QSAR model for *in vivo* skin sensitisation (local lymph node assay) (v1.0)

ProtoTOX by ProtoQSAR

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 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

ProtoTOX is part of

ProtoPRED

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

📞 +34 962 021 811   ✉ protopred@protoqsar.com

https://protopred.protoqsar.com/