

## 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 Skłodowska-Curie grant agreement No 896848.

## Endpoint

### Physical-chemical properties: Zeta potential.

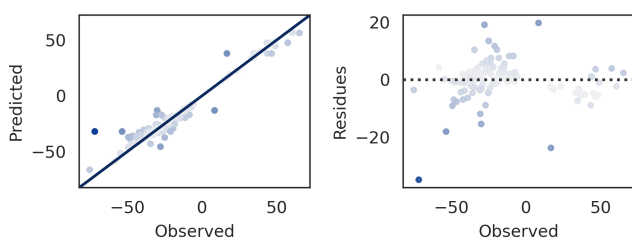
The zeta potential is the charge that develops at the interface between a solid surface and its liquid medium. Zeta potential can be used as a proxy for surface charge and may provide information in the dispersion stability and agglomeration/deagglomeration of particles. Surface charge may influence 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

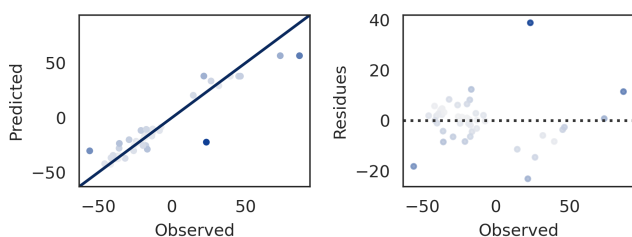
The models was developed with a dataset including metal oxides (MOx), quantum dots (QD) and noble metals (M) nanomaterials, covered by organic ligands/surfactants. It requires also the inclusion of the size (diameter) of the nanoparticle.

## Metrics

### Training set



### Validation set



Parameters	Training	Validation
R <sup>2</sup> 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

ProtoNANO 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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