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 (Absorption, Distribution, Metabolism and Excretion) of chemical substances.

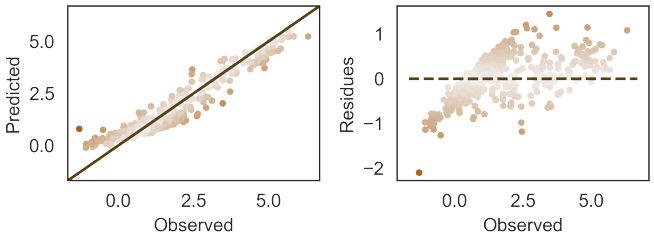
Endpoint

Toxicokinetic: half life

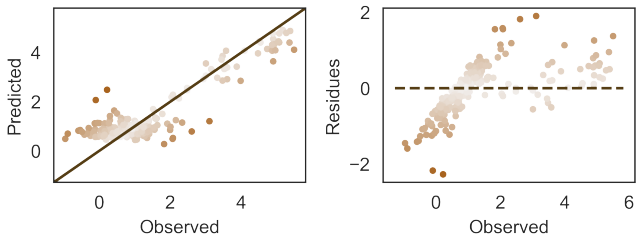
The half life for a drug is the time required for the concentration of the drug to reach half of its original value. It has a major effect on both the size of the dose that is given and the frequency of dosing.

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

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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