QSAR model for Thyroid-stimulating hormone (TSH, or thyrotropin) receptor (TSHR) agonism (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 agonism

The thyroid stimulating hormone receptor (TSHR) is a G-protein-coupled receptor on the thyroid gland cells that binds thyroid stimulating hormone (TSH) to trigger thyroid hormone production and thyroid gland growth. Thyroid stimulating hormone receptor agonism refers to the activation of the thyroid-stimulating hormone receptor (TSHR), a G protein-coupled receptor located in the thyroid gland, by endogenous TSH or TSH-like compounds. Agonism of TSHR promotes the synthesis and release of thyroid hormones (T3 and T4), which are critical for growth, metabolism, and development.

Metrics

Training set

Experimental values	QSAR predictions	
	inactive	**agonist**
inactive	189	17
agonist	11	188

Validation set

Experimental values	QSAR predictions	
	inactive	**agonist**
inactive	45	25
agonist	19	49

Parameters	Training	Validation
Accuracy	0.93	0.68
Sensitivity / recall	0.94	0.72
Specificity	0.92	0.64
Precision	0.92	0.66
Negative predictive value	0.94	0.70
F-score	0.93	0.69
Matthews Correlation Coefficient	0.86	0.36
Critical Success Index	0.87	0.53
Area under the ROC	0.93	0.68