Supplementary Information

Nano-QSAR modeling for ecosafe design of second generation TiO_2-based nano-photocatalysts

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TABLE S1. Materials, methods and sample characteristic

Materials

Titanium(IV) isopropoxide (TIP) (97%), $PdCl_2$ (5 wt.% in 10 wt.% HCl) $HAuCl_4$ (Au≈52%) and K_2PtCl_4 (98%) were purchased from Sigma-Aldrich. Cyclohexane, isopropyl alcohol, hydrazine, acetone, AOT (dioctylsulfosuccinate sodium salt), $AgNO_3$, (POCH S.A. Poland) were used without further purification.

Preparation of monometallic and bimetallic nanoparticles supported on TiO_2 by microemulsion and sol-gel method

Noble metal (Au, Ag, Pt) modified TiO_2 were obtained by hydrolysis of TIP (titanium tetraisopropoxide) in a water/AOT/cyclohexane microemulsion containing one or combination of two metal precursors in water cores. Mixing was carried out for 1 h under nitrogen; the metal ions were then reduced by dropwise addition of a microemulsion containing the reducing agent (hydrazine). The titanium tetraisopropoxide was added into the microemulsion system containing noble metal nanoparticles. The microemulsions were mixed and purged with nitrogen, washed, dried and calcined for 3 h at different temperatures. Pure TiO_2 was synthesized in the same approach without addition of metal precursors. TiO_2 modified with Au, Ag, Pt and Pd nanoparticles were prepared using the sol–gel method by hydrolysis reaction of TIP) with water. Firstly, 25 cm^3 TIP was dispersed in 25 cm^3 ethanol at the room temperature followed by 30 min solution mixing. After that, 14.2 cm^3 of water was added to the alkoxide solution and white precipitate was formed. Finally, a certain amount of $AgNO_3$, $HAuCl_4$, K_2PtCl_4, or/and $PdCl_2$, was dissolved in deionized water and mixed with TiO2 gel for 1 h. All the samples were obtained by the sequential addition of metal precursors to TiO_2 gel. The obtained photocatalysts were dried at 80◦C and thencalcined in air at 400°C for 3 h.

TABLE S2. Experimental characteristic of obtained $Me_{mix}@TiO_2$ photocatalysts.

clear TiO_2					
Kind	**2θ**	**intensity**	**amount of anatase (A)/brookite (B) [%]**	**Crystallite size of anatase [Å]**	**Lattice lenght of anatase structure [Å] a=b≠c**
A	25.32	3419	36/64	58.74	a=3.79654 ±0.000668
					c=9.518378±0.00268
4.5 Ag					
Kind	**2θ**	**intensity**	**amount of anatase/brookite [%]**	**Crystallite size of**	**Lattice lenght of anatase structure [Å] a=b≠c**
A	25.33	3667		55.23	a=3.788592±0.001051
					c=9.488774±0.003057
2.5 Ag_0.1Pt					
Kind	**2θ**	**intensity**	**amount of anatase/brookite [%]**	**Crystallite size of anatase [Å]**	**Lattice lenght of anatase structure [Å] a=b≠c**
A	25.3	3624	30/70	56.35	a=3,818419±0,002
					c=9,515961±0,008
1.5Ag_0.25Pt					
Kind	**2θ**	**intensity**	**amount of anatase/brookite [%]**	**Crystallite size of anatase [Å]**	**Lattice lenght of anatase structure [Å] a=b≠c**
A	25.3	4134	29/71	456/B54.97	a=3,7853±0,005
					c=9,4621±0,0114
Pt	39.8	531			
Pt	46.3	442			
0.5Ag_0.5Pt					
Kind	**2θ**	**intensity**	**amount of anatase/brookite [%]**	**Crystallite size of anatase [Å]**	**Lattice lenght of anatase structure [Å] a=b≠c**
A	25.5	36.2	37/63	(54.2 nm)	a=3,7364±0,0004
					c=9,0256±0,001

