

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.

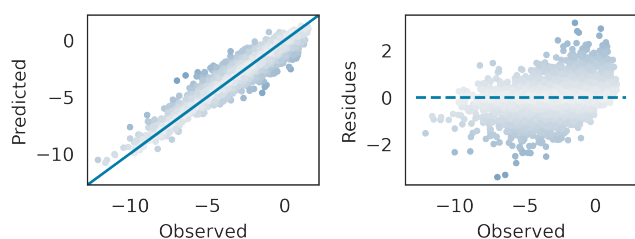
Endpoint

Physical-chemical properties: Water solubility.

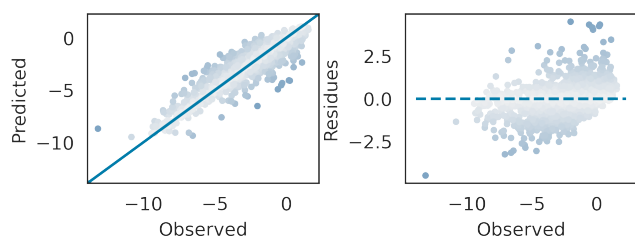
The solubility of a substance in water is specified by the saturation mass concentration of the substance in water at a given temperature. The solubility in water is specified in units of mass per volume of solution.

Metrics

Training set



Validation set



Parameters	Training	Validation
R ² score	0.91	0.82
Mean absolute error (MAE)	0.50	0.69
Mean squared error (MSE)	0.45	0.87
Median absolute error	0.38	0.53
Explained variance	0.91	0.82