

Electronic Supplementary Information

Computer-aided Nanotoxicology: Risk Assessment of Metal Oxide Nanoparticles via nano-QSAR

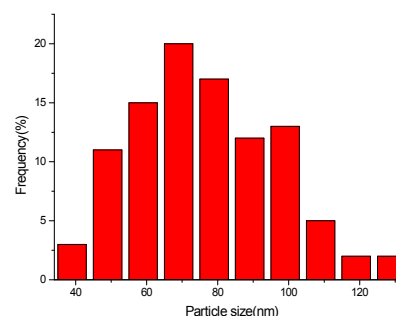
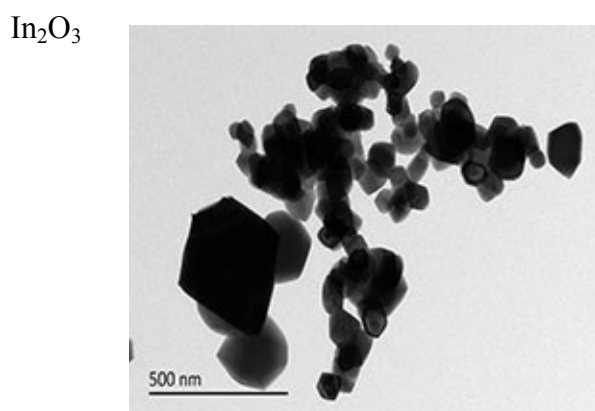
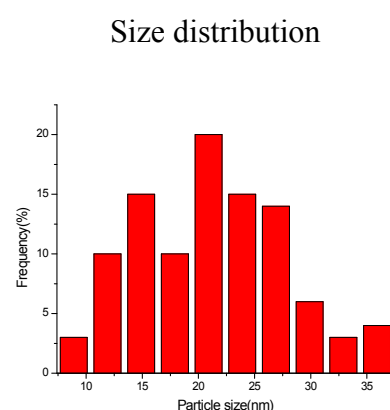
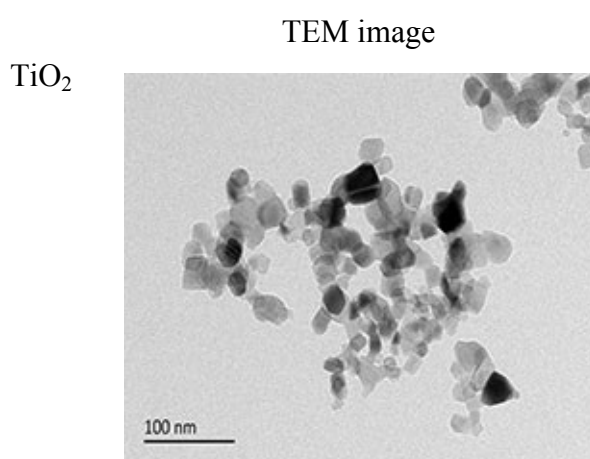
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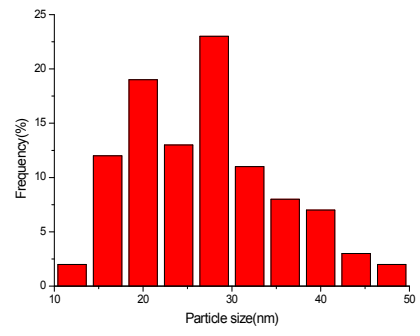
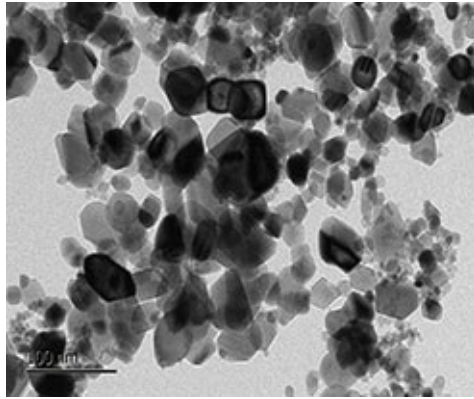
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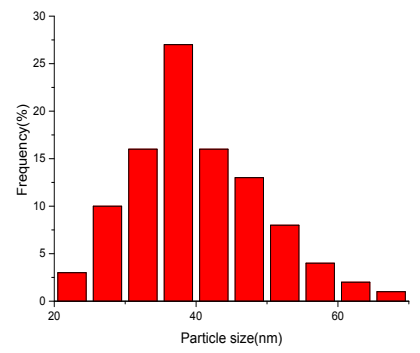
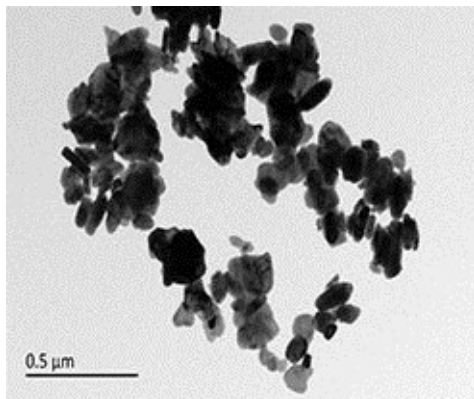
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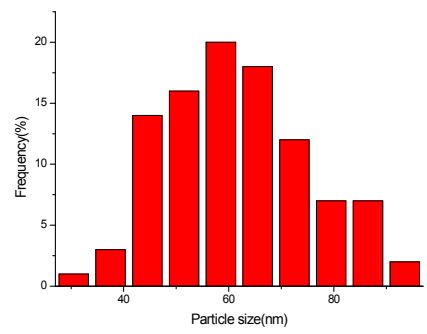
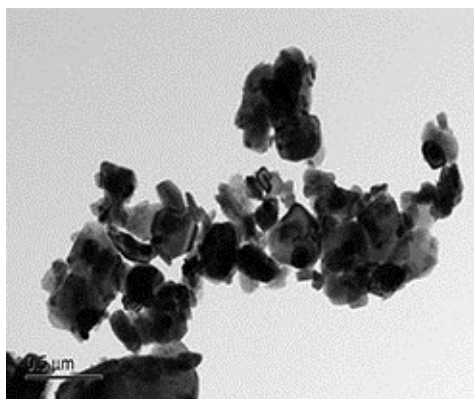
SnO₂



