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

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 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