BEILSTEIN JOURNAL OF NANOTECHNOLOGY

Supporting Information

for

A review on the structural characterization of nanomaterials for nano-QSAR models

Salvador Moncho, Eva Serrano-Candelas, Jesús Vicente de Julián-Ortiz and Rafael Gozalbes

Beilstein J. Nanotechnol. **2024,** *15,* 854–866. doi:10.3762/bjnano.15.71

All models evaluated in the review, as well as the classification of selected descriptors according to the proposed categories

List of contents:

Table S1: List of models evaluated in the review, as well as the classification of selected descriptors according to the classification presented in this paper. Abbreviatures used in the table: CN: coordination numbers; CNT: carbon nanotubes; Ei: energy of i (CB, conduction band; form, formation, VB, valence band): $El_{(w)}$: descriptors calculated or from literature relating to pure elements (w if weighted for compounds); EC: descriptors based in the electron configuration; EN: descriptors related with electronegativity; Ful.: fullerenes; IS: Ionic strength in the reaction media; LDM: liquid drop model descriptors; Molec.: common molecular descriptors obtained from the SMILES for organic molecules; M_i: descriptor referring only to the metal atom; MOx: metal oxides (element among parenthesis if there is a single composition); NOM: Amount of organic matter in the test media; ON: oxidation number of the metal; Pr_i: binary descriptor indicating the presence/absence of a component or experimental condition; PT: position in the periodic table, QDs: quantum dots; QM: descriptors calculated using electronic methods; S_i: size of the nanomaterial described by its diameter (a subindex can be included referring to different methods or media); SA: surface area; SP: sedimentation potential (calculated); SPR: signaling-pathway responses; Target: the target cell is included as a descriptors (directly or by a perturbation method); R1 and R2: magnetic relaxitivities; ZP: zeta potential; $\#_i$: count of atoms of element/type i.

				Classification					
	Reference	**Endpoint**	**NM type**	**A**	**B**	**C**	**D**	**E**	**F**
[1]	Hu, 2009	LD_{50} (cytotoxicity in *E. coli*)	MOx	M_{charge}					
[2]	Fourches, 2010	Cellular uptake in PaCa2 human cells	MOx (Fe)		Molec.				
		Toxicity vector in human cells (4 types)	Mixed			S			
[3]	Sayes, 2010	Membrane damage in human lung cells (LDH test)	MOx			S_{TEM}, S_{Water}, S_{buff}	ZP, R1, R2		
[4]	Burello, 2011b	Oxidative stress potential	MOx	M_{ON}					
[5]	Liu, 2011	Cytotoxicity in BEAS-2	MOx	$\#_{M,O}$, M_{mass}, PT					

				Classification					
	Reference	**Endpoint**	**NM type**	**A**	**B**	**C**	**D**	**E**	**F**
[6]	Puzyn, 2011	pEC_{50} (cytotoxicity in *E. coli*)	MOx	QM					
[7]	Rallo, 2011	Luciferase in murine RAW cells	M/Mox				SPR		
[8]	Chau, 2012	Cellular uptake in PaCa2 human cells	MOx (Fe)		Molec				
[9]	Epa, 2012	Smooth cell apoptosis	Mixed	Pr_{Fe2O3}	$Pr_{Dextran}$, Acidity				
		Cellular uptake (HUVEC/ PaCa2)	MOx (Fe)		Molec.				
[10]	Patel, 2012	Cytotoxicity in RAW and BEAS-2B cells	Mixed						
[11]	Toropov, 2012	pEC_{50} (cytotoxicity in *E. coli*)	MOx						
[12]	Ahmed, 2013	pEC_{50} (HIV-protease binding)	Ful.	QM	Molec.				
[13]	Liu, 2013a	Cytotoxicity	MOx			S	ZP, R1, R2		
[14]	Liu, 2013b	EZ metric (Zebrafish embryo)	Mixed					precursors	
[15]	Liu, 2013c	Cytotoxicity in BEASE/RAW (MTS)	MOx						
[16]	Kar, 2014	pEC_{50} (cytotoxicity in *E. coli*)	MOx	EN, M_{charge}					

