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

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 antagonism refers to the binding of substances to ERβ that prevent its activation. These antagonists inhibit the effects of natural estrogens at this receptor, potentially affecting cellular proliferation, differentiation, and immune modulation in ERβ-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