QSAR model for *in vivo* skin sensitisation (local lymph node assay) (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 sensitisation. OECD 429: Skin sensitisation: LLNA.

A skin sensitizer is an agent that will lead to an allergic response in susceptible individuals following skin contact. As a consequence of a secondary - usually organ-specific - subsequent re-exposure, adverse health effects on the skin.

Metrics

Training set

Experimental values	QSAR predictions	
	non-sensitizer	**sensitizer**
non-sensitizer	76	11
sensitizer	24	164

Validation set

Experimental values	QSAR predictions	
	non-sensitizer	**sensitizer**
non-sensitizer	12	7
sensitizer	17	35

Parameters	Training	Validation
Accuracy	0.87	0.66
Sensitivity / recall	0.87	0.67
Specificity	0.87	0.63
Precision	0.94	0.83
Negative predictive value	0.76	0.41
F-score	0.90	0.74
Matthews Correlation Coefficient	0.72	0.27
Critical Success Index	0.82	0.59
Area under the ROC	0.87	0.65

ProtoREACH 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.

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