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

ProtoREACH by ProtoQSAR

ProtoREACH

ProtoREACH is a computational (*in silico*) tool specially focused on 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.

REACH also promotes alternative methods for the hazard assessment of substances in order to reduce the number of tests on animals. The requirements for registering a chemical substance are organized as annexes of the REACH regulation. Different annexes must be used depending on the substance mass produced or imported by each company.

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