Pt	39.77	461			
6.5 Ag_0.5 Pt					
Kind	**2θ**	**intensity**	**amount of anatase/brookite [%]**	**Crystallite size of anatase [Å]**	**Lattice lenght of anatase structure [Å] a=b≠c**
A	25.24	3252	29/71	150	a=3,806±0,0041 c=9,4876±0,0133
Pt	39.76	615			
Pt	46.2	445			
1.25 Pt					
Kind	**2θ**	**intensity**	**amount of anatase/brookite [%]**	**Crystallite size of anatase [Å]**	**Lattice lenght of anatase structure [Å] a=b≠c**
A	25.32	3768	36/64	56.5	a=3.792803±0.000658 c=9.497447±0.002704
0.5 Au_0.1 Pt					
Kind	**2θ**	**intensity**	**amount of anatase/brookite [%]**	**Crystallite size of anatase [Å]**	**Lattice lenght of anatase structure [Å] a=b≠c**
A	25.3	3689	31/69	60.19	a=3,8199±0,0026 c=9,5358±0,0067
Au	44.6	290?			
Au	64.7	372			

0.5 Ag					
Kind	**2θ**	**intensity**	**amount of anatase/brookite [%]**	**Crystallite size of anatase [Å]**	**Lattice lenght of anatase structure [Å]**
A	25.3	7007	31/69	100.12	a=3,782202±0,001545 c=9,425336±0,006059
6.5 Ag					
Kind	**2θ**	**intensity**	**amount of anatase/brookite**	**Crystallite size of anatase [Å]**	**Lattice lenght of anatase structure [Å]**
A	25.28	3338		56.48	a=3.794686±0.000524 c=9.49257±0.002055
R	28.05	623			
4.5 Ag_0.1Pt					
Kind	**2θ**	**intensity**	**amount of anatase/brookite [%]**	**Crystallite size of anatase [Å]**	**Lattice lenght of anatase structure [Å]**
A	25.4	3388	27/73	219.7	a=3,788±0,004 c=9,4605±0,0082
2.5 ag_0.25Pt					
Kind	**2θ**	**intensity**	**amount of anatase/brookite**	**Crystallite size of anatase [Å]**	**Lattice lenght of anatase structure [Å]**
A	25.4	3837	29/71	32.28	a=3,767267±0,04 c=9,567995±0,09
Pt	39.7	511			
Pt	46.25	436			
1.5Ag_0.5Pt					
Kind	**2θ**	**intensity**	**amount of anatase/brookite [%]**	**Crystallite size of anatase [Å]**	**Lattice lenght of anatase structure [Å]**
A	25.3	3711	37/63	(51.12 nm)	a=3,8153±0,0047 c=9,4929±0,0067

Pt	39.78	499			
Pt	46.2	402			
0.1 Pt					
Kind	**2θ**	**intensity**	**amount of anatase/brookite [%]**	**Crystallite size of anatase [Å]**	**Lattice lenght of anatase structure [Å]**
A	25.3	4381	32/68	63.75	a=3,8119±0,002 c=9,5111±0,005
0.1 Au					
Kind	**2θ**	**intensity**	**amount of anatase/brookite [%]**	**Crystallite size of anatase [Å]**	**Lattice lenght of anatase structure [Å]**
A	25.3	3522	32/68	64.67	a=3.829351±0.001906 c=9.488823±0.007422
0.5 Au_0.1 Pt					
Kind	**2θ**	**intensity**	**amount of anatase/brookite [%]**	**Crystallite size of anatase [Å]**	**Lattice lenght of anatase structure [Å]**
A	25.3	5006	30/70	75.18	a=3,791±0,001 c=9,5179±0,0053
Au?	38.3	1353			
Au	44.6	319			
Au	64.7	377			

