QSAR model for plasma protein binding (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.

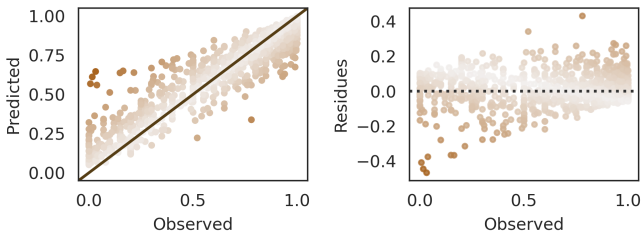
Endpoint

Toxicokinetic: plasma-protein binding

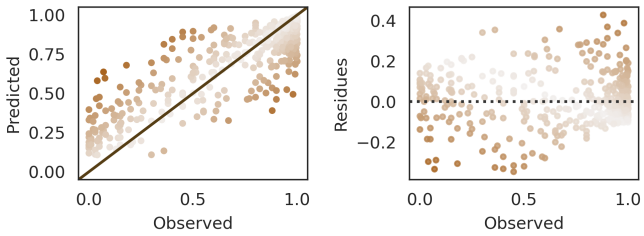
Plasma protein binding is one of the major mechanisms of drug uptake and distribution is through PPB, thus the binding of a drug to proteins in plasma has a strong influence on its pharmacodynamic behavior. PPB can directly influence the oral bioavailability because the free concentration of the drug is at stake when a drug binds to serum proteins in this process.

Metrics

Training set



Validation set



Parameters	Training	Validation
R^2 score	0.89	0.73
Mean absolute error (MAE)	0.07	0.13
Mean squared error (MSE)	0.01	0.03
Median absolute error	0.05	0.09
Explained variance	0.89	0.73

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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