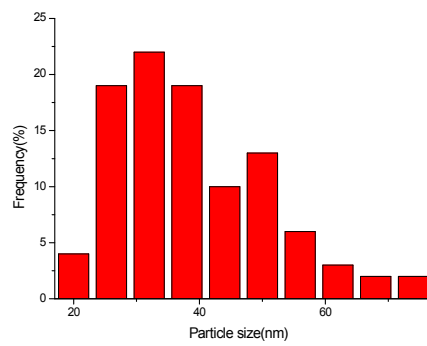
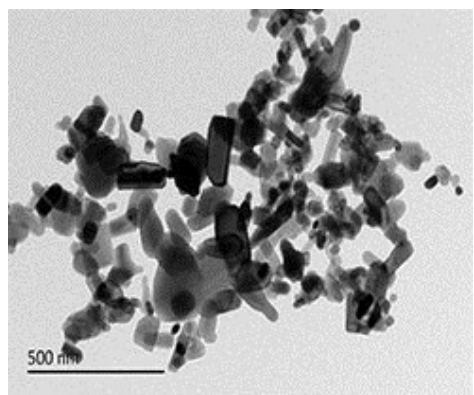
WO₃



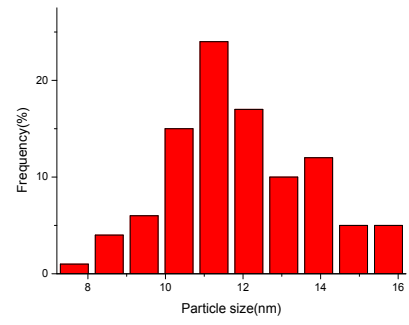
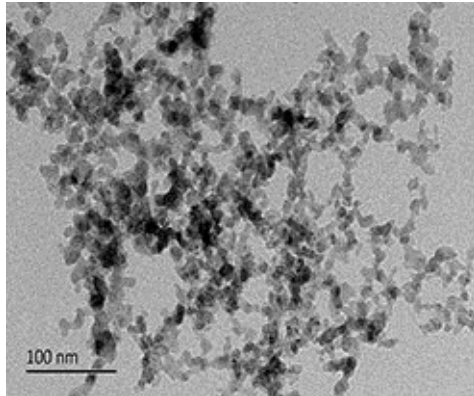
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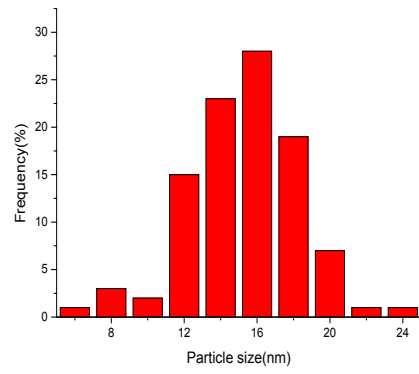
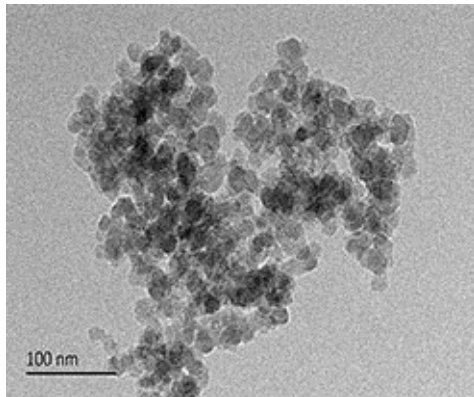
ZnO



