

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

GenoITS

GenoITS is a computational workflow focused on the prediction of genotoxicity using the Integrated Testing Strategy proposed by REACH. GenoITS uses 5 different QSAR models to perform the complete workflow, one per each kind of study demanded by REACH (gene mutation in bacteria; *in vitro* cytogenicity; *in vitro* gene mutation; *in vivo* cytogenicity; *in vivo* gene mutation). ProtoITS also allows the users to supply their own experimental data.

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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

GenoITS is part of



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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