QSAR model for human liver microsomal stability (v2.0)

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 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	1019	163
Non-stable	64	935

Validation set

Experimental values	QSAR predictions	
	Stable	**Non-stable**
Stable	276	120
Non-stable	70	263

Parameters	Training	Validation
Accuracy	0.90	0.74
Sensitivity / recall	0.94	0.79
Specificity	0.86	0.70
Precision	0.85	0.69
Negative predictive value	0.94	0.80
F-score	0.89	0.73
Matthews Correlation Coefficient	0.80	0.49
Critical Success Index	0.80	0.58
Area under the ROC	0.90	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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