QSAR model for Glucocorticoid Receptor (GR) antagonism (v1.0)

ProtoED
by **ProtoQSAR**

ProtoED

ProtoED is a computational (*in silico*) tool focused on the prediction of endpoints related with the toxicity of chemical substances. It includes a variety of *in vitro* and *in vivo* tests in humans, animals, microorganisms and cell lines.

ProtoED mainly includes, but is not limited to, endpoints used by REACH, a European Union regulation, adopted to improve the protection of human health and the environment from the risks that can be posed by chemicals, while enhancing the competitiveness of the EU chemicals industry.

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

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