

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.

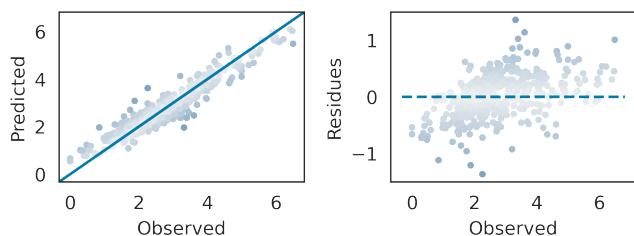
Endpoint

Environmental fate parameters: Adsorption/desorption in soil.

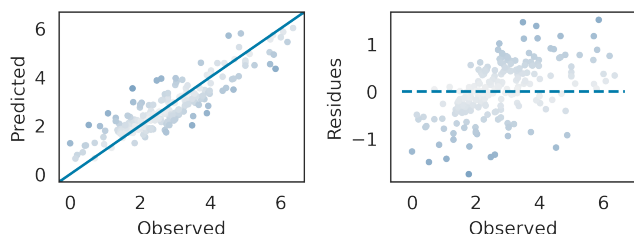
The organic carbon normalized adsorption coefficient (K_{oc}) is the ratio of a substance concentration sorbed in the organic matter component of soil or sediment to that in the aqueous phase at equilibrium. Adsorption is caused by temporary (reversible) or permanent bonding between the substance and a surface (e.g. due to van der Waals interactions, hydrogen bonding to hydroxyl groups, ionic interactions, covalent bonding, etc.).

Metrics

Training set



Validation set



Parameters	Training	Validation
R^2 score	0.91	0.80
Mean absolute error (MAE)	0.28	0.46
Mean squared error (MSE)	0.13	0.33
Median absolute error	0.22	0.38
Explained variance	0.91	0.80