QSAR model for *in vitro* cytogenicity study in mammalian cells (chromosomal aberration) (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. *In vitro* Mammalian Chromosome Aberration 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. The *in vitro* mammalian chromosome aberration test is a measure of *in vitro* chromosomal mutagenicity. The test evaluates structural and numerical chromosome aberrations. The test identifies substances that induce structural chromosome aberrations in cultured mammalian established cell lines, cell strains or primary cell cultures.

Metrics

Training set

Experimental values	QSAR predictions	
	non-cytotoxic	cytotoxic
non-cytotoxic	48	17
cytotoxic	16	46

Validation set

Experimental values	QSAR predictions	
	non-cytotoxic	cytotoxic
non-cytotoxic	24	10
cytotoxic	9	21

Parameters	Training	Validation
Accuracy	0.74	0.70
Sensitivity / recall	0.74	0.70
Specificity	0.74	0.71
Precision	0.73	0.68
Negative predictive value	0.75	0.73
F-score	0.74	0.69
Matthews Correlation Coefficient	0.48	0.41
Critical Success Index	0.58	0.53
Area under the ROC	0.74	0.70