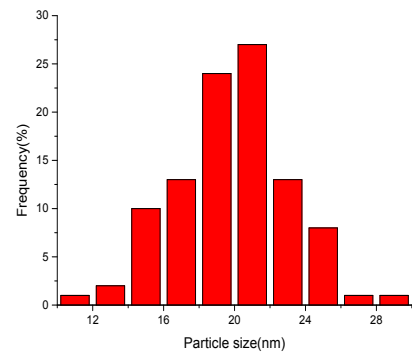
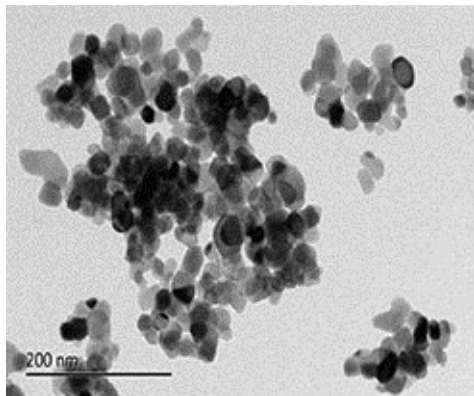
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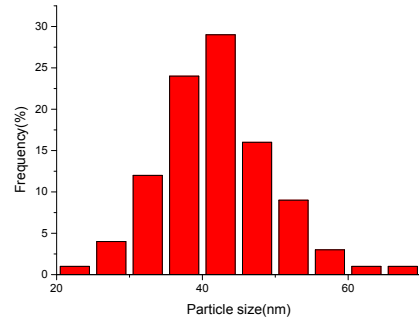
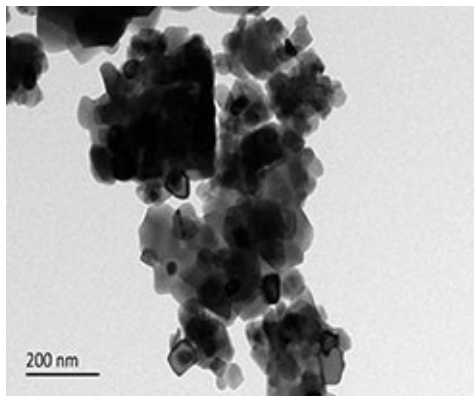
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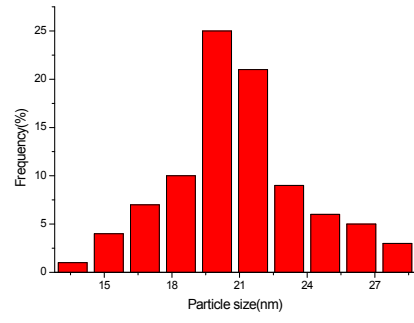
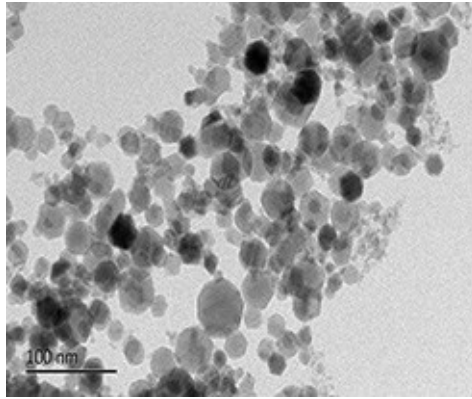
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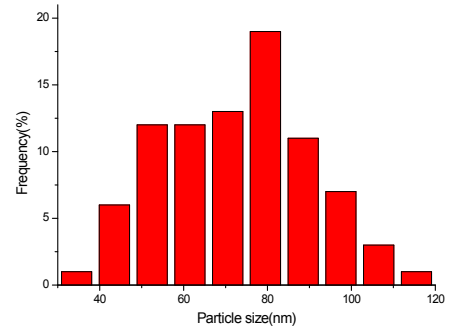
