# QSAR model for acute oral toxicity (2000 mg/kg bw) (v2.0)

**ProtoTOX**
by ProtoQSAR

## ProtoTOX

ProtoTOX is a computational (*in silico*) tool focused on the prediction of endpoints related with the toxicity of chemical substances. It includes a variety of *in vitro* and *in vivo* tests in humans, animals, microorganisms and cell lines.

ProtoTOX 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

### Human health effects: Acute oral toxicity

Acute oral toxicity refers to whether a single exposure (or multiple exposures within 24 hours) to the substance of interest, administered orally could be associated with adverse effects on human health. This model classifies a substance as "Toxic" if the LD50 is below 2000 mg/kg bw (this corresponds to the numeric cut-off criteria for CLP regulation between not-classified substances and categories 1 to 4 in oral acute toxicity).

## Metrics

### Training set

| Experimental values | QSAR predictions | |
|---|---|---|
| | **Non-toxic** | **Toxic** |
| **Non-toxic** | 2321 | 265 |
| **Toxic** | 776 | 3874 |

### Validation set

| Experimental values | QSAR predictions | |
|---|---|---|
| | **Non-toxic** | **Toxic** |
| **Non-toxic** | 834 | 344 |
| **Toxic** | 527 | 1397 |

| Parameters | Training | Validation |
|---|---|---|
| Accuracy | 0.86 | 0.72 |
| Sensitivity / recall | 0.83 | 0.73 |
| Specificity | 0.90 | 0.71 |
| Precision | 0.94 | 0.80 |
| Negative predictive value | 0.75 | 0.61 |
| F-score | 0.88 | 0.76 |
| Matthews Correlation Coefficient | 0.71 | 0.42 |
| Critical Success Index | 0.79 | 0.62 |
| Area under the ROC | 0.87 | 0.72 |

ProtoTOX 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

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