QSAR model for *in vitro* gene mutation study in mammalian cells (*Hprt* assay) (v1.1)

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: Mutagenicity/Genotoxicity. *In Vitro* Mammalian Cell Gene Mutation Tests using the *Hprt* and *xprt* genes.

Mutagenicity refers to the induction of permanent transmissible changes in the amount or structure of the genetic material of cells or organisms. The purpose of the *in vitro* mammalian cell gene mutation test is to detect gene mutations induced by chemicals. The cell lines used in these tests measure forward mutations in reporter genes, specifically the endogenous hypoxanthine-guanine phosphoribosyl transferase gene. *Hprt* gene mutation assay identifies substances that induce gene mutations in the *Hprt* gene of established cell lines.

Metrics

Training set

Experimental values	QSAR predictions	
	non-mutagenic	mutagenic
non-mutagenic	283	50
mutagenic	4	35

Validation set

Experimental values	QSAR predictions	
	non-mutagenic	mutagenic
non-mutagenic	108	35
mutagenic	5	12

Parameters	Training	Validation
Accuracy	0.85	0.75
Sensitivity / recall	0.90	0.71
Specificity	0.85	0.76
Precision	0.41	0.26
Negative predictive value	0.99	0.96
F-score	0.56	0.37
Matthews Correlation Coefficient	0.55	0.31
Critical Success Index	0.39	0.23
Area under the ROC	0.87	0.73

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

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