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

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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