QSAR model for *in vivo* skin irritation (v1.0)

ProtoREACH by ProtoQSAR

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: 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