

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

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 antagonism occurs when compounds bind to the GR but do not activate it, thereby preventing the effects of endogenous glucocorticoids. This antagonism can be used therapeutically but may also disrupt homeostatic regulation of inflammation and metabolism.

Metrics

Training set

Experimental values	QSAR predictions	
	inactive	antagonist
inactive	1331	114
antagonist	159	1277

Validation set


Experimental values	QSAR predictions	
	inactive	antagonist
inactive	436	46
antagonist	74	405


Parameters	Training	Validation
Accuracy	0.91	0.88
Sensitivity / recall	0.89	0.85
Specificity	0.92	0.90
Precision	0.92	0.90
Negative predictive value	0.89	0.85
F-score	0.90	0.87
Matthews Correlation Coefficient	0.81	0.75
Critical Success Index	0.82	0.77
Area under the ROC	0.91	0.88

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/>

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