

QSAR model for Estrogen Receptor Beta (ER β) 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: Estrogen receptor beta antagonism

Estrogen Receptor Beta (ER β) 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 antagonism refers to the binding of substances to ER β that prevent its activation. These antagonists inhibit the effects of natural estrogens at this receptor, potentially affecting cellular proliferation, differentiation, and immune modulation in ER β -expressing tissues.

Metrics

Training set

Experimental values	QSAR predictions	
	inactive	antagonist
inactive	350	66
antagonist	37	268

Validation set


Experimental values	QSAR predictions	
	inactive	antagonist
inactive	128	26
antagonist	27	76

Parameters	Training	Validation
Accuracy	0.86	0.79
Sensitivity / recall	0.88	0.74
Specificity	0.84	0.83
Precision	0.80	0.75
Negative predictive value	0.90	0.83
F-score	0.84	0.74
Matthews Correlation Coefficient	0.71	0.57
Critical Success Index	0.72	0.59
Area under the ROC	0.86	0.78

ProtoED is part of



ProtoPRED platform allows the easy, fast and user-friendly prediction of different properties of chemical compounds, using proprietary (Q)SAR models.

 +34 962 021 811

 protopred@protoqsar.com

<https://protopred.protoqsar.com/>

© 2025 ProtoQSAR S.L.