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

ProtoICH

by **ProtoQSAR**

ProtoICH

ProtoICH is a computational (*in silico*) tool specially focused on **ICH M7 Guideline**, aimed to reduce the potential carcinogenic risk of impurities. ICH M7 Guideline proposes the use of computational methods as an alternative for mutagenicity assays. It requires the prediction by means of two computational metodologies: a **statistical method (QSAR)** and an **expert-rule based method**. Moreover, it requires the detection of aflatoxins, N-nitrosamines and azoxy compounds (carcinogenicity **cohort of concern**).

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

ProtoICH 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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