

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: Mutagenicity/Genotoxicity. Mammalian erythrocyte micronucleus test.

Mutagenicity refers to the induction of permanent transmissible changes in the amount or structure of the genetic material of cells or organisms. Genotoxicity is a broader term and refers to processes which alter the structure, information content or segregation of DNA and are not necessarily associated with mutagenicity. *In vivo* mammalian erythrocyte micronucleus test is a measure of *in vivo* chromosomal mutagenicity. The test identifies substances that cause micronuclei in erythroblasts sampled from bone marrow and/or peripheral blood cells of animals, usually rodents. These micronuclei originate from acentric fragments or whole chromosomes, and the test thus has the potential to detect both clastogenic and aneugenic substances.

Metrics

Training set

Experimental values	QSAR predictions	
	non-cytotoxic	cytotoxic
non-cytotoxic	60	22
cytotoxic	29	92

Validation set


Experimental values	QSAR predictions	
	non-cytotoxic	cytotoxic
non-cytotoxic	23	13
cytotoxic	10	23

Parameters	Training	Validation
Accuracy	0.75	0.67
Sensitivity / recall	0.76	0.70
Specificity	0.73	0.64
Precision	0.81	0.64
Negative predictive value	0.67	0.70
F-score	0.78	0.67
Matthews Correlation Coefficient	0.49	0.34
Critical Success Index	0.64	0.50
Area under the ROC	0.75	0.67

ProtoREACH 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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