QSAR model for partition coefficient (log D) (v1.0)

ProtoPHYSCHEM by ProtoQSAR

ProtoPHYSCHEM

ProtoPHYSCHEM is a computational (*in silico*) tool focused on the prediction of endpoints related with the physicochemical properties of chemical substances.

ProtoPHYSCHEM mainly includes, but is not limited to, endpoints used by REACH, a European Union regulation, adopted to improve the protection of human health and the environment from the risks that can be posed by chemicals, while enhancing the competitiveness of the EU chemicals industry.

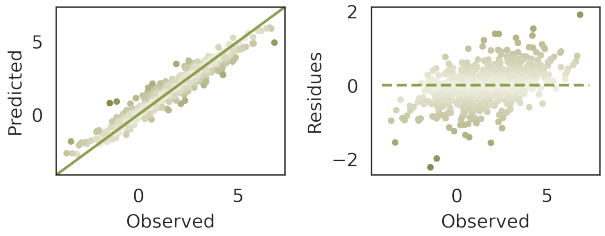
Endpoint

Physical-chemical properties: Octanol-water partition coefficient (Kow). Partition Coefficient (n-octanol/water) at constant pH (7,4)

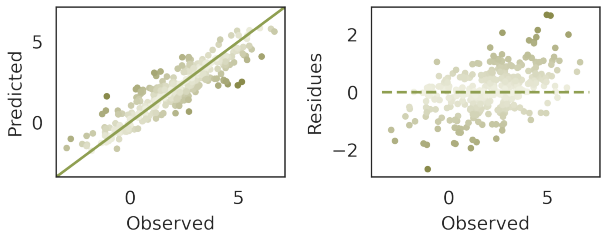
The n-octanol/water partition coefficient (Dow, also referred as D) is defined as the ratio of the equilibrium concentrations of a dissolved substance in a two-phase system consisting of the largely immiscible solvents n-octanol and water. On the contrary to Kow, D is determined for ionizale compounds at a fixed pH, because it is a more realistic measure for PBT and chemical safety assessment for those substances which dissociate within an environmentally relevant pH range (pKa 5-9).

Metrics

Training set



Validation set



Parameters	Training	Validation
R^2 score	0.94	0.82
Mean absolute error (MAE)	0.34	0.60
Mean squared error (MSE)	0.20	0.61
Median absolute error	0.25	0.49
Explained variance	0.94	0.82

ProtoPHYSCHEM is part of ProtoPRED

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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