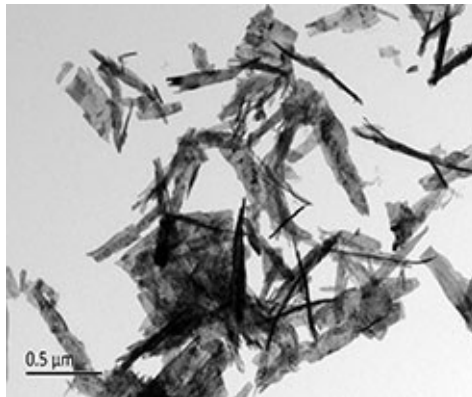
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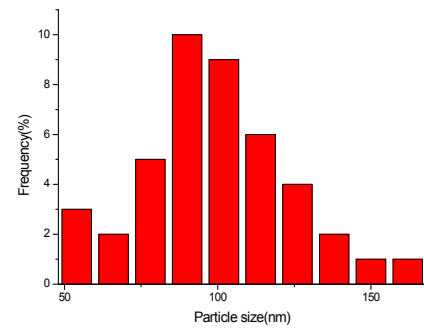
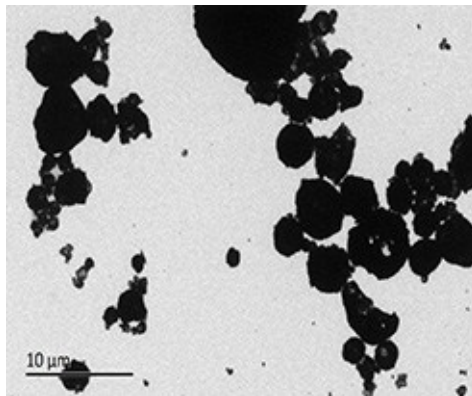
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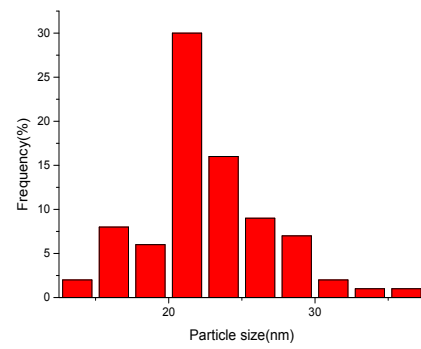
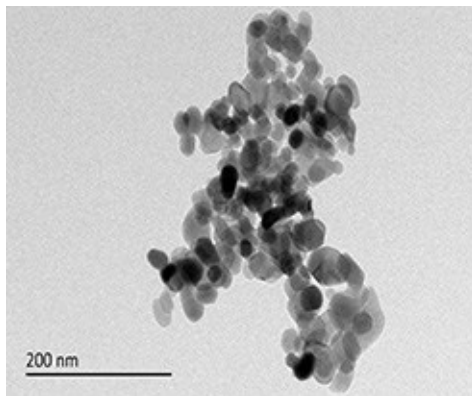
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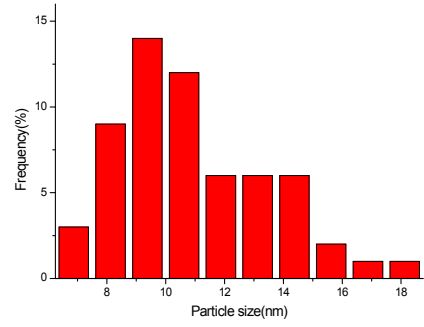
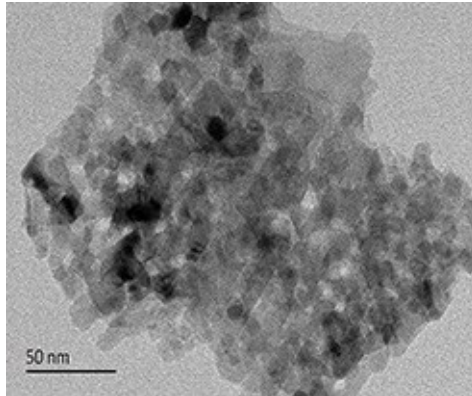
Yb_2O_3



