QSAR model for Androgen Receptor (AR) agonism (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 agonism.

The androgen receptor belongs to the superfamily of nuclear receptors that mediates the actions of lipophilic ligands, such as steroids, retinoids, and thyroid hormones. By binding and activating the AR, these agonists induce the AR dissociation from heat shock proteins and translocate to the nucleus, where they can effectively bind to DNA-specific sequences (androgen response elements or AREs), and ultimately the regulation of target gene transcription. This process produces a diverse range of biological effects crucial for male sexual differentiation and other physiological processes.

Metrics

Training set

Experimental values	QSAR predictions	
	inactive	**agonist**
inactive	237	21
agonist	34	220

Validation set

Experimental values	QSAR predictions	
	inactive	**agonist**
inactive	72	15
agonist	16	69

Parameters	Training	Validation
Accuracy	0.89	0.82
Sensitivity / recall	0.87	0.81
Specificity	0.92	0.83
Precision	0.91	0.82
Negative predictive value	0.87	0.82
F-score	0.89	0.82
Matthews Correlation Coefficient	0.79	0.64
Critical Success Index	0.80	0.69
Area under the ROC	0.89	0.82

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.

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