

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

Ecotoxic effects: Toxicity to microorganisms.

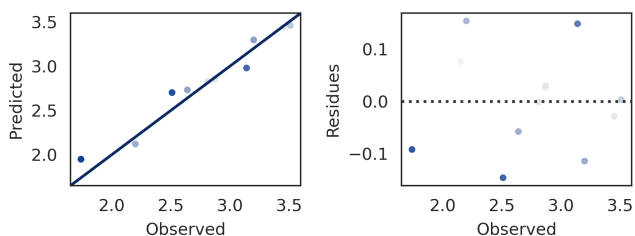
The cytotoxicity versus *Escherichia coli* bacteria is a measure of the potential toxicity over microorganisms. It can have environmental consequences, but also can serve to elucidate the effects on higher, more complex organisms.

Nanomaterials

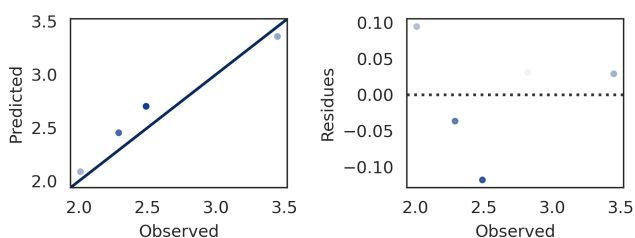
The models was developed with bare MOx nanoparticles with a diameter ~40 nm and does not consider the size.

Metrics

Training set



Validation set



Parameters	Training	Validation
R ² score	0.96	0.93
Mean absolute error (MAE)	0.08	0.11
Mean squared error (MSE)	0.01	0.02
Median absolute error	0.07	0.09
Explained variance	0.96	0.95

ProtoNANO is part of

ProtoPRED

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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