QSAR model for Cytotoxicity in human 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.

ProtoNANO was developed as a part of the NanoQSAR research project. This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No 896848.

Endpoint

Human health effects: cytotoxicity

The cytotoxicity versus human primary cells, is a mesure of the potential toxicity of the nanomaterials. QD has extremely useful properties, but they can promote cytotoxicity mainly by the inherent toxicity of the components of the QD core (mainly selenium and cadmium).

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	77	6
Toxic	8	67

Validation set

Experimental values	QSAR predictions	
	Non-toxic	Toxic
Non-toxic	26	7
Toxic	9	11

Parameters	Training	Validation
Accuracy	0.91	0.70
Sensitivity / recall	0.89	0.55
Specificity	0.93	0.79
Precision	0.92	0.61
Negative predictive value	0.91	0.74
F-score	0.91	0.58
Matthews Correlation Coefficient	0.82	0.35
Critical Success Index	0.83	0.41
Area under the ROC	0.91	0.67

ProtoNANO is part of ProtoPRED

ProtoPRED platform allows the easy, fast and user-friendly prediction of different properties of chemical compounds, by proprietary (Q)SAR models.

+34 962 021 811 protopred@protoqsar.com

https://protopred.protoqsar.com/