QSAR model for *in vivo* skin 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: Skin irritation/corrosion.

Dermal irritation is defined as the production of reversible damage of the skin following the application of a test substance for up to 4 hours, while dermal corrosion is the production of irreversible damage of the skin; namely, visible necrosis through the epidermis and into the epidermis, following the application of a test substance for up to 4 hours.

Metrics

Training set

Experimental values	QSAR predictions	
	non-irritant	irritant
non-irritant	130	63
irritant	36	218

Validation set

Experimental values	QSAR predictions	
	non-irritant	irritant
non-irritant	27	35
irritant	17	72

Parameters	Training	Validation
Accuracy	0.78	0.66
Sensitivity / recall	0.86	0.81
Specificity	0.67	0.44
Precision	0.78	0.67
Negative predictive value	0.78	0.61
F-score	0.81	0.73
Matthews Correlation Coefficient	0.55	0.26
Critical Success Index	0.69	0.58
Area under the ROC	0.77	0.62

ProtoTOX is part of ProtoPRED

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/

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