

## 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.

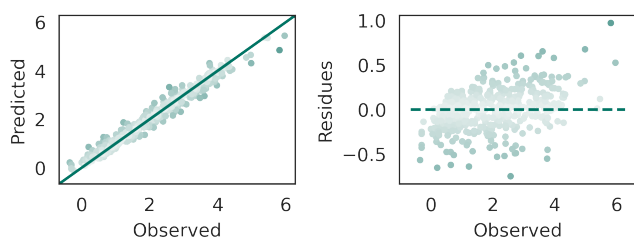
## Endpoint

**Environmental fate parameters: Bioconcentration. BCF fish. Bioconcentration: Flow-through Fish Test.**

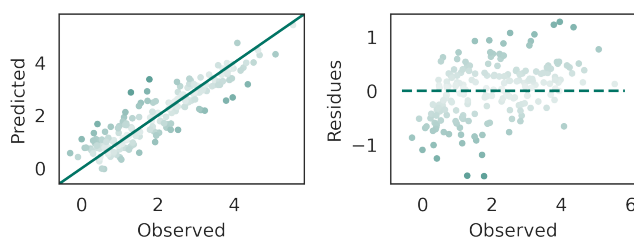
Bioconcentration refers to the accumulation of a substance dissolved in water by an aquatic organism. The bioconcentration factor (BCF) is the ratio of the concentration of a substance in an organism to the concentration in water.

## Metrics

### Training set



### Validation set



| Parameters                | Training | Validation |
|---------------------------|----------|------------|
| R <sup>2</sup> 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       |

ProtoECO is part of



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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