QSAR model for cytotoxicity in tumoral cells (QDs) (v1.0)

ProtoNANO

ProtoNANO is a computational (*in silico*) tool focused on the prediction of endpoints related with the physicochemical, toxicological and ecotoxicological properties of nanomaterials.

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Endpoint

Other

The cytotoxicity versus cells lines growth from tumoural cells, is a mesure of the potential toxicity of the nanomaterials, but specifically of their potency toward tumoural cells. The antitumoral capacity of QD has been reported elsewhere, due to their particular molecular characteristics, which include optical, electronic, and engineered biocompatibility in physiological environments. Moreover, they can be coated to specifically arise cancer cells.

Nanomaterials

The models was developed with quantum dots (QD) of variable composition in the core and the shell. It requires the inclusion of the size and two experimental conditions: exposure time and concentration.

Metrics

Training set

Experimental values	QSAR predictions	
	Non-toxic	**Toxic**
Non-toxic	158	17
Toxic	75	283

Validation set

Experimental values	QSAR predictions	
	Non-toxic	**Toxic**
Non-toxic	49	20
Toxic	31	80

Parameters	Training	Validation
Accuracy	0.83	0.72
Sensitivity / recall	0.79	0.72
Specificity	0.90	0.71
Precision	0.94	0.80
Negative predictive value	0.68	0.61
F-score	0.86	0.76
Matthews Correlation Coefficient	0.66	0.42
Critical Success Index	0.75	0.61
Area under the ROC	0.85	0.72