			Classification					
Reference	**Endpoint**	**NM type**	**A**	**B**	**C**	**D**	**E**	**F**
[17] Kleandrova, 2014	Multiple: ecotoxicity and toxicity	M/MOx	$EI_{(w)}$					
[18] Liu, 2014	10 SPRs and 4 cytotoxicity indicators in RAW/BEAS-2B	M/Mox						
[19] Pathakoti, 2014	pEC_{50} (cytotoxicity in *E. coli*)	MOx	QM		S_{TEM}, S_{hydro}, SA, Mass, V	ZP_{water}, ZP_{media}		Pr_{Light}
[20] Singh, 2014	several	Mixed						
[21] Sizochenko, 2014	pEC_{50} (cytotoxicity in *E. coli* and HaCaT)	MOx			LDM			
[22] Toropov, 2014	Mutagenicity (Ames test in TA100)	Ful.						Pr_{S9}, $Pr_{Irradiation}$, Dose
[23] Venigalla, 2014	pEC_{50} (cytotoxicity in *E. coli*)	MOx						
[24] Gajewicz, 2015	HaCaT	MOx						
[25] Kaweeteerawat, 2015	pEC_{50} (cytotoxicity in *E. coli*)	MOx						
[26] Mikolajczyk, 2015	Zeta Potential	MOx						

				Classification				
Reference	**Endpoint**	**NM type**	**A**	**B**	**C**	**D**	**E**	**F**
[27] Sizochenko, 2015	Cytotoxicity in BEASE/RAW (MTS)	MOx						
[28] Toropov, 2015b	Mutagenicity (Ames test in TA100)	Ful./CNT				Id		Pr_{S9}, $Pr_{incub.}$, Dose
[29] Toropov , 2015a	Mutagenicity (Ames test in TA100)	CNT						Pr_{S9}, $Pr_{incub.}$, Dose
[30] Toropova, 2015	Cell viability (HK-2/LLC-PK1)	SiO_2		$\#_M$		S_{bin}		Dose, time
[31] Cassano, 2016	pEC_{25} (WST-1) Several	SiO_2				S_{bin}, R_{bin}	ZP_{bin}	Time, CL,
[32] Jagiello, 2016	HIV-protease binding	Ful.						
[33] Kar, 2016	pEC_{50} (cytotoxicity in *E. coli* and HaCaT)	MOx						
[34] Le, 2016	Cell viability/LDH	MOx (Zn)						
[35] Manganelli, 2016	Cell viability in HEK cells	SiO_2			S			Dose, Time
[36] Mu, 2016	E.Coli	MOx	EN, $M_{softness}$, M_{IP}					

Reference	Endpoint	NM type	Classification					
			A	B	C	D	E	F
[37] Pan, 2016	E. Coli / HaCaT	MOx						
[38] Toropova, 2016a	Mutagenicity (Ames test in TA100 and E. coli)	Ful.						Pr_{S9}, Pr_{irrad}, Dose
[39] Toropova, 2016b	Mutagenicity (Ames test in TA100)	CNT				Id		Pr_{S9},, Dose
[40] Toropova, 2016c	pEC_{50} (cytotoxicity in *E. coli* and HaCaT)	MOx	SMILES					Target
[41] Basant, 2017	pEC_{50} (cytotoxicity in *E. coli* and HaCaT)	MOx	several					Pr_{Light}, Target
[42] Concu, 2017	Toxicity (general)	M/Mox	EI_{Volume}, EN, $EI_{Polarizability}$		S, shape		EC_{50}_oth	time
[43] Fjodorova, 2017	pEC_{50} (cytotoxicity to *E. coli)*	MOx	$\#_{M,O}$, EN, PT, M_{charge}					
[44] Manganelli, 2017	Cell viability	SiO_2			S_{bin}			Dose, Time
[45] Sizochenko, 2017	Zebrafish Hatching Enzyme ZHE1	MOx						
[46] Zhou, 2017	pEC_{50} (cytotoxicity to *E. coli)*	MOx						

