# QSAR model for *in vivo* gene mutation study in somatic cells (comet assay) (v1.0)

ProtoTOX by ProtoQSAR

## 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/Genotoxicity. *In vivo* comet assay in mouse.**

The comet assay is a method for measuring DNA strand breaks in eukaryotic cells. Single cells/nuclei embedded in agarose on a slide are lysed with detergent and high salt concentration. This lysis step digests the cellular and nuclear membranes and allows the release of coiled DNA loops generally called nucleoids and DNA fragments. Electrophoresis at high pH results in structures resembling comets, which, by using appropriate fluorescent stains, can be observed by fluorescence microscopy; DNA fragments migrate away from the “head” into the “tail” based on their size, and the intensity of the comet tail relative to the total intensity (head plus tail) reflects the amount of DNA breakage.

## Metrics

### Training set

| Experimental values | QSAR predictions | |
|---|---|---|
| | non-mutagenic | mutagenic |
| non-mutagenic | 90 | 10 |
| mutagenic | 5 | 80 |

### Validation set

| Experimental values | QSAR predictions | |
|---|---|---|
| | non-mutagenic | mutagenic |
| non-mutagenic | 31 | 7 |
| mutagenic | 6 | 36 |

| Parameters | Training | Validation |
|---|---|---|
| Accuracy | 0.92 | 0.84 |
| Sensitivity / recall | 0.94 | 0.86 |
| Specificity | 0.90 | 0.82 |
| Precision | 0.89 | 0.84 |
| Negative predictive value | 0.95 | 0.84 |
| F-score | 0.91 | 0.85 |
| Matthews Correlation Coefficient | 0.84 | 0.67 |
| Critical Success Index | 0.84 | 0.73 |
| Area under the ROC | 0.92 | 0.84 |

ProtoTOX 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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