

QSAR model for Androgen Receptor (AR) 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: 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 platform allows the easy, fast and user-friendly prediction of different properties of chemical compounds, using proprietary (Q)SAR models.

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