

ProtoREACH

ProtoREACH is a computational (*in silico*) tool specially focused on 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.

REACH also promotes alternative methods for the hazard assessment of substances in order to reduce the number of tests on animals. The requirements for registering a chemical substance are organized as annexes of the REACH regulation. Different annexes must be used depending on the substance mass produced or imported by each company.

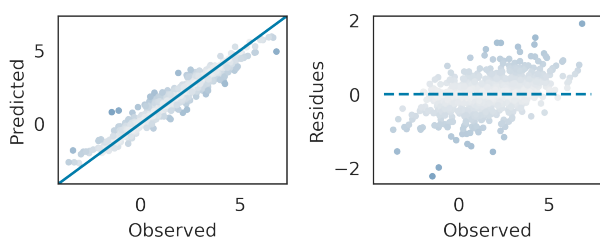
Endpoint

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

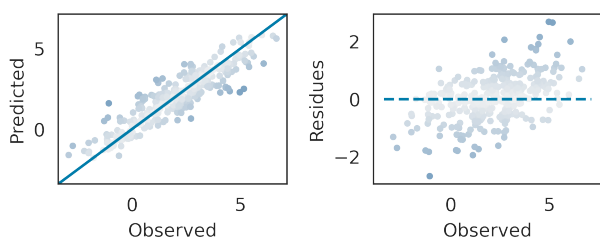
The n-octanol/water partition coefficient (Dow, also referred as D) is defined as the ratio of the equilibrium concentrations of a dissolved substance in a two-phase system consisting of the largely immiscible solvents n-octanol and water. On the contrary to Kow, D is determined for ionizable compounds 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