2.5% Ag					
Kind	**2θ**	**intensity**	**amount of anatase/brookite**	**Crystallite size of anatase**	**Lattice lenght of anatase structure [Å]**
A	25.3	6281	28/72	75.35	a=3,794±0,002 c=9,503±0,004
1.5Ag_0.1Pt					
Kind	**2θ**	**intensity**	**amount of anatase/brookite**	**Crystallite size of anatase**	**Lattice lenght of anatase structure [Å]**
A	25.3	3759	29/71	368	a=3,7835±0,002 c=9,5037±0,0076
0.5Ag_0.25Pt					
Kind	**2θ**	**intensity**	**amount of anatase/brookite**	**Crystallite size of anatase**	**Lattice lenght of anatase structure [Å]**
A	25.3	3859	32/68	63.93	a=3,799528±0,0029 c=9,5171±0,011
6.5Ag_0.25Pt					
Kind	**2θ**	**intensity**	**amount of anatase/brookite [%]**	**Crystallite size of anatase [Å]**	**Lattice lenght of anatase structure [Å]**
A	25.2	3260		127	a=3,8033±0,0037 c=9,4655±0,0121
Pt	39.86	584			
Pt	46.3	428			
4.5 Ag_0.5Pt					
Kind	**2θ**	**intensity**	**amount of anatase/brookite [%]**	**Crystallite size of anatase [Å]**	**Lattice lenght of anatase structure [Å]**
A	25.3	3661	31/69	76.96	a=3,7965±0,0017 c=9,4867±0,0059
Pt	39.7	515			

Pt	46.3?	439			
0.5 Pt					
Kind	**2θ**	**intensity**	**amount of anatase/brookite**	**Crystallite size of anatase**	**Lattice lenght of anatase structure [Å]**
A	25.29	3917	36/64	66.24	a=3.80218±0.000695 c=9.51724±0.004139
Pt	40.13	308			
Pt	46.3	308			
0.5 Au_0.1 Pt					
Kind	**2θ**	**intensity**	**amount of anatase/brookite [%]**	**Crystallite size of anatase [Å]**	**Lattice lenght of anatase structure [Å]**
A	25.3	3791	31/69	63.03	a=3,8265±0,0028 c=9,5393±0,006
Au	44.6	327			
Au	64.6	402			
0.1 Au_0.1 Pt					
Kind	**2θ**	**intensity**	**amount of anatase/brookite [%]**	**Crystallite size of anatase [Å]**	**Lattice lenght of anatase structure [Å]**
A	25.3	3023	32/68	54.66	a=3,825767±0,0018 c=9,4718±0,0073
1.5 Ag					
Kind	**2θ**	**intensity**	**amount of anatase/brookite [%]**	**Crystallite size of anatase [Å]**	**Lattice lenght of anatase structure [Å]**
A	25.3	6636	32/68	98	a=3,813±0,004 c=9,483±0,009
0.5Ag_0.1 Pt					
Kind	**2θ**	**intensity**	**amount of anatase/brookite [%]**	**Crystallite size of anatase [Å]**	**Lattice lenght of anatase structure [Å]**
A	25.3	4333	29/71	112.71	a=3,7525±0,0038 c=9,5235±0,006
6.5 Ag 0.1 Pt					
Kind	**2θ**	**intensity**	**amount of anatase/brookite [%]**	**Crystallite size of anatase [Å]**	**Lattice lenght of anatase structure [Å]**
A	25.3	3329	35.4/61.1/3(rutile)	57.04	a=3.791733±0.005176 c=9.49295±0.014334
4.5 Ag_0.25Pt					
Kind	**2θ**	**intensity**	**amount of anatase/brookite**	**Crystallite size of**	**Lattice lenght of anatase structure [Å]**
A	25.3	3510	31/69	128.86	a=3,8106±0,0038 c=9,4722±0,0133
Pt	39.66	656			
Pt	46.3	477			
2.5 Ag 0.5 Pt					
Kind	**2θ**	**intensity**	**amount of anatase/brookite**	**Crystallite size of**	**Lattice lenght of anatase structure [Å]**
A	25.29	3269	35/65	138.7	a=3,733865±0,001 c=9,025991±0,003
Pt	39.8	508			
Pt	46.3	426			
0.25 Pt					

