QSAR model for adsorption/desorption (v1.0)

ProtoECO by ProtoQSAR

ProtoECO

ProtoECO is a computational (*in silico*) tool focused on the prediction of endpoints related with ecotoxicity and the environmental effects chemical substances. This includes properties related to the distribution and degradation of substances in the environment as well as their toxic effects in the biota.

ProtoECO 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.

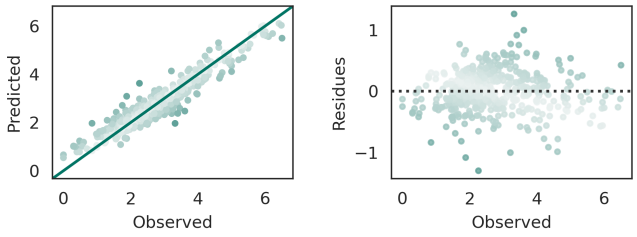
Endpoint

Environmental fate parameters: Adsorption/desorption in soil.

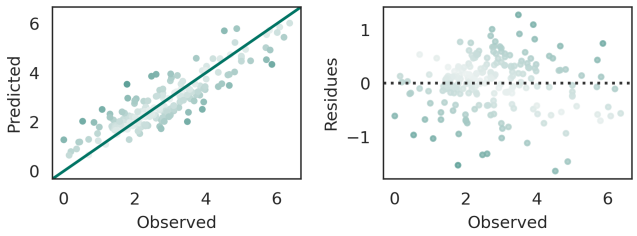
The organic carbon normalized adsorption coefficient (Koc) is the ratio of a substance concentration sorbed in the organic matter component of soil or sediment to that in the aqueous phase at equilibrium. Adsorption is caused by temporary (reversible) or permanent bonding between the substance and a 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

ProtoECO 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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