QSAR model for Thyroid Receptor Beta (TRβ) 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 receptor beta agonism

Thyroid Hormone Receptor Beta (TRβ) is a nuclear receptor that binds to thyroid hormone and plays a crucial role in regulating gene expression in various organs such as the liver, kidney, and thyroid. It is one of the major isoforms of thyroid hormone receptors and is involved in specific physiological functions within the body. Thyroid receptor beta agonism refers to a chemical compound that mimics the action of thyroid hormone, specifically targeting TRβ. Agonism leads to activation of target gene expression linked to thyroid hormone.

Metrics

Training set

Experimental values	QSAR predictions	
	inactive	**agonist**
inactive	123	2
agonist	6	114

Validation set

Experimental values	QSAR predictions	
	inactive	**agonist**
inactive	38	5
agonist	2	39

Parameters	Training	Validation
Accuracy	0.97	0.92
Sensitivity / recall	0.95	0.95
Specificity	0.98	0.88
Precision	0.98	0.89
Negative predictive value	0.95	0.95
F-score	0.97	0.92
Matthews Correlation Coefficient	0.94	0.84
Critical Success Index	0.93	0.85
Area under the ROC	0.97	0.92

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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