

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 toxicity by oral route.

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 platform allows the easy, fast and user-friendly prediction of different properties of chemical compounds, using proprietary (Q)SAR models.

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