QSAR model for half life (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.

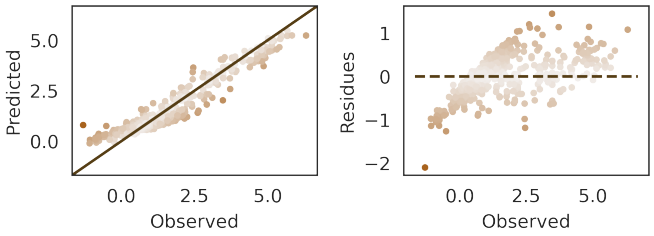
Endpoint

Toxicokinetic: half life

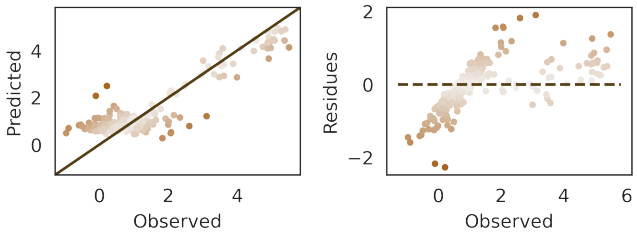
The half-life for a drug is the time required for the concentration of the drug to reach half of its original value. It has a major effect on both the size of the dose that is given and the frequency of dosing.

Metrics

Training set



Validation set



Parameters	Training	Validation
R^2 score	0.91	0.80
Mean absolute error (MAE)	0.32	0.51
Mean squared error (MSE)	0.17	0.42
Median absolute error	0.25	0.43
Explained variance	0.91	0.80