

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.

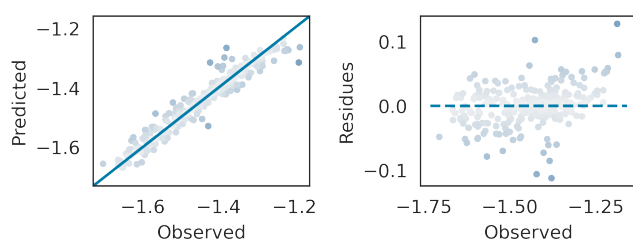
Endpoint

Physical-chemical properties: Surface tension.

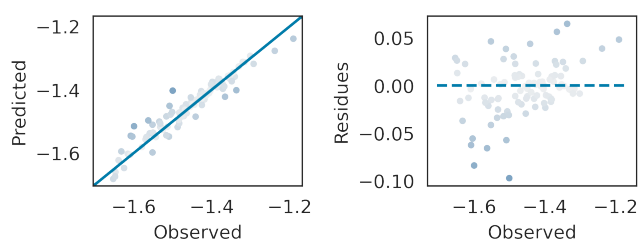
The free surface enthalpy per unit of surface area is referred to as surface tension. The surface tension is given as: N/m or mN/m (1mN/m = 1 dyne/cm). The surface tension of an aqueous solution of a substance can be used to determine whether the substance is surface active (surfactant).

Metrics

Training set



Validation set



Parameters	Training	Validation
R ² score	0.93	0.92
Mean absolute error (MAE)	0.02	0.02
Mean squared error (MSE)	0.00	0.00
Median absolute error	0.01	0.01
Explained variance	0.93	0.92