Supplementary information

From Basic Physics to Mechanisms of Toxicity: "Liquid Drop" Approach Applied to Develop Predictive Classification Models for Toxicity of Metal Oxide Nanoparticles

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Table S1. Specifications of developed model for toxicity towards *E.coli*

Compound	Observed values log ($1/EC_{50}$)	Predicted values log ($1/EC_{50}$)	Predicted standard deviation log (1/EC50))	Set
ZrO_2	2.150	1.902	0.148	test
NiO	3.450	3.242	0.368	test
Sb_2O_3	2.640	2.956	0.382	test
Al_2O_3	2.490	2.570	0.168	training
Bi_2O_3	2.820	2.850	0.027	training
SnO_2	2.010	1.902	0.148	training
TiO_2	1.740	1.832	0.206	training
V_2O_3	3.140	2.888	0.345	training
Y_2O_3	2.870	2.870	0.000	training
CoO	3.510	3.370	0.313	training
Cr_2O_3	2.510	2.538	0.209	training
Fe_2O_3	2.290	2.378	0.120	training
In_2O_3	2.810	2.822	0.027	training
La_2O_3	2.870	2.87	0.000	training
SiO_2	2.200	1.924	0.252	training

Figure S1. Plot of experimentally determined (observed) versus predicted log values of $1/EC_{50}$ for model of toxicity towards *E.coli*

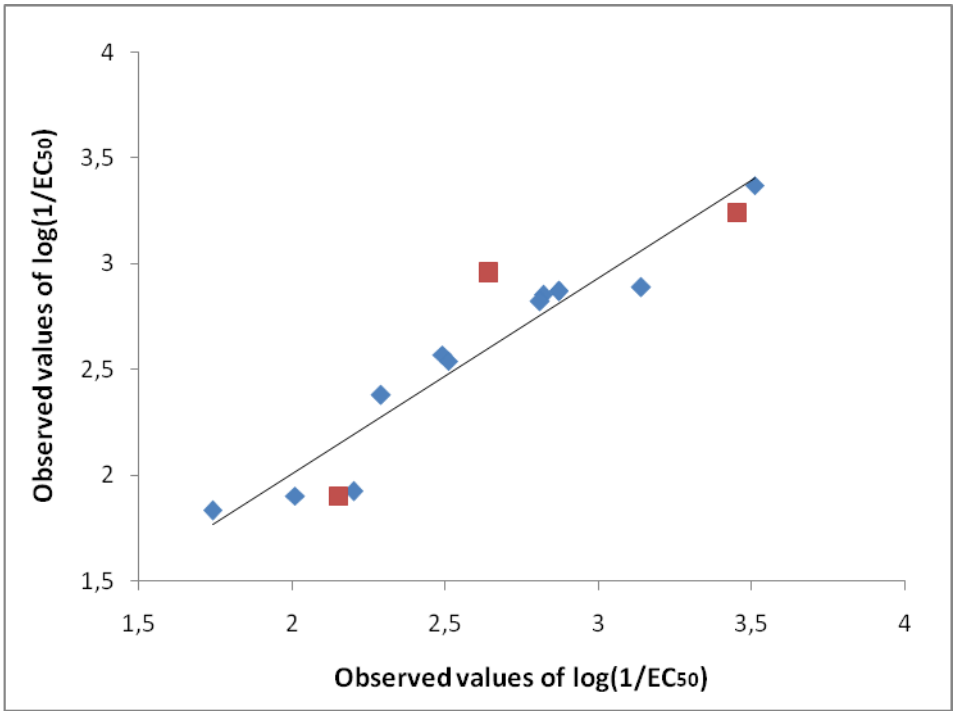

Table S2. Specifications of developed model for toxicity towards *HaCaT*

Compound	Observed values log (1/LC_{50})	Predicted values log (1/LC_{50})	Predicted standard deviation log (1/LC50))	Set
ZrO_2	2.020	2.110	0.066	test
CoO	2.830	2.786	0.493	test
Cr_2O_3	2.300	2.160	0.073	test
Al_2O_3	1.850	1.912	0.131	training
Bi_2O_3	2.500	2.534	0.076	training
SiO_2	2.120	1.962	0.187	training
SnO_2	2.670	2.544	0.201	training
TiO_2	1.760	1.818	0.130	training
WO_3	2.560	2.560	0.000	training
Y_2O_3	2.210	2.146	0.088	training
ZnO	3.320	3.118	0.452	training
Fe_2O_3	2.050	2.082	0.072	training
In_2O_3	2.920	2.816	0.178	training
La_2O_3	2.870	2.880	0.022	training
Mn_2O_3	2.640	2.510	0.178	training
NiO	2.490	2.490	0.000	training
Sb_2O_3	2.310	2.388	0.533	training

Figure S2. Plot of experimentally determined (observed) versus predicted log values of 1/LC_{50} for model of toxicity towards *HaCaT*