QSAR model for *in vivo* eye irritation (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: 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