QSAR model for *in vitro* cytogenicity study in mammalian cells (chromosomal aberration) (v1.0)

ProtoTOX by **ProtoQSAR**

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 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

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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