Reference	Endpoint	NM type	Classification					
			A	B	C	D	E	F
[47] Choi, 2018	Cell viability several	MOx	E_{CB}, E_{VB}, ΔH_f		S_{TEM}, S_{DLS}			
[48] De, 2018	pEC_{50} (cytotoxicity to *E. coli*/HaCaT) and % EI (Zebrafish)	MOx	M_{ON}, EN, Valence			Tox_{other}		
[49] Mikolajczyk, 2018	pEC50 (cytotoxicity to CHO-K1)	MOx (Ti)	M_{IP}, M_{EA}, M_{hard}, M_{ads}					
[50] Shin, 2018	Immobilization *D. magna*	several	EI, Several	Coating	S_{TEM}, S_{agg}, Shape	ZP		$Pr_{Exp.\ cond}$ Time, IS, NOM, Number DM,
[51] Sizochenko, 2018	pEC50 (several targets)	MOx	M_{ch}, EI_{ion_rad}, EN, E_{gap}		$R_{Wigner\text{-}Seitz}$			
[52] Trinh, 2018		Ful.						
[52] Buglak, 2019	cell viability several	CNT			S, Lenght, Area			Dose,Time ,CL, Method
[53] Cai, 2019	EC50 (*D. Magna*)	MOx (Ti)						

			Classification					
Reference	**Endpoint**	**NM type**	**A**	**B**	**C**	**D**	**E**	**F**
[54] Choi, 2019	% (cell viability in HaCaT and BEAS)	MOx/Ag	$\#_{elements}$		S_{TEM}, S_{DLS}	Surface charge		Assay, dose
[55] Kuz'min, 2019	E.Coli/Hacat	MOx	several		LDM, S			
[56] Mikolajczyk, 2019	pEC_{50} (cytoxocity on CHO-K1)	MOx (Ti)		EN				
	Photodegradation of phenol	MOx (Ti)		$\%_{Pd}$, SP	SA_{BET}			
[57] Ojha, 2019	Cellular uptake in PaCa2/HUVEC/U937	MOx (Fe)						
[58] Ambure, 2020	Cytoxicity/Genotoxicity	MOx		Molec				
[59] Cao, 2020	Cytoxicity A549 cells	MOx	M_{charge}, $M_{\%w}$					
[60] Halder, 2020	Genotoxicity	MOx	$EI_{(w)}$					
[61] Huang, 2020	Inflammatory potential IL1beta production	MOx						
[62] Kotzabasaki, 2020	Cell viability	FeOx						
[63] Kudrinskiy, 2020	MIC (S. cerevisae)	Ag			S, SA	ZP, Cmax, kPO		

				Classification				
Reference	**Endpoint**	**NM type**	**A**	**B**	**C**	**D**	**E**	**F**
[64] Papadiamantis, 2020	Cell viability	MOx	Crystal, CN		S, SA, TSA, Shydro,	ZP, PZZP,		Assay
[65] RybińskaFryca, 2020	Photodegradation of phenol	MOx (Ti)		$\#_{N,C}$	SA_{BET}		Precursor (IL, cation, anion)	
	pEC_{50} (cytotoxicity to *E. coli)*	MOx (Ti)		EN, $M_{\%mol}$				
	Zeta potential (in media)		HOMO/$\#_M$		S_{TEM}	ZP_{water}		
[66] Gul, 2021	cell viability	Several					Synthesys method	
[67] Jung, 2021	pLC_{50} (fish)	Ag			S	ZP, $pLC_{50Daphn}$		
[68] Kumar, 2021	cell viability	QDs						
[69] Qi, 2021	pEC50 (cytotoxicity to CHO-K1)	MOx (Ti)		$M_{mol\_fraction}$				
[70] Sifonte, 2021	pEC_{50} HaCaT	MOx						
[71] Toropova, 2021	Cell viability	MOx	Formula, H_{form}, Ecb, Evb, EN.		S_{TEM}, S_{hydro}			CL, Species, Origin, Cell-type, Time,

