QSAR model for caco-2 permeability (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: Caco-2 permeability

The Caco-2 cell line is derived from a human colon carcinoma. The cells have characteristics that resemble intestinal epithelial cells, such as the formation of a polarised monolayer, well-defined brush border on the apical surface and intercellular junctions. The Caco-2 cell line is commonly used as a substitute for the human intestinal epithelium to assess in vivo drug permeability. This choice is attributed to its morphological and functional similarities with human enterocytes.

Metrics

Training set
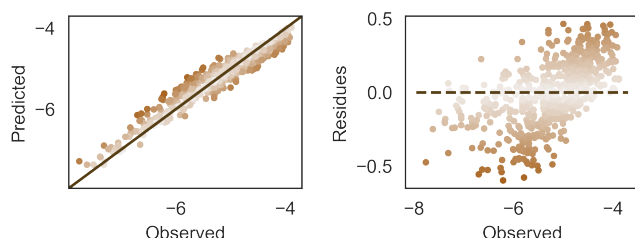
Validation set
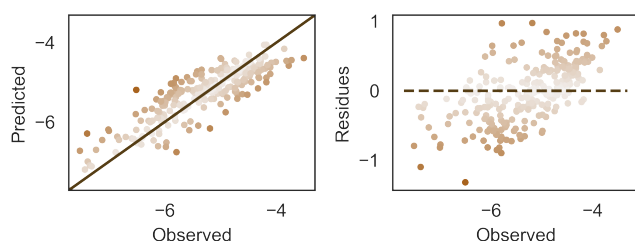
Parameters	Training	Validation
R^2 score	0.92	0.75
Mean absolute error (MAE)	0.17	0.31
Mean squared error (MSE)	0.05	0.16
Median absolute error	0.15	0.26
Explained variance	0.92	0.75

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.

+34 962 021 811   protopred@protoqsar.com

https://protopred.protoqsar.com/