QSAR model for bioconcentration factor (v1.0)

ProtoREACH

by **ProtoQSAR**

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.
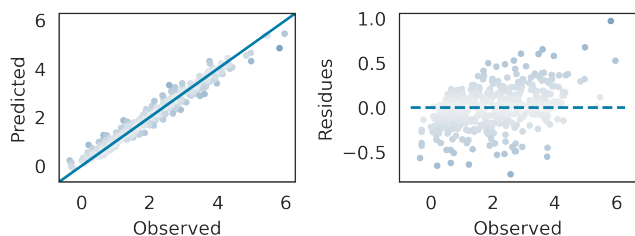
Endpoint

Environmental fate parameters: Bioconcentration. BCF fish. Bioconcentration: Flow-through Fish Test.
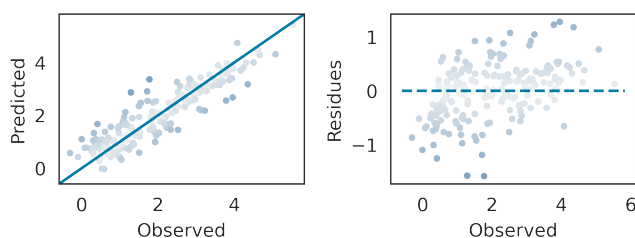
Bioconcentration refers to the accumulation of a substance dissolved in water by an aquatic organism. The bioconcentration factor (BCF) is the ratio of the concentration of a substance in an organism to the concentration in water.

Metrics

Training set

Validation set

Parameters	Training	Validation
R^2 score	0.97	0.84
Mean absolute error (MAE)	0.17	0.40
Mean squared error (MSE)	0.05	0.26
Median absolute error	0.13	0.32
Explained variance	0.97	0.84

ProtoREACH 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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