QSAR model for partition Coefficient, Log P (M) (v1.0)

ProtoNANO

ProtoNANO is a computational (*in silico*) tool focused on the prediction of endpoints related with the physicochemical, toxicological and ecotoxicological properties of nanomaterials.

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Endpoint

Physical-chemical properties: Octanol-water partition coefficient (Kow).

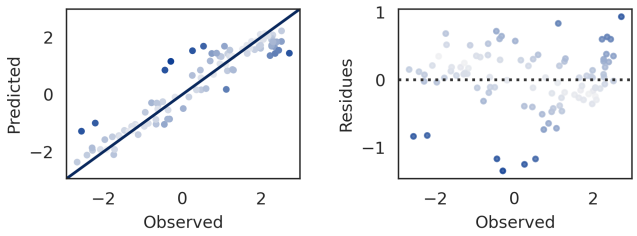
The n-octanol/water partition coefficient (Kow) is defined as the ratio of the equilibrium concentrations of a dissolved substance in a two-phase system consisting of the largely immiscible solvents n-octanol and water. The Kow is typically defined as the partition coefficient of the neutral, undissociated form of a substance.

Nanomaterials

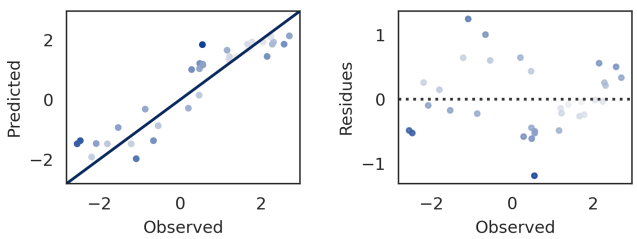
The models was developed with noble metal partilces (Au, Pd, Pt) covered by organic ligands/surfactants.

Metrics

Training set



Validation set



Parameters	Training	Validation
R^2 score	0.90	0.86
Mean absolute error (MAE)	0.37	0.50
Mean squared error (MSE)	0.24	0.34
Median absolute error	0.30	0.49
Explained variance	0.90	0.87