QSAR model for Cytotoxicity in *E. coli* (MOx) (v1.0)

ProtoNANO by **ProtoQSAR**

ProtoNANO

Proto**NANO** 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

Ecotoxic effects: Toxicity to microorganisms

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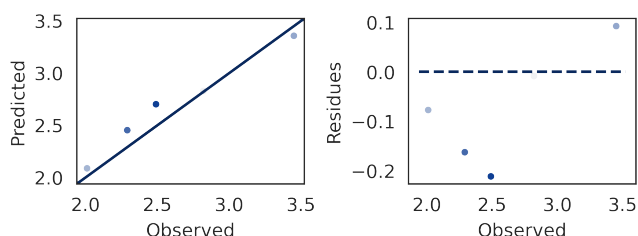
Nanomaterials

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

Metrics

Training set
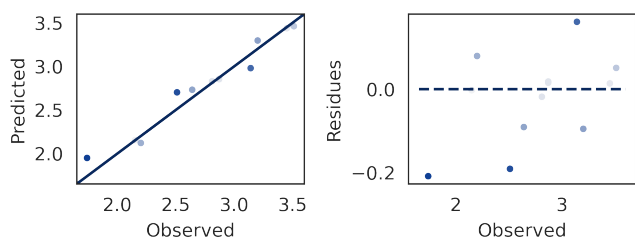
Validation set

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