

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: Eye irritation/corrosion.

An eye irritating substance causes irritating effects or damages after contact with the eyes.

Metrics

Training set

Experimental values	QSAR predictions	
	non-irritant	irritant
non-irritant	1206	182
irritant	68	592

Validation set

Experimental values	QSAR predictions	
	non-irritant	irritant
non-irritant	393	78
irritant	42	171

Parameters	Training	Validation
Accuracy	0.88	0.82
Sensitivity / recall	0.90	0.80
Specificity	0.87	0.83
Precision	0.76	0.69
Negative predictive value	0.95	0.90
F-score	0.83	0.74
Matthews Correlation Coefficient	0.74	0.61
Critical Success Index	0.70	0.59
Area under the ROC	0.88	0.82

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.

+34 962 021 811

protopred@protoqsar.com

<https://protopred.protoqsar.com/>

© 2022 ProtoQSAR, S.L.