QSAR model for Estrogen Receptor Beta (ERβ) agonism (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: Estrogen receptor beta agonism

Estrogen Receptor Beta (ERβ) is a subtype of estrogen receptor that is involved in mediating the protective effects of estradiol against stroke injury in the brain. It plays a unique role in the neuroprotection provided by physiological levels of estradiol. Estrogen receptor beta agonism involves the binding of specific compounds to ERβ. Agonist binding activates ERβ, leading to modulation of gene expression.

Metrics

Training set

Experimental values	QSAR predictions	
	inactive	agonist
inactive	350	7
agonist	31	204

Validation set

Experimental values	QSAR predictions	
	inactive	agonist
inactive	150	6
agonist	20	82

Parameters	Training	Validation
Accuracy	0.94	0.90
Sensitivity / recall	0.87	0.80
Specificity	0.98	0.96
Precision	0.97	0.93
Negative predictive value	0.92	0.88
F-score	0.91	0.86
Matthews Correlation Coefficient	0.87	0.79
Critical Success Index	0.84	0.76
Area under the ROC	0.92	0.88

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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