

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/Genotoxicity. Mammalian erythrocyte micronucleus 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. *In vivo* mammalian erythrocyte micronucleus test is a measure of *in vivo* chromosomal mutagenicity. The test identifies substances that cause micronuclei in erythroblasts sampled from bone marrow and/or peripheral blood cells of animals, usually rodents. These micronuclei originate from acentric fragments or whole chromosomes, and the test thus has the potential to detect both clastogenic and aneugenic substances.

Metrics

Training set

| Experimental values | QSAR predictions | |
|---------------------|------------------|-----------|
| | non-cytotoxic | cytotoxic |
| non-cytotoxic | 60 | 22 |
| cytotoxic | 29 | 92 |

Validation set

| Experimental values | QSAR predictions | |
|---------------------|------------------|-----------|
| | non-cytotoxic | cytotoxic |
| non-cytotoxic | 23 | 13 |
| cytotoxic | 10 | 23 |

| Parameters | Training | Validation |
|----------------------------------|----------|------------|
| Accuracy | 0.75 | 0.67 |
| Sensitivity / recall | 0.76 | 0.70 |
| Specificity | 0.73 | 0.64 |
| Precision | 0.81 | 0.64 |
| Negative predictive value | 0.67 | 0.70 |
| F-score | 0.78 | 0.67 |
| Matthews Correlation Coefficient | 0.49 | 0.34 |
| Critical Success Index | 0.64 | 0.50 |
| Area under the ROC | 0.75 | 0.67 |

GenoITS is part of



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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