QSAR model for developmental toxicity (v1.0)



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: 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

Experimental values

> non-toxic toxic

Training set

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

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Validation set			
	QSAR predictions		
	non-toxic	toxic	
	25	16	

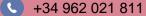
Parameters	Training	Validation
Accuracy	0.84	0.58
Sensitivity / recall	0.79	0.57
Specificity	0.90	0.61
Precision	0.92	0.68
Negative predictive value	0.75	0.49
F-score	0.85	0.62
Matthews Correlation Coefficient	0.69	0.17
Critical Success Index	0.74	0.45
Area under the ROC	0.85	0.59

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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