

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.

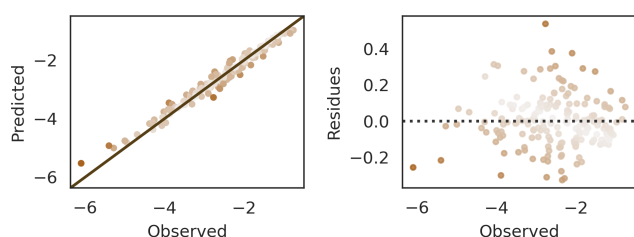
Endpoint

Toxicokinetic: skin permeability.

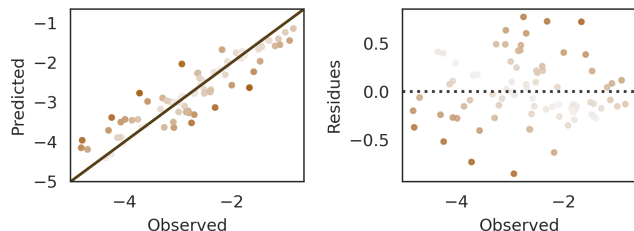
Skin permeability is a measure of the absorption of a compound through the outer surface of the skin.

Metrics

Training set



Validation set



Parameters	Training	Validation
R ² score	0.97	0.84
Mean absolute error (MAE)	0.13	0.30
Mean squared error (MSE)	0.03	0.16
Median absolute error	0.09	0.24
Explained variance	0.97	0.84

ProtoADME is part of



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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