

ProtoNANO

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

ProtoNANO was developed as a part of the NanoQSAR research project. This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 896848.

Endpoint

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

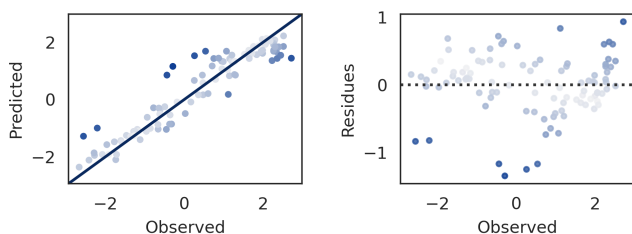
The n-octanol/water partition coefficient (Kow) is defined as the ratio of the equilibrium concentrations of a dissolved substance in a two-phase system consisting of the largely immiscible solvents n-octanol and water. The Kow is typically defined as the partition coefficient of the neutral, undissociated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

Nanomaterials

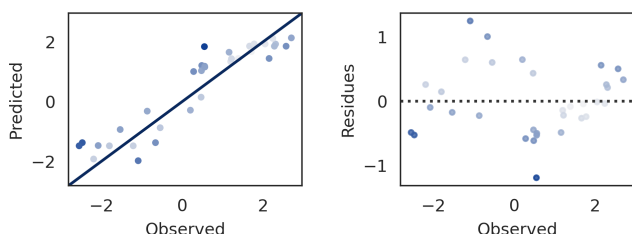
The models was developed with noble metal partilces (Au, Pd, Pt) covered by organic ligands/surfactants.

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

ProtoNANO 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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