QSAR model for Zeta Potential (M/Mox/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

Physical-chemical properties: Zeta potential

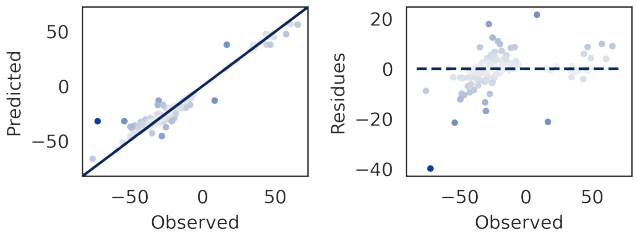
The zeta potential is the charge that develops at the interface between a solid surface and its liquid medium. Zeta potential can be used as a proxy for surface charge and may provide information in the dispersion stability and agglomeration/deagglomeration of particles. Surface charge may influence systemic distribution and cellular uptake of a nanoform, and ultimately its toxicity. Additionally, there is evidence of its link with the inflammogenicity of nanomaterials.

Nanomaterials

The models was developed with a dataset including metal oxides (MOx), quantum dots (QD) and noble metals (M) nanomaterials, covered by organic ligands/surfactants. It requires also the inclusion of the size (diameter) of the nanoparticle.

Metrics

Training set



Parameters	Training	Validation
R^2 score	0.94	0.89
Mean absolute error (MAE)	4.23	6.55
Mean squared error (MSE)	46.89	117.98
Median absolute error	2.30	3.59
Explained variance	0.94	0.89

Validation set