QSAR model for human liver microsomal stability (v1.0)

ProtoADME by ProtoQSAR

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: Human liver microsomal stability

The metabolic stability assays offer a method to calculate the rate of clearance of a test compound over time in microsomal incubations, as a measure of clearance.

Metrics

Training set

Experimental values	QSAR predictions	
	Stable	**Non-stable**
Stable	1435	98
Non-stable	51	812

Validation set

Experimental values	QSAR predictions	
	Stable	**Non-stable**
Stable	411	97
Non-stable	95	199

Parameters	Training	Validation
Accuracy	0.94	0.76
Sensitivity / recall	0.94	0.68
Specificity	0.94	0.81
Precision	0.89	0.67
Negative predictive value	0.97	0.81
F-score	0.92	0.67
Matthews Correlation Coefficient	0.87	0.49
Critical Success Index	0.84	0.51
Area under the ROC	0.94	0.74

ProtoADME is part of ProtoPRED

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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