QSAR model for carcinogenicity (v1.0)

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: Carcinogenicity. Carcinogenicity Studies.

Chemicals are defined as carcinogenic if they induce tumours, increase tumour incidence and/or malignancy or shorten the time to tumour occurrence.

Metrics

Training set

Experimental values	QSAR predictions	
	Non-carcinogen	**Carcinogen**
Non-carcinogen	286	14
Carcinogen	13	174

Validation set

Experimental values	QSAR predictions	
	Non-carcinogen	**Carcinogen**
Non-carcinogen	74	27
Carcinogen	20	44

Parameters	Training	Validation
Accuracy	0.94	0.72
Sensitivity / recall	0.93	0.69
Specificity	0.95	0.73
Precision	0.93	0.62
Negative predictive value	0.96	0.79
F-score	0.93	0.65
Matthews Correlation Coefficient	0.88	0.41
Critical Success Index	0.87	0.48
Area under the ROC	0.94	0.71

ProtoREACH 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/

©2026 ProtoQSAR S.L.