Kind	2θ	intensity	amount of anatase/brookite	Crystallite size of	Lattice lenght of anatase structure [Å]
A	25.3	3695	32/68	63.94	a=3,8172±0,0017 c=9,4895±0,0043
0.25 Au					
Kind	**2θ**	**intensity**	**amount of**	**Crystallite**	**Lattice lenght of**
A	25.3	3634	32/68	62.13	a=3,817±0,0017 c=9,4793±0,0057
Au??	44.4	360			
Au	64.6	420			
0.5 Au_0.1 Pt					
Kind	**2θ**	**intensity**	**amount of anatase/brookite**	**Crystallite size of**	**Lattice lenght of anatase structure [Å]**
A	25.3	9035	34/66	172.5	a=3,7807±0,0005 c=9,5191±0,0018
Au	38.3	1546			
Au	44.5	305			
Au	65.1?	298			

The efficiency of phenol degradation after 1 h irradiation [%] for samples obtained by sol gel method

Sample label	Amount of noble metal precursor[mol.%]				BET surface area [m^2/g]	Under Vis light [%]	Under UV-Vis light [%]
	Ag	Pt	Au	Pd			
0.1Ag	0	0	0	0	61	12.9	61.8
0.5Ag	0.1	0	0	0	91	6.4	64.4
1.5Ag	0.5	0	0	0	89	16.6	70.3
2.5Ag	1.5	0	0	0	91	24.4	73.5
4.5Ag	2.5	0	0	0	67.5	9.2	73.5
0.1Ag_0.1Au	4.5	0	0	0	106.5	23	63
0.5Ag_0.1Au	0.1	0	0.1	0	112	1.5	52.9
1.5Ag_0.1Au	0.5	0	0.1	0	90.2	15.8	65.6
2.5Ag_0.1Au	1.5	0	0.1	0	79	8.1	60
0.1Ag_0.5Au	2.5	0	0.1	0	103	8.6	51.4
2.5Ag_0.5Au	0.1	0	0.5	0	90.4	0	64.6
4.5Ag_0.5Au	2.5	0	0.5	0	111.4	4.2	69.5
0.1Ag_0.1Pt	4.5	0	0.5	0	92	31.5	85.4
0.5Ag_0.1Pt	0.1	0.1	0	0	94	12.8	68.4
1.5Ag_0.1Pt	0.5	0.1	0	0	145.6	17.1	85.6
2.5Ag_0.1Pt	1.5	0.1	0	0	86	6.9	71.1
0.1Ag_0.5Pt	2.5	0.1	0	0	112.5	60.1	96.8
2.5Ag_0.5Pt	0.1	0.5	0	0	119	66	96.1
0.1Ag_0.1Pd	2.5	0.5	0	0	79	14	77.4
0.5Ag_0.1Pd	0.1	0	0	0.1	77.5	14.4	72.1
1.5Ag_0.1Pd	0.5	0	0	0.1	98	19.6	96.0
2.5Ag_0.1Pd	1.5	0	0	0.1	98	25.4	94.9
0.1Ag_0.5Pd	2.5	0	0	0.1	115	45.4	99.2
2.5Ag_0.5Pd	0.1	0	0	0.5	107	39.2	99.5
4.5Ag_0.5Au	2.5	0	0	0.5	99	1.8	100
0.1Ag_0.1Pt_0.1Au	4.5	0	0.5	0	94	11.5	84.4
0.1Pt_0.1Au_0.1Pd	0.1	0.1	0.1	0	92	49.1	100
0.1Ag_0.1Pt_0.1Pd	0	0.1	0.1	0.1	89	78.5	100
0.1Ag_0.1Au_0.1Pd	0.1	0.1	0	0.1	85	8.0	92.8
0.1Ag_0.1Pt_0.1Au_0.1Pd	0.1	0	0.1	0.1	94	49.9	100

Table 3. List of toxicity data splitting.

