

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.

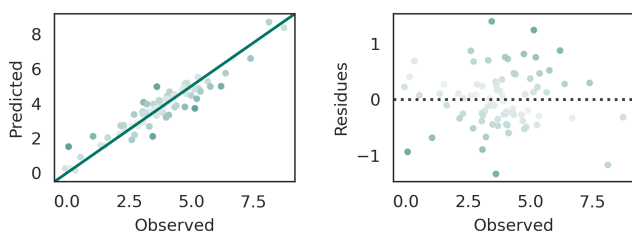
Endpoint

Ecotoxic effects: Acute toxicity to fish. Fish, Acute Toxicity Test.

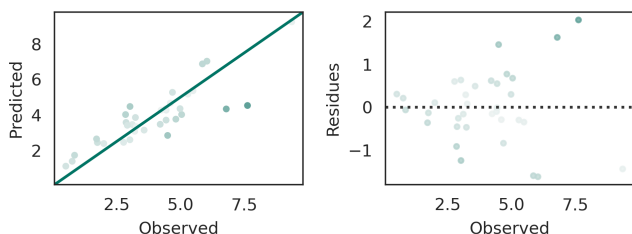
Short-term aquatic toxicity to fish (also generally referred to as 'acute' toxicity) is assessed by exposing fish to relatively high concentrations of a chemical for a relatively short period of time (usually 96h). The effect of a chemical substance on the mortality of fish is measured.

Metrics

Training set



Validation set



Parameters	Training	Validation
R ² score	0.89	0.73
Mean absolute error (MAE)	0.43	0.71
Mean squared error (MSE)	0.30	0.93
Median absolute error	0.36	0.62
Explained variance	0.89	0.73

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.

+34 962 021 811

protopred@protoqsar.com

<https://protopred.protoqsar.com/>

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