

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.

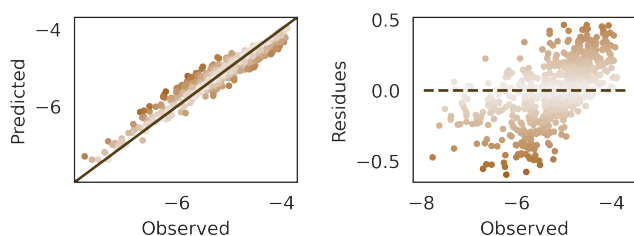
Endpoint

Toxicokinetic: Caco-2 permeability

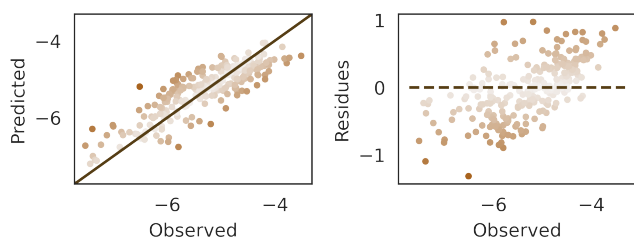
The Caco-2 cell line is derived from a human colon carcinoma. The cells have characteristics that resemble intestinal epithelial cells such as the formation of a polarised monolayer, well-defined brush border on the apical surface and intercellular junctions.

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 platform allows the easy, fast and user-friendly prediction of different properties of chemical compounds, by proprietary (Q)SAR models.

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