ID	Name	Split	Exp. endpoint	Pred. by model eq. 6	Pred. by model eq. 7
1	0.1Pt	Training	4.53	4.69	4.65
2	0.1Au	Training	4.56	4.69	4.65
3	0.25Au	Training	4.62	4.69	4.69
27	0.5Ag_0.1Pt	Test	4.64	4.79	4.74
4	0.25Au_0.25Pt	Training	4.66	4.69	4.75
5	0.05Au_0.05Pt	Training	4.67	4.69	4.65
6	0.25Pt	Training	4.67	4.69	4.69
28	0.5Au_0.5Pt	Test	4.68	4.69	4.86
7	0.1Au_0.1Pt_400	Training	4.68	4.69	4.67
8	0.5Au_0.25Pt	Training	4.70	4.69	4.81
9	0.1Au_0.25Pt	Training	4.70	4.69	4.71
29	1.25Pt	Test	4.71	4.69	4.92
10	0.5Ag	Training	4.72	4.79	4.72
11	0.5Pt	Training	4.73	4.69	4.74
12	0.5Ag_0.25Pt	Training	4.73	4.79	4.78
30	0.5Au_0.1Pt_400	Test	4.75	4.69	4.77
13	0.25Au_0.1Pt	Training	4.76	4.69	4.71
14	1.5Ag_0.1Pt	Training	4.84	4.97	4.93
31	1.5Ag	Test	4.89	4.97	4.90
15	0.5Ag_0.5Pt	Training	4.94	4.79	4.84
16	1.5Ag_0.25Pt	Training	5.01	4.97	4.96
17	2.5Ag_0.1Pt	Training	5.06	5.15	5.11
32	1.5Ag_0.5Pt	Test	5.26	4.97	5.02
18	2.5Ag_0.5Pt	Training	5.32	5.15	5.20
19	2.5Ag	Training	5.35	5.15	5.09
20	2.5Ag_0.25Pt	Training	5.37	5.15	5.15
33	4.5Ag_0.1Pt	Test	5.54	5.51	5.48
21	6.5Ag_0.1Pt	Training	5.63	5.88	5.85
22	4.5Ag_0.25Pt	Training	5.65	5.51	5.51
23	4.5Ag_0.5Pt	Training	5.65	5.51	5.57
34	4.5Ag	Test	5.70	5.51	5.46
24	6.5Ag_0.5Pt	Training	5.80	5.88	5.94
25	6.5Ag_0.25Pt	Training	5.84	5.88	5.88
26	6.5Ag	Training	5.88	5.88	5.83

