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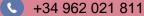
Experimental values	QSAR predictions		
	non-irritant	irritant	
non-irritant	27	35	
irritant	17	72	

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



ProtoPRED platform allows the easy, fast and user-friendly prediction of different properties of chemical compounds, by proprietary (Q)SAR models.







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