Reference	Endpoint	NM type	Classification					
			A	B	C	D	E	F
								Dose, Assay
[72] Varsou, 2021	Immobilization of *D. Magna*	Ag/MOx (Ti)			S_{TEM}, S_{DLS},	ZP, Cond. El Mob.	Aging	
[73] Yuan, 2021	Cell proliferation rate HK2	M+MOx (Ti)						
[74] Zhang, 2021	Interaction energy (calculated) with SARS-CoV-2 proteins	Ful./CNT/ Graph.			D, L, SA, Angle			
[75] Shin, 2021	Cell viability in human lung cells	MOx (Ti)	EC	EC				
[76] Banerjee, 2023	pEC_{50} (cytotoxicity to CHO-K1)	MOx (Ti)	EN, EA, ΔH_f		SA			
[77] Na, 2023	$EC_{10/50}$ (toxicity to *A. fischeri*)	MOx			S_{NM}, S_{DLS}, SA	ZP		

References

1. Hu, X.; Cook, S.; Wang, P.; Hwang, H. min *Science of the Total Environment* **2009**, *407*, 3070–3072, doi:10.1016/j.scitotenv.2009.01.033
2. Fourches, D.; Pu, D.; Tassa, C.; Weissleder, R.; Shaw, S.Y.; Mumper, R.J.; Tropsha, A. *ACS Nano* **2010**, *4*, 5703–5712, doi:10.1021/nn1013484
3. Sayes, C.; Ivanov, I. , doi:10.1111/j.1539-6924.2010.01438.x
4. Burello, E.; Worth, A.P. *Nanotoxicology* **2011**, *5*, 228–235, doi:10.3109/17435390.2010.502980
5. Liu, R.; Rallo, R.; George, S.; Ji, Z.; Nair, S.; Nel, A.E.; Cohen, Y. *Small* **2011**, *7*, doi:10.1002/smll.201002366
6. Puzyn, T.; Rasulev, B.; Gajewicz, A.; Hu, X.; Dasari, T.P.; Michalkova, A.; Hwang, H.M.; Toropov, A.; Leszczynska, D.; Leszczynski, J. *Nat Nanotechnol* **2011**, *6*, 175–178, doi:10.1038/nnano.2011.10
7. Rallo, R.; France, B.; Liu, R.; Nair, S.; George, S.; Damoiseaux, R.; Giralt, F.; Nel, A.; Bradley, K.; Cohen, Y. *Environ Sci Technol* **2011**, *45*, 1695–1702, doi:10.1021/ES103606X/SUPPL_FILE/ES103606X_SI_001.PDF
8. Chau, Y.T.; Yap, C.W. *RSC Adv* **2012**, *2*, 8489–8496, doi:10.1039/c2ra21489j
