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

ProtoED by ProtoQSAR

ProtoED

ProtoED is a computational tool designed to predict whether a compound will act as an agonist or antagonist on various hormonal receptors, facilitating the assessment of the compound's potential to disrupt the endocrine system.

By employing QSAR models, ProtoED offers an efficient alternative to experimental assays by enabling rapid and accurate predictions of compound-receptor interactions, serving as a valuable tool in chemical and pharmacological research.

This module promotes the use of alternative methods, helping to reduce the need for *in vivo* testing and supporting decision-making processes regarding potential risks to human health and the environment.

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