Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Electronic Supplementary Information

Table S1. Results obtained from regression based nano-QSAR models. Experimental and predicted EC_{50} values of 34 modified TiO_2 nanoparticles are reported.

No.	Sample	Amount of noble metal [mol %]			Size [nm]	MW [mol/L]	BET Surface Area [m^2/g]	Observed $log(EC_{50})^{-1}$ data [molar]	**Model I**			**Model II**		
		Ag	Pt	Au					Improved SMILES	DCW	Predicted $log(EC_{50})^{-1}$ data	Improved SMILES	DCW	Predicted $log(EC_{50})^{-1}$ data
1	0.5Ag	0.5	0	0	10.01	53.93	158.00	4.72	[Ag]B1[Pt]C0[Au]D0E3F0G5	50.427	4.746	[Ag]B1[Pt]C0[Au]D0E2F0G8	83.625	4.690
2	1.5Ag	1.5	0	0	9.80	161.80	162.00	4.89	[Ag]B2[Pt]C0[Au]D0E3F2G5	51.219	4.856	[Ag]B2[Pt]C0[Au]D0E2F2G8	85.846	4.919
3	2.5Ag	2.5	0	0	7.53	269.67	163.00	5.35	[Ag]B3[Pt]C0[Au]D0E2F3G5	54.694	5.339	[Ag]B3[Pt]C0[Au]D0E2F3G8	88.125	5.154
4	4.5Ag	4.5	0	0	5.52	485.41	183.00	5.70	[Ag]B4[Pt]C0[Au]D0E1F6G7	57.059	5.667	[Ag]B4[Pt]C0[Au]D0E1F6G9	92.641	5.620
5	6.5Ag	6.5	0	0	5.64	701.14	148.00	5.88	[Ag]B5[Pt]C0[Au]D0E1F8G4	58.077	5.809	[Ag]B5[Pt]C0[Au]D0E1F8G8	94.778	5.841
6	0.5Ag_0.1Pt	0.5	0.1	0	11.27	73.44	161.00	4.64	[Ag]B1[Pt]C2[Au]D0E4F0G5	49.738	4.650	[Ag]B1[Pt]C2[Au]D0E2F1G8	83.565	4.684
7	1.5Ag_0.1Pt	1.5	0.1	0	36.80	181.31	141.00	4.84	[Ag]B2[Pt]C2[Au]D0E8F2G3	51.332	4.871	[Ag]B2[Pt]C2[Au]D0E8F2G8	85.486	4.882
8	2.5Ag_0.1Pt	2.5	0.1	0	5.63	289.18	152.00	5.06	[Ag]B3[Pt]C2[Au]D0E1F4G4	53.348	5.152	[Ag]B3[Pt]C2[Au]D0E1F3G8	88.303	5.173
9	4.5Ag_0.1Pt	4.5	0.1	0	21.97	504.91	115.00	5.54	[Ag]B4[Pt]C2[Au	56.266	5.557	[Ag]B4[Pt]C2[A	92.514	5.607

									]D0E7F6G1			u]D0E5F6G7		
10	6.5Ag_0.1Pt	6.5	0.1	0	5.70	720.65	130.00	5.63	[Ag]B5[Pt]C2[Au]D0E1F8G2	57.230	5.691	[Ag]B5[Pt]C2[Au]D0E1F9G7	92.775	5.634
11	0.5Ag_0.25Pt	0.5	0.25	0	6.40	102.71	138.00	4.73	[Ag]B1[Pt]C3[Au]D0E1F1G2	50.058	4.694	[Ag]B1[Pt]C3[Au]D0E1F1G8	85.778	4.912
12	1.5Ag_0.25Pt	1.5	0.25	0	45.60	210.57	172.00	5.01	[Ag]B2[Pt]C3[Au]D0E9F2G6	53.127	5.121	[Ag]B2[Pt]C3[Au]D0E9F2G9	85.409	4.874
13	2.5Ag_0.25Pt	2.5	0.25	0	3.23	318.44	144.00	5.37	[Ag]B3[Pt]C3[Au]D0E0F4G3	54.586	5.324	[Ag]B3[Pt]C3[Au]D0E1F4G8	90.233	5.372
14	4.5Ag_0.25Pt	4.5	0.25	0	12.87	534.18	151.00	5.65	[Ag]B4[Pt]C3[Au]D0E5F6G4	58.070	5.808	[Ag]B4[Pt]C3[Au]D0E3F6G8	91.064	5.458
15	6.5Ag_0.25Pt	6.5	0.25	0	12.70	749.91	135.00	5.84	[Ag]B5[Pt]C3[Au]D0E5F8G2	57.889	5.783	[Ag]B5[Pt]C3[Au]D0E3F9G7	92.546	5.610
16	0.5Ag_0.5Pt	0.5	0.5	0	5.42	151.48	165.00	4.94	[Ag]B1[Pt]C4[Au]D0E1F2G5	51.391	4.880	[Ag]B1[Pt]C4[Au]D0E1F2G8	85.281	4.861
17	1.5Ag_0.5Pt	1.5	0.5	0	5.12	259.34	164.00	5.26	[Ag]B2[Pt]C4[Au]D0E1F3G5	54.075	5.253	[Ag]B2[Pt]C4[Au]D0E1F3G8	88.153	5.157
18	2.5Ag_0.5Pt	2.5	0.5	0	13.87	367.21	181.00	5.32	[Ag]B3[Pt]C4[Au]D0E5F5G7	54.512	5.313	[Ag]B3[Pt]C4[Au]D0E3F4G9	90.376	5.387
19	4.5Ag_0.5Pt	4.5	0.5	0	7.70	582.95	166.00	5.65	[Ag]B4[Pt]C4[Au]D0E2F7G5	56.993	5.658	[Ag]B4[Pt]C4[Au]D0E2F7G8	93.707	5.730
20	6.5Ag_0.5Pt	6.5	0.5	0	15.00	798.68	134.00	5.80	[Ag]B5[Pt]C4[Au]D0E6F9G2	58.155	5.819	[Ag]B5[Pt]C4[Au]D0E3F9G7	93.606	5.720
21	0.1Pt	0	0.1	0	6.38	19.51	134.60	4.53	[Ag]B0[Pt]C2[Au]D0E1F0G2	48.534	4.483	[Ag]B0[Pt]C2[Au]D0E1F0G7	82.276	4.551
22	0.25Pt	0	0.25	0	6.39	48.77	163.38	4.67	[Ag]B0[Pt]C3[Au	50.793	4.797	[Ag]B0[Pt]C3[A	82.074	4.530

