimental values	QSAR predictions	
	Negative	**Positive**
Negative	56	36
Positive	44	113

Parameters	Training	Validation
Accuracy	0.89	0.68
Sensitivity / recall	0.88	0.72
Specificity	0.92	0.61
Precision	0.96	0.76
Negative predictive value	0.79	0.56
F-score	0.92	0.74
Matthews Correlation Coefficient	0.77	0.32
Critical Success Index	0.84	0.59
Area under the ROC	0.90	0.66