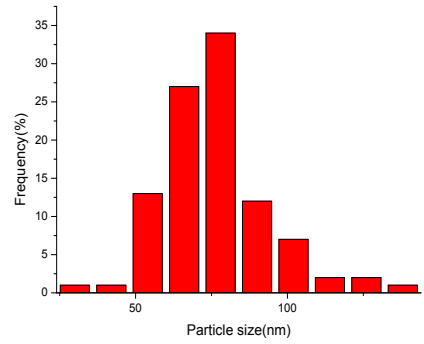
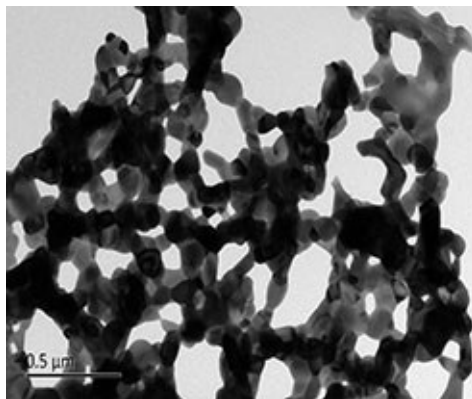
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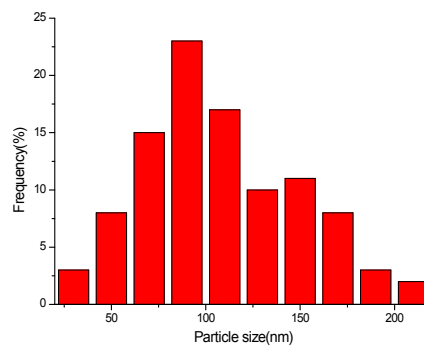
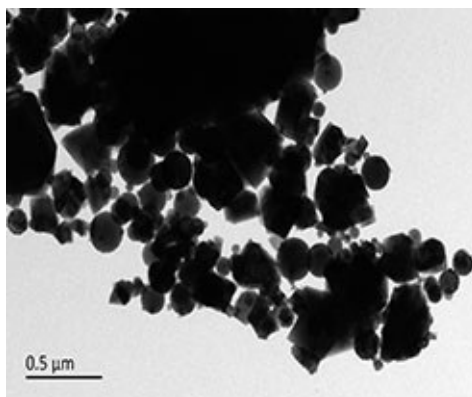
NiO