									]D0E1F0G5			u]D0E1F0G8		
23	0.5Pt	0	0.5	0	6.62	97.54	129.20	4.73	[Ag]B0[Pt]C4[Au]D0E1F1G2	48.341	4.456	[Ag]B0[Pt]C4[Au]D0E2F1G7	83.272	4.653
24	1.25Pt	0	1.25	0	5.65	243.86	152.10	4.71	[Ag]B0[Pt]C5[Au]D0E1F3G4	50.229	4.718	[Ag]B0[Pt]C5[Au]D0E1F3G8	84.956	4.827
25	0.1Au	0	0	0.1	6.47	19.70	187.80	4.56	[Ag]B0[Pt]C0[Au]D2E1F0G8	49.491	4.616	[Ag]B0[Pt]C0[Au]D2E1F0G9	84.941	4.826
26	0.25Au	0	0	0.25	6.21	49.24	168.10	4.62	[Ag]B0[Pt]C0[Au]D3E1F0G6	49.787	4.657	[Ag]B0[Pt]C0[Au]D3E1F0G9	83.342	4.661
27	0.5Au_0.1Pt	0	0.1	0.5	6.02	117.99	196.40	4.75	[Ag]B0[Pt]C2[Au]D4E1F1G9	50.305	4.729	[Ag]B0[Pt]C2[Au]D4E1F1G9	83.496	4.676
28	0.1Au_0.1Pt	0	0.1	0.1	5.97	39.21	190.59	4.68	[Ag]B0[Pt]C2[Au]D2E1F0G8	49.837	4.664	[Ag]B0[Pt]C2[Au]D2E1F0G9	83.077	4.633
29	0.25Au_0.25Pt	0	0.25	0.25	6.22	98.01	154.10	4.66	[Ag]B0[Pt]C3[Au]D3E1F1G4	49.834	4.663	[Ag]B0[Pt]C3[Au]D3E1F1G8	83.970	4.725
30	0.5Au_0.5Pt	0	0.5	0.5	6.34	196.03	151.07	4.68	[Ag]B0[Pt]C4[Au]D4E1F2G4	50.032	4.691	[Ag]B0[Pt]C4[Au]D4E1F2G8	83.687	4.696
31	0.5Au_0.25Pt	0	0.25	0.5	5.11	147.25	153.48	4.70	[Ag]B0[Pt]C3[Au]D4E1F2G4	50.325	4.732	[Ag]B0[Pt]C3[Au]D4E1F2G8	82.627	4.587
32	0.1Au_0.25Pt	0	0.25	0.1	4.97	68.47	105.00	4.70	[Ag]B0[Pt]C3[Au]D2E1F0G0	49.823	4.662	[Ag]B0[Pt]C3[Au]D2E1F1G6	82.722	4.597
33	0.25Au_0.1Pt	0	0.1	0.25	4.54	68.75	150.45	4.76	[Ag]B0[Pt]C2[Au]D3E1F0G4	49.735	4.650	[Ag]B0[Pt]C2[Au]D3E1F1G8	83.797	4.707
34	0.05Au_0.05Pt	0	0.05	0.05	6.48	19.60	164.97	4.67	[Ag]B0[Pt]C1[Au]D1E1F0G5	49.903	4.673	[Ag]B0[Pt]C1[Au]D1E1F0G8	82.491	4.573