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