

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

ProtoREACH

ProtoREACH is a computational (*in silico*) tool specially focused on 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.

REACH also promotes alternative methods for the hazard assessment of substances in order to reduce the number of tests on animals. The requirements for registering a chemical substance are organized as annexes of the REACH regulation. Different annexes must be used depending on the substance mass produced or imported by each company.

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 |

ProtoREACH is part of



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

 +34 962 021 811

 protopred@protoqsar.com

<https://protopred.protoqsar.com/>

© 2024 ProtoQSAR S.L.