9. Epa, V.C.; Burden, F.R.; Tassa, C.; Weissleder, R.; Shaw, S.; Winkler, D.A. *Nano Lett* **2012**, *12*, 5808–5812, doi:10.1021/nl303144k
10. Patel, T.R. Ph.D. Thesis: Bayesian Methods in the Quantitative Risk Assessment and Toxicity Profiling of Engineered Nanomaterials, University of California Los Angeles, 2012
11. Toropov, A.A.; Toropova, A.P.; Benfenati, E.; Gini, G.; Puzyn, T.; Leszczynska, D.; Leszczynski, J. *Chemosphere* **2012**, *89*, 1098–1102, doi:10.1016/j.chemosphere.2012.05.077
12. Ahmed, L.; Rasulev, B.; Turabekova, M.; Leszczynska, D.; Leszczynski, J. *Org Biomol Chem* **2013**, *11*, doi:10.1039/c3ob40878g
13. Liu, R.; Rallo, R.; Weissleder, R.; Tassa, C.; Shaw, S.; Cohen, Y. *Small* **2013**, *9*, 1842–1852, doi:10.1002/smll.201201903
14. Liu, X.; Tang, K.; Harper, S.; Harper, B.; Steevens, J.A.; Xu, R. *Int J Nanomedicine* **2013**, *8*, 31–43, doi:10.2147/IJN.S40742
15. Liu, R.; Zhang, H.Y.; Ji, Z.X.; Rallo, R.; Xia, T.; Chang, C.H.; Nel, A.; Cohen, Y. *Nanoscale* **2013**, *5*, 5644–5653, doi:10.1039/C3NR01533E
16. Kar, S.; Gajewicz, A.; Puzyn, T.; Roy, K.; Leszczynski, J. *Ecotoxicol Environ Saf* **2014**, *107*, 162–169, doi:10.1016/j.ecoenv.2014.05.026
17. Kleandrova, V. V.; Luan, F.; González-Díaz, H.; Ruso, J.M.; Speck-Planche, A.; Cordeiro, M.N.D.S. *Environ Sci Technol* **2014**, *48*, 14686–14694, doi:10.1021/es503861x
18. Liu, R.; France, B.; George, S.; Rallo, R.; Zhang, H.; Xia, T.; Nel, A.E.; Bradley, K.; Cohen, Y. *Analyst* **2014**, *139*, 943–953, doi:10.1039/C3AN01409F
19. Pathakoti, K.; Huang, M.J.; Watts, J.D.; He, X.; Hwang, H.M. *J Photochem Photobiol B* **2014**, *130*, 234–240, doi:10.1016/j.jphotobiol.2013.11.023

