QSAR model for Androgen Receptor (AR) 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: 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