# QSAR model for fish acute toxicity (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

**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
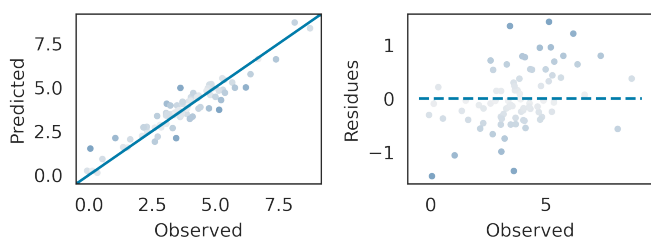


### Validation set
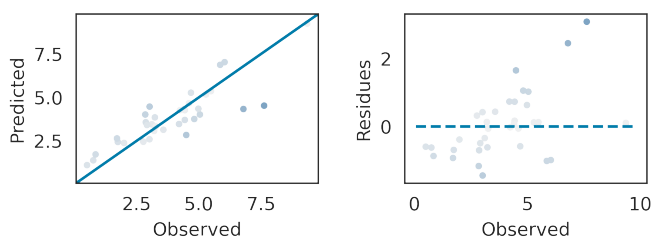


| Parameters | Training | Validation |
|---|---|---|
| $R^2$ score | 0.89 | 0.73 |
| Mean absolute error (MAE) | 0.43 | 0.71 |
| Mean squared error (MSE) | 0.30 | 0.93 |
| Median absolute error | 0.36 | 0.62 |
| Explained variance | 0.89 | 0.73 |

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.

+34 962 021 811    protopred@protoqsar.com