QSAR model for Thyroid Receptor Beta (TRβ) antagonism (v1.0)

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 beta antagonism

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 antagonism refers to the inhibition of TRβ activation by compounds that occupy the receptor without triggering its transcriptional activity. This can interfere with systemic thyroid hormone signaling and contribute to metabolic dysfunctions.

Metrics

Training set

Experimental values	QSAR predictions	
	inactive	**antagonist**
inactive	358	27
antagonist	13	368

Validation set

Experimental values	QSAR predictions	
	inactive	**antagonist**
inactive	110	21
antagonist	5	122

Parameters	Training	Validation
Accuracy	0.95	0.90
Sensitivity / recall	0.97	0.96
Specificity	0.93	0.84
Precision	0.93	0.85
Negative predictive value	0.96	0.96
F-score	0.95	0.90
Matthews Correlation Coefficient	0.90	0.80
Critical Success Index	0.90	0.82
Area under the ROC	0.95	0.90

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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