QSAR model for acute oral 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

Human health effects: Acute oral toxicity

Accute 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.

Metrics

Training set

Experimental values	QSAR predictions	
	Non-toxic	**Toxic**
Non-toxic	63	8
Toxic	13	36

Validation set

Experimental values	QSAR predictions	
	Non-toxic	**Toxic**
Non-toxic	17	7
Toxic	6	11

Parameters	Training	Validation
Accuracy	0.82	0.68
Sensitivity / recall	0.73	0.65
Specificity	0.89	0.71
Precision	0.82	0.61
Negative predictive value	0.83	0.74
F-score	0.77	0.63
Matthews Correlation Coefficient	0.63	0.35
Critical Success Index	0.63	0.46
Area under the ROC	0.81	0.68

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.

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