QSAR model for volume of distribution (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.

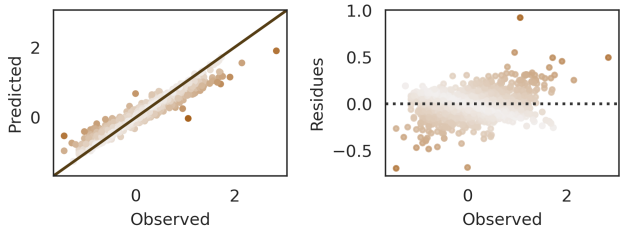
Endpoint

Toxicokinetic: Volume of distribution.

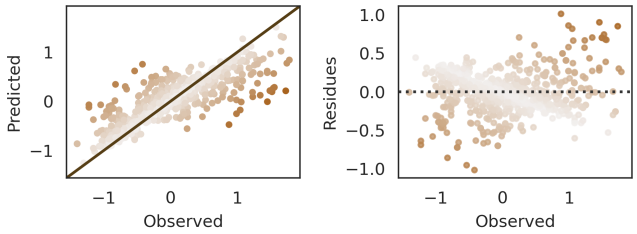
The Volume of distribution (VD) is a theoretical concept that connects the administered dose with the actual initial concentration present in the circulation and it is an important parameter to describe the in vivo distribution for drugs. In practical, we can speculate the distribution characters for an unknown compound according to its VD value, such as its condition binding to plasma protein, its distribution amount in body fluid and its uptake amount in tissues.

Metrics

Training set



Validation set



Parameters	Training	Validation
R^2 score	0.94	0.70
Mean absolute error (MAE)	0.10	0.23
Mean squared error (MSE)	0.02	0.12
Median absolute error	0.06	0.13
Explained variance	0.94	0.70

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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