

# QSAR model for Thyroid-stimulating hormone (TSH, or thyrotropin) receptor (TSHR) antagonism (v1.0)

## ProtoED

ProtoED 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.

ProtoED 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: Thyroid stimulating hormone receptor antagonism

thyroid gland cells that binds thyroid stimulating hormone (TSH) to trigger thyroid hormone production and thyroid gland growth. Thyroid stimulating hormone receptor antagonism is the inhibition of TSHR activity by compounds that block TSH binding or receptor activation. This can reduce thyroid hormone production and disturb endocrine balance, with implications for metabolic rate and neurodevelopment.

## Metrics

### Training set

| Experimental values | QSAR predictions |            |
|---------------------|------------------|------------|
|                     | inactive         | antagonist |
| inactive            | 134              | 11         |
| antagonist          | 10               | 145        |

### Validation set


| Experimental values | QSAR predictions |            |
|---------------------|------------------|------------|
|                     | inactive         | antagonist |
| inactive            | 30               | 20         |
| antagonist          | 11               | 40         |

| Parameters                       | Training | Validation |
|----------------------------------|----------|------------|
| Accuracy                         | 0.93     | 0.69       |
| Sensitivity / recall             | 0.94     | 0.78       |
| Specificity                      | 0.92     | 0.60       |
| Precision                        | 0.93     | 0.67       |
| Negative predictive value        | 0.93     | 0.73       |
| F-score                          | 0.93     | 0.72       |
| Matthews Correlation Coefficient | 0.86     | 0.39       |
| Critical Success Index           | 0.87     | 0.56       |
| Area under the ROC               | 0.93     | 0.69       |

ProtoED 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](mailto:protopred@protoqsar.com)

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

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