20. Singh, K.P.; Gupta, S. *RSC Advances* **2014**, *4*, 13215–13230
21. Sizochenko, N.; Rasulev, B.; Gajewicz, A.; Kuz'Min, V.; Puzyn, T.; Leszczynski, J. *Nanoscale* **2014**, *6*, doi:10.1039/c4nr03487b
22. Toropov, A.A.; Toropova, A.P. *Chemosphere* **2014**, *104*, 262–264, doi:10.1016/j.chemosphere.2013.10.079
23. Venigalla, S.; Dhail, S.; Ranjan, P.; Jain, S.; Chakraborty, T. *Former: Ann. West Univ. Timisoara-Series Chem* **2014**, *23*, 123–130
24. Gajewicz, A.; Schaeublin, N.; Rasulev, B.; Hussain, S.; Leszczynska, D.; Puzyn, T.; Leszczynski, J. *Nanotoxicology* **2015**, *9*, 313–325, doi:10.3109/17435390.2014.930195
25. Kaweeteerawat, C.; Ivask, A.; Liu, R.; Zhang, H.; Chang, C.H.; Low-Kam, C.; Fischer, H.; Ji, Z.; Pokhrel, S.; Cohen, Y.; et al. *Environ Sci Technol* **2015**, *49*, 1105–1112, doi:10.1021/es504259s
26. Mikolajczyk, A.; Gajewicz, A.; Rasulev, B.; Schaeublin, N.; Maurer-Gardner, E.; Hussain, S.; Leszczynski, J.; Puzyn, T. *Chemistry of Materials* **2015**, *27*, 2400–2407, doi:10.1021/cm504406a
27. Sizochenko, N.; Rasulev, B.; Gajewicz, A.; Mokshyna, E.; Kuz'min, V.E.; Leszczynski, J.; Puzyn, T. *RSC Adv* **2015**, *5*, 77739–77745, doi:10.1039/C5RA11399G
28. Toropov, A.A.; Toropova, A.P. *Chemosphere* **2015**, *139*, 18–22, doi:10.1016/j.chemosphere.2015.05.042
29. Toropov, A.A.; Toropova, A.P. *Chemosphere* **2015**, *124*, 40–46, doi:10.1016/j.chemosphere.2014.10.067
30. Toropova, A.P.; Toropov, A.A.; Benfenati, E. *SAR QSAR Environ Res* **2015**, *26*, 29–40, doi:10.1080/1062936X.2014.984327
31. Cassano, A.; Robinson, R.L.M.; Palczewska, A.; Puzyn, T.; Gajewicz, A.; Tran, L.; Manganelli, S.; Cronin, M.T.D. *ATLA Alternatives to Laboratory Animals* **2016**, *44*, doi:10.1177/026119291604400603
32. Jagiello, K.; Grzonkowska, M.; Swirog, M.; Ahmed, L.; Rasulev, B.; Avramopoulos, A.; Papadopoulos, M.G.; Leszczynski, J.; Puzyn, T. *Journal of Nanoparticle Research* **2016**, *18*, doi:10.1007/s11051-016-3564-1
33. Kar, S.; Gajewicz, A.; Roy, K.; Leszczynski, J.; Puzyn, T. *Ecotoxicol Environ Saf* **2016**, *126*, 238–244, doi:10.1016/j.ecoenv.2015.12.033
34. Le, T.C.; Yin, H.; Chen, R.; Chen, Y.; Zhao, L.; Casey, P.S.; Chen, C.; Winkler, D.A. *Small* **2016**, *12*, 3568–3577, doi:10.1002/SMLL.201600597
35. Manganelli, S.; Leone, C.; Toropov, A.A.; Toropova, A.P.; Benfenati, E. *Chemosphere* **2016**, *144*, 995–1001, doi:10.1016/J.CHEMOSPHERE.2015.09.086
36. Mu, Y.; Wu, F.; Zhao, Q.; Ji, R.; Qie, Y.; Zhou, Y.; Hu, Y.; Pang, C.; Hristozov, D.; Giesy, J.P.; et al. *Nanotoxicology* **2016**, *10*, 1207–1214, doi:10.1080/17435390.2016.1202352
37. Pan, Y.; Li, T.; Cheng, J.; Telesca, D.; Zink, J.I.; Jiang, J. *RSC Adv* **2016**, *6*, 25766–25775, doi:10.1039/C6RA01298A
38. Toropova, A.P.; Toropov, A.A.; Veselinović, A.M.; Veselinović, J.B.; Benfenati, E.; Leszczynska, D.; Leszczynski, J. *Ecotoxicol Environ Saf* **2016**, *124*, 32–36, doi:10.1016/j.ecoenv.2015.09.038
39. Toropova, A.P.; Toropov, A.A.; Rallo, R.; Leszczynska, D.; Leszczynski *Int. J. Environ. Res* **2016**, *10*, 59–64