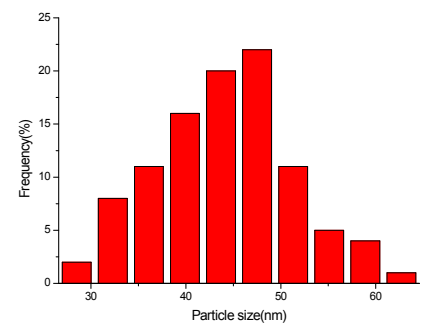
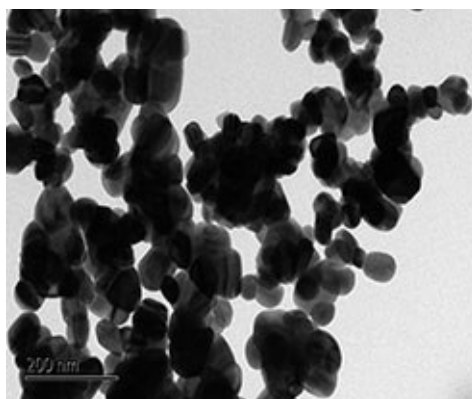
La₂O₃



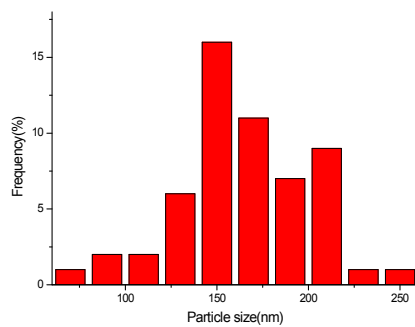
Sb₂O₃



HfO₂



Bi_2O_3



Mn_2O_3

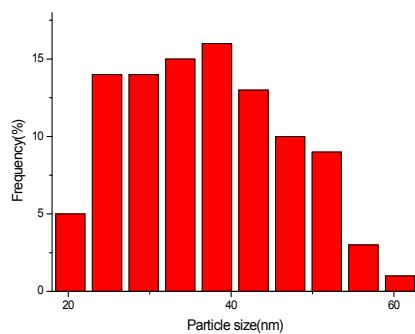
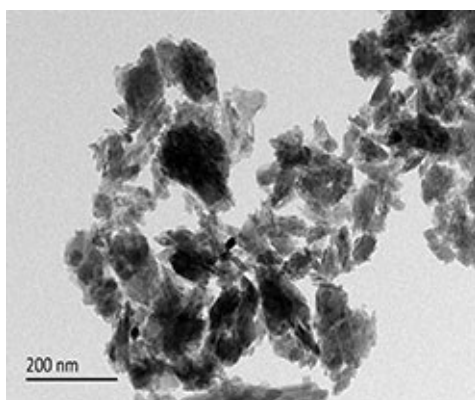


Fig.S1: The morphology and particle size distribution of different MeOx NPs

Table S1: The results of Y-randomisation test of the four nano-QSAR models

Probe of Y-scrambling	A549 cells							
	Model I		Model II		Model III		Model IV	
	Training set	Test set	Training set	Test set	Training set	Test set	Training set	Test set
R_1^2	0.006	0.001	0.001	0.136	0.133	0.165	0.015	0.004
R_2^2	0.085	0.125	0.071	0.145	0.000	0.076	0.000	0.138
R_3^2	0.013	0.102	0.057	0.060	0.011	0.042	0.040	0.055
R_4^2	0.006	0.101	0.206	0.070	0.106	0.125	0.017	0.099
R_5^2	0.092	0.148	0.109	0.060	0.013	0.282	0.000	0.291
R_6^2	0.069	0.019	0.056	0.030	0.077	0.060	0.004	0.105
R_7^2	0.155	0.217	0.014	0.055	0.204	0.210	0.024	0.363
R_8^2	0.026	0.274	0.117	0.149	0.024	0.058	0.001	0.086
R_9^2	0.041	0.372	0.017	0.132	0.035	0.149	0.070	0.174
R_{10}^2	0.011	0.002	0.070	0.078	0.002	0.226	0.004	0.323
Average R_x^2	0.050	0.136	0.072	0.092	0.060	0.139	0.018	0.164
Original R^2	0.865	0.817	0.972	0.948	0.902	0.864	0.996	0.879