Table S4. Statistic parameters towards development of Nano-QSPR model.*

No	Name	Suitable to	Coefficient	Description of Coefficient
1	The correlation coefficient The root mean square error of calibration	Measure of goodness-of-fit	$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i^{obs} - y_i^{pred})^2}{\sum_{i=1}^{n}(y_i^{obs} - \tilde{y}^{obs})^2}$ $RMSEC = \sqrt{\frac{\sum_{i=1}^{n}(y_i^{obs} - y_i^{pred})^2}{n}}$	where: y_j^{obs} – experimental (observed) value of the property for the i^{th} compound from the training set; y_i^{pred} – predicted value for i^{th} compound from the training set; y^{obs} – the mean experimental value of the property in the training set; n – the number of compounds in the training set.
	The cross-validated coefficient The root mean square error of calibration	Measure stability of the model	$Q^2_{LOO} = 1 - \frac{\sum_{i=1}^{n}(y_i^{obs} - y_i^{predcv})^2}{\sum_{i=1}^{n}(y_i^{obs} - \tilde{y}^{obs})^2}$ $RMSECV = \sqrt{\frac{\sum_{i=1}^{n}(y_i^{obs} - y_i^{predcv})^2}{n}}$	where: y_j^{obs} – experimental (observed) value of the property for the i^{th} compound; y_i^{predcv} – cross-validated predicted valuef or i^{th} compound; y – the mean experimental value of the property in the training set; n – the number of compounds in the training set.
3	The external-validation coefficient The root mean square error of prediction	Measure external predictivity	$Q^2_{EXT} = 1 - \frac{\sum_{j=1}^{k}(y_j^{obs} - y_j^{pred})^2}{\sum_{j=1}^{k}(y_j^{obs} - \hat{y}^{obs})^2}$ $RMSEP = \sqrt{\frac{\sum_{j=1}^{k}(y_j^{obs} - y_j^{pred})^2}{k}}$	where: y_j^{obs} – experimental (observed) value of the property for the j^{th} compound from the validation set; y_i^{pred} – predicted valuef or j^{th}compound from the validation set; $\hat{y}^{obs}$ – the mean experimental value of the property in the validation set; k – the number of compounds in the validation set. Squared correlation coefficient values between the observed and predicted values of the compounds with/without intercept (r^2/ r_0^2).
4	Concordance Correlation Coefficient	The accuracy and different variants of r^2_m Restrictive parameter for expressing external predictivity Mean absolute error	$CCC = \frac{2\sum_{j=1}^{k_{EXT}}(r_m^2 = r^2(1 - \sqrt{r^2 - r_0^2}))}{\sum_{j=1}^{k_{EXT}}(y_j^{obs} - \hat{y}^{obs})^2 + \sum_{j=1}^{}(y_j^{} - y^{})^2 + k_{EXT}(\hat{y}^{obs} - \hat{y}^{pred})^2}$ $MEA = \frac{1}{k}\sum y_j^{obs} - y_j^{pred}$	

*Please note that are details according to statistics calculations are described in presented study:

A. Golbraikh, A. Tropsha, *Journal of Molecular Graphics and Modelling*, 2002, **20**, 269-276. (Please see, MS, References section, position 42)

P. Gramatica, *QSAR & Combinatorial Science,* 2007, **26**, 694-701 (Please see, MS, References section, position 60)

K. Roy, S. Kar and P. Ambure, *Chemometrics and Intelligent Laboratory Systems,* 2015, ***145***, 22-29. (Please see, MS, References section, position 61)

K. Roy, N. R. Das, P. Ambure and N. B. Aher, *Chemometrics and Intelligent Laboratory Systems,* 2016, **152**, 18-33 (Please see, MS, References section, position 62)

Table S5. Parameters used in development of applicability domain.*

Coefficient	Description of coefficient
$h_i = \mathbf{x_i^T}(\mathbf{X^T X})(\mathbf{X^T X})^{-1}\mathbf{x_i}$	where the leverage value h_i for each i^{th} compound is calculated from the descriptor matrix (**X**), $\mathbf{x_i}$ is a row vector of molecular descriptors for a particular (i^{th}) compound. The value of h_i greater than the warning h^* value indicates that the structure of a compound substantially differs from those used for the calibration. Therefore, the compound is located outside the optimum prediction space. The h^* value is calculated as in eq. 16
$h^* = \frac{\mathbf{3(p+1)}}{\boldsymbol{n}}$	where p is the number of variables used in the model, n is the number of training compounds

*P. Gramatica, *QSAR & Combinatorial Science*, 2007, **26**, 694-701.

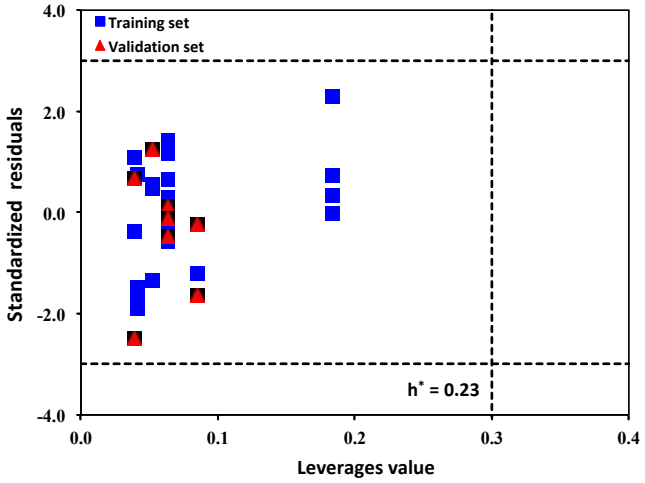
P. Gramatica, S. Cassani and N. Chirico, *Journal of Computational Chemistry*, 2014, **35**, 1036-1044.

