QSAR model for Thyroid Receptor Alpha (TRα) agonism (v1.0)

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 alpha agonism

Thyroid hormone receptor alpha (TRα) is defined as a type of receptor that binds to the active thyroid hormone T3, primarily expressed in certain brain areas and the heart. Thyroid receptor alpha agonism is a mechanism by which substances interact with thyroid receptor alpha (TRα).

Metrics

Training set

Experimental values	QSAR predictions	
	inactive	**agonist**
inactive	101	6
agonist	10	96

Validation set

Experimental values	QSAR predictions	
	inactive	**agonist**
inactive	37	0
agonist	6	30

Parameters	Training	Validation
Accuracy	0.92	0.92
Sensitivity / recall	0.91	0.83
Specificity	0.94	1.00
Precision	0.94	1.00
Negative predictive value	0.91	0.86
F-score	0.92	0.91
Matthews Correlation Coefficient	0.85	0.85
Critical Success Index	0.86	0.83
Area under the ROC	0.92	0.92

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