QSAR model for in vitro gene mutation study in bacteria (Ames test) (v1.0)



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. OECD 471: Bacterial reverse mutation test.

Mutagenicity refers to the induction of permanent transmissible changes in the amount or structure of the genetic material of cells or organisms. The Bacterial reverse mutation test evaluates gene mutations. The test uses amino-acid requiring strains of bacteria to detect (reverse) gene mutations (point mutations and frameshifts).

Metrics

Training set

Experimental values	QSAR predictions		
	non-mutagenic	mutagenic	
non-mutagenic	2048	203	
mutagenic	154	2463	

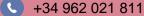
	Validation set		
Experimental values	QSAR predictions		
	non-mutagenic	mutagenic	
non-mutagenic	553	196	
mutagenic	190	685	

Parameters	Training	Validation
Accuracy	0.93	0.76
Sensitivity / recall	0.94	0.78
Specificity	0.91	0.74
Precision	0.92	0.78
Negative predictive value	0.93	0.74
F-score	0.93	0.78
Matthews Correlation Coefficient	0.85	0.52
Critical Success Index	0.87	0.64
Area under the ROC	0.93	0.76



ProtoPRED platform allows the easy, fast and user-friendly prediction of different properties of chemical compounds, by proprietary (Q)SAR models.







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