QSAR model for Glucocorticoid Receptor (GR) 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: Glucocorticoid receptor agonism

The glucocorticoid receptor (GR) is an evolutionarily conserved nuclear receptor superfamily protein that mediates the diverse actions of glucocorticoids as a ligand-dependent transcription factor. This receptor is a protein that shuttles from the cytoplasm to the nucleus upon binding to its ligand glucocorticoid hormone, where it modulates the transcription rates of glucocorticoid-responsive genes positively or negatively. Glucocorticoid receptor agonism involves the binding of glucocorticoid hormones or synthetic glucocorticoids to the GR.

Metrics

Training set

Experimental values	QSAR predictions	
	inactive	**agonist**
inactive	546	11
agonist	47	550

Validation set

Experimental values	QSAR predictions	
	inactive	**agonist**
inactive	171	16
agonist	27	172

Parameters	Training	Validation
Accuracy	0.95	0.89
Sensitivity / recall	0.92	0.86
Specificity	0.98	0.91
Precision	0.98	0.91
Negative predictive value	0.92	0.86
F-score	0.95	0.89
Matthews Correlation Coefficient	0.90	0.78
Critical Success Index	0.90	0.80
Area under the ROC	0.95	0.89