

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: in vivo pre-natal-developmental

A reproductive and/or developmental toxic substance may affect fertility and can cause health effects in offspring after recurring contact by ingestion, inhalation, or skin contact. This study is designed to provide information on substance-induced effects on growth and survival of the foetuses, and increased incidences in external, skeletal and soft tissue malformations and variations in foetuses.

Metrics

Training set

Experimental values	QSAR predictions	
	non-toxic	toxic
non-toxic	85	9
toxic	28	107

Validation set


Experimental values	QSAR predictions	
	non-toxic	toxic
non-toxic	25	16
toxic	26	34

Parameters	Training	Validation
Accuracy	0.84	0.58
Sensitivity / recall	0.79	0.57
Specificity	0.90	0.61
Precision	0.92	0.68
Negative predictive value	0.75	0.49
F-score	0.85	0.62
Matthews Correlation Coefficient	0.69	0.17
Critical Success Index	0.74	0.45
Area under the ROC	0.85	0.59

ProtoREACH 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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