QSAR model for Androgen Receptor (AR) antagonism (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: Androgen receptor antagonism

The androgen receptor belongs to the superfamily of nuclear receptors that mediates the actions of lipophilic ligands, such as steroids, retinoids, and thyroid hormones. Androgen receptor antagonism is a biological mechanism in which certain substances, such as pharmaceutical agents or environmental chemicals, bind to the androgen receptor (AR) without activating it. Instead, these substances block the receptor's activity, thereby preventing endogenous androgens from exerting their physiological effects. This inhibition can alter gene expression patterns and interfere with normal androgen-mediated development or function.

Metrics

Training set

Experimental values	QSAR predictions	
	inactive	**antagonist**
inactive	578	118
antagonist	100	598

Validation set

Experimental values	QSAR predictions	
	inactive	**antagonist**
inactive	176	58
antagonist	61	172

Parameters	Training	Validation
Accuracy	0.84	0.75
Sensitivity / recall	0.86	0.74
Specificity	0.83	0.75
Precision	0.84	0.75
Negative predictive value	0.85	0.74
F-score	0.85	0.74
Matthews Correlation Coefficient	0.69	0.49
Critical Success Index	0.73	0.59
Area under the ROC	0.84	0.75