QSAR model for Estrogen Receptor Beta (ERβ) agonism (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 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