

QSAR model for Estrogen Receptor Alpha (ER α) 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 alpha agonism

Estrogen receptor alpha (ER α) is a member of the nuclear receptor superfamily of transcription factors whose activity is primarily regulated by binding of estrogen/estradiol (E2). E2 plays an indispensable role in growth, development, reproduction, and maintenance of numerous physiological systems in mammals. Estrogen receptor alpha agonism is a process where certain substances, including endogenous estrogens or synthetic estrogenic compounds, bind to the ER α . Upon activation, ER α initiates transcriptional regulation of estrogen-responsive genes involved in development, metabolism, and cell proliferation.

Metrics

Training set

Experimental values	QSAR predictions	
	inactive	agonist
inactive	672	73
agonist	73	607

Validation set

Experimental values	QSAR predictions	
	inactive	agonist
inactive	224	97
agonist	83	209

Parameters	Training	Validation
Accuracy	0.90	0.71
Sensitivity / recall	0.89	0.72
Specificity	0.90	0.70
Precision	0.89	0.68
Negative predictive value	0.90	0.73
F-score	0.89	0.70
Matthews Correlation Coefficient	0.79	0.41
Critical Success Index	0.81	0.54
Area under the ROC	0.90	0.71

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.

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