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

ProtoED
by **ProtoQSAR**

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 receptor alpha antagonism

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 antagonism occurs when compounds bind to TRα but do not activate it, effectively blocking thyroid hormone signaling and potentially leading to metabolic and developmental disturbances.

Metrics

Training set

Experimental values	QSAR predictions	
	inactive	antagonist
inactive	188	28
antagonist	7	203

Validation set

Experimental values	QSAR predictions	
	inactive	antagonist
inactive	61	13
antagonist	3	67

Parameters	Training	Validation
Accuracy	0.92	0.89
Sensitivity / recall	0.97	0.96
Specificity	0.87	0.82
Precision	0.88	0.84
Negative predictive value	0.96	0.95
F-score	0.92	0.89
Matthews Correlation Coefficient	0.84	0.79
Critical Success Index	0.85	0.81
Area under the ROC	0.92	0.89

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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