40. Toropova, A.P.; Toropov, A.A.; Manganelli, S.; Leone, C.; Baderna, D.; Benfenati, E.; Fanelli, R. *NanoImpact* **2016**, *1*, 60–64, doi:10.1016/j.impact.2016.04.003
41. Basant, N.; Gupta, S. *Nanotoxicology* **2017**, *11*, 339–350, doi:10.1080/17435390.2017.1302612
42. Concu, R.; Kleandrova, V. V.; Speck-Planche, A.; Cordeiro, M.N.D.S. *http://dx.doi.org/10.1080/17435390.2017.1379567* **2017**, *11*, 891–906, doi:10.1080/17435390.2017.1379567
43. Fjodorova, N.; Novic, M.; Gajewicz, A.; Rasulev, B. *Nanotoxicology* **2017**, *11*, 475–483, doi:10.1080/17435390.2017.1310949
44. Manganelli, S.; Benfenati, E. *Methods in Molecular Biology* **2017**, *1601*, 275–290, doi:10.1007/978-1-4939-6960-9_22/FIGURES/6
45. Sizochenko, N.; Leszczynska, D.; Leszczynski, J. *Nanomaterials* **2017**, *7*, doi:10.3390/nano7100330
46. Zhou, Z.; Tang, X.; Dai, W.; Shi, J.; Chen, H. *Can J Chem* **2017**, *95*, 863–866, doi:10.1139/cjc-2017-0172
47. Choi, J.S.; Ha, M.K.; Trinh, T.X.; Yoon, T.H.; Byun, H.G. *Sci Rep* **2018**, *8*, doi:10.1038/s41598-018-24483-z
48. De, P.; Kar, S.; Roy, K.; Leszczynski, J. *Environ Sci Nano* **2018**, *5*, doi:10.1039/C8EN00809D
49. Mikolajczyk, A.; Gajewicz, A.; Mulkiewicz, E.; Rasulev, B.; Marchelek, M.; Diak, M.; Hirano, S.; Zaleska-Medynska, A.; Puzyn, T. *Environ Sci Nano* **2018**, *5*, doi:10.1039/c8en00085a
50. Shin, H.K.; Seo, M.; Shin, S.E.; Kim, K.Y.; Park, J.W.; No, K.T. *Environ Sci Nano* **2018**, *5*, 765–775, doi:10.1039/c7en01127j
51. Sizochenko, N.; Mikolajczyk, A.; Jagiello, K.; Puzyn, T.; Leszczynski, J.; Rasulev, B. *Nanoscale* **2018**, *10*, 582–591, doi:10.1039/C7NR05618D
52. Trinh, T.X.; Choi, J.S.; Jeon, H.; Byun, H.G.; Yoon, T.H.; Kim, J. *Chem Res Toxicol* **2018**, *31*, 183–190, doi:10.1021/acs.chemrestox.7b00303
53. Cai, Y.; Nowack, B.; Wigger, H. *NanoImpact* **2019**, *15*, doi:10.1016/j.impact.2019.100180
54. Choi, J.S.; Trinh, T.X.; Yoon, T.H.; Kim, J.; Byun, H.G. *Chemosphere* **2019**, *217*, 243–249, doi:10.1016/j.chemosphere.2018.11.014
55. Kuz'min, V.E.; Ognichenko, L.N.; Sizochenko, N.; Chapkin, V.A.; Stelmakh, S.I.; Shyrykalova, A.O.; Leszczynski, J. *International Journal of Quantitative Structure-Property Relationships* **2018**, *4*, 28–40, doi:10.4018/ijqspr.2019010103
56. Mikolajczyk, A.; Sizochenko, N.; Mulkiewicz, E.; Malankowska, A.; Rasulev, B.; Puzyn, T. *Nanoscale* **2019**, *11*, 11808–11818, doi:10.1039/C9NR01162E
57. Ojha, P.K.; Kar, S.; Roy, K.; Leszczynski, J. *Nanotoxicology* **2019**, *13*, 14–34, doi:10.1080/17435390.2018.1529836
58. Ambure, P.; Ballesteros, A.; Huertas, F.; Camilleri, P.; Barigye, S.J.; Gozalbes, R. *International Journal of Quantitative Structure-Property Relationships* **2020**, *5*, 83–100, doi:10.4018/ijqspr.20201001.oa2
59. Cao, J.; Pan, Y.; Jiang, Y.; Qi, R.; Yuan, B.; Jia, Z.; Jiang, J.; Wang, Q. *Green Chemistry* **2020**, *22*, 3512–3521, doi:10.1039/d0gc00933d
60. Halder, A.K.; Melo, A.; Cordeiro, M.N.D.S. *Chemosphere* **2020**, *244*, doi:10.1016/j.chemosphere.2019.125489

