

QSAR model for *in vivo* mammalian somatic cell genotoxicity study (micronucleus assay) (v1.0)

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. Mammalian erythrocyte micronucleus test.

Mutagenicity refers to the induction of permanent transmissible changes in the amount or structure of the genetic material of cells or organisms. Genotoxicity is a broader term and refers to processes which alter the structure, information content or segregation of DNA and are not necessarily associated with mutagenicity. *In vivo* mammalian erythrocyte micronucleus test is a measure of *in vivo* chromosomal mutagenicity. The test identifies substances that cause micronuclei in erythroblasts sampled from bone marrow and/or peripheral blood cells of animals, usually rodents. These micronuclei originate from acentric fragments or whole chromosomes, and the test thus has the potential to detect both clastogenic and aneugenic substances.

Metrics

Training set

Experimental values	QSAR predictions	
	non-cytotoxic	cytotoxic
non-cytotoxic	60	22
cytotoxic	29	92

Validation set

Experimental values	QSAR predictions	
	non-cytotoxic	cytotoxic
non-cytotoxic	23	13
cytotoxic	10	23

Parameters	Training	Validation
Accuracy	0.75	0.67
Sensitivity / recall	0.76	0.70
Specificity	0.73	0.64
Precision	0.81	0.64
Negative predictive value	0.67	0.70
F-score	0.78	0.67
Matthews Correlation Coefficient	0.49	0.34
Critical Success Index	0.64	0.50
Area under the ROC	0.75	0.67

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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