61. Huang, Y.; Li, X.; Xu, S.; Zheng, H.; Zhang, L.; Chen, J.; Hong, H.; Kusko, R.; Li, R. *Environ Health Perspect* **2020**, *128*, 1–13, doi:10.1289/EHP6508
62. Kotzabasaki, M.I.; Sotiropoulos, I.; Sarimveis, H. *RSC Adv* **2020**, *10*, 5385–5391, doi:10.1039/c9ra09475j
63. Kudrinskiy, A.; Zherebin, P.; Gusev, A.; Shapoval, O.; Pyee, J.; Lisichkin, G.; Krutyakov, Y. *Nanomaterials* **2020**, *10*, 1–22, doi:10.3390/nano10081459
64. Papadiamantis, A.G.; Jänes, J.; Voyiatzis, E.; Sikk, L.; Burk, J.; Burk, P.; Tsoumanis, A.; Ha, M.K.; Yoon, T.H.; Valsami-Jones, E.; et al. *Nanomaterials* **2020**, *10*, 1–19, doi:10.3390/nano10102017
65. Rybińska-Fryca, A.; Mikolajczyk, A.; Puzyn, T. *Nanoscale* **2020**, *12*, 20669–20676, doi:10.1039/d0nr05220e
66. Gul, G.; Yildirim, R.; Ileri-Ercan, N. *Environ Sci Nano* **2021**, *8*, 937–949, doi:10.1039/D0EN01240H
67. Jung, U.; Lee, B.; Kim, G.; Shin, H.K.; Kim, K.T. *Chemosphere* **2021**, *283*, doi:10.1016/j.chemosphere.2021.131164
68. Kumar, A.; Kumar, P. *J Hazard Mater* **2021**, *402*, 123777, doi:10.1016/J.JHAZMAT.2020.123777
69. Qi, R.; Pan, Y.; Cao, J.; Yuan, B.; Wang, Y.; Jiang, J. *Environ Sci Nano* **2021**, *8*, 927–936, doi:10.1039/D0EN01266A
70. Peláez Sifonte, E.; Antonio Castro-Smirnov, F.; Adrian Soutelo Jimenez, A.; Raúl González Diez, H.; Guzmán Martínez, F. *Journal of Nanoparticle research* **2021**, *23*, 161, doi:10.1007/s11051-021-05288-0
71. Toropova, A.P.; Toropov, A.A.; Leszczynski, J.; Sizochenko, N. *Environ Toxicol Pharmacol* **2021**, *86*, doi:10.1016/j.etap.2021.103665
72. Varsou, D.D.; Ellis, L.J.A.; Afantitis, A.; Melagraki, G.; Lynch, I. *Chemosphere* **2021**, *285*, doi:10.1016/j.chemosphere.2021.131452
73. Yuan, B.; Wang, P.; Sang, L.; Gong, J.; Pan, Y.; Hu, Y. *Ecotoxicol Environ Saf* **2021**, *208*, doi:10.1016/j.ecoenv.2020.111634
74. Zhang, F.; Wang, Z.; Vijver, M.G.; Peijnenburg, W.J.G.M. *Ecotoxicol Environ Saf* **2021**, *219*, doi:10.1016/j.ecoenv.2021.112357
75. Shin, H.K.; Kim, S.; Yoon, S. *NanoImpact* **2021**, *21*, 100298, doi:10.1016/J.IMPACT.2021.100298
76. Banerjee, A.; Kar, S.; Pore, S.; Roy, K. *https://doi.org/10.1080/17435390.2023.2186280* **2023**, *17*, 78–93, doi:10.1080/17435390.2023.2186280
77. Na, M.; Nam, S.H.; Moon, K.; Kim, J. *Environ Sci Nano* **2023**, *10*, 325–337, doi:10.1039/D2EN00672C