Table S6. List of quantum-mechanical descriptors calculated for photocatalyst obtained by microemulsion method .

Sample label	[mol %]	[mol %]	[mol %]	[nm]	[mol/L]	[kJ/mol]	[kJ/mol]	[kJ/mol]	[kJ/mol]	[eV]	[m^2/g]	[°C]	The efficiency of phenol degradation after 1 h irradiation under [%]	
	Amount of Ag	Amount of Pt	Amount of Au	Size of NPs	MW	Electron affinity[a]	Ionization[a]	Absolut electronnegativity[b]	Absolut hardness[a]	Ea	BET surface area	Calcination temp.	visible light [%]	UV-Vis light [%]
0.5Ag	0.50	0.00	0.00	10.01	53.93	62.80	365.50	214.15	151.35	-1153.02	158.00	400.00	25.90	52.50
1.5Ag	1.50	0.00	0.00	9.80	161.80	188.40	1096.50	642.45	454.05	-1152.92	162.00	400.00	12.40	57.30
2.5Ag	2.50	0.00	0.00	7.53	269.67	314.00	1827.50	1070.75	756.75	-1152.82	163.00	400.00	6.60	68.90
4.5Ag	4.50	0.00	0.00	5.52	485.41	565.20	3289.50	1927.35	1362.15	-1152.61	183.00	400.00	8.90	89.00
6.5Ag	6.50	0.00	0.00	5.64	701.14	816.40	4751.50	2783.95	1967.55	-1152.41	148.00	400.00	0.90	94.00
0.5Ag_0.1Pt	0.50	0.10	0.00	11.27	73.44	83.33	452.50	267.92	184.59	-1153.02	161.00	400.00	7.90	68.50
1.5Ag_0.1Pt	1.50	0.10	0.00	36.80	181.31	208.93	1183.50	696.22	487.29	-1152.91	141.00	400.00	11.80	69.70
2.5Ag_0.1Pt	2.50	0.10	0.00	5.63	289.18	334.53	1914.50	1124.52	789.99	-1152.81	152.00	400.00	21.80	79.40
4.5Ag_0.1Pt	4.50	0.10	0.00	21.97	504.91	585.73	3376.50	1981.12	1395.39	-1152.61	115.00	400.00	13.70	96.40
6.5Ag_0.1Pt	6.50	0.10	0.00	5.70	720.65	836.93	4838.50	2837.72	2000.79	-1152.40	130.00	400.00	27.10	95.30
0.5Ag_0.25Pt	0.50	0.25	0.00	6.40	102.71	114.13	583.00	348.56	234.44	-1153.01	138.00	400.00	14.80	77.70
1.5Ag_0.25Pt	1.50	0.25	0.00	45.60	210.57	239.73	1314.00	776.86	537.14	-1152.90	172.00	400.00	16.70	75.80
2.5Ag_0.25Pt	2.50	0.25	0.00	3.23	318.44	365.33	2045.00	1205.16	839.84	-1152.80	144.00	400.00	7.30	80.40
4.5Ag_0.25Pt	4.50	0.25	0.00	12.87	534.18	616.53	3507.00	2061.76	1445.24	-1152.60	151.00	400.00	26.10	93.90
6.5Ag_0.25Pt	6.50	0.25	0.00	12.70	749.91	867.73	4969.00	2918.36	2050.64	-1152.39	135.00	400.00	9.30	87.70
0.5Ag_0.5Pt	0.50	0.50	0.00	5.42	151.48	165.45	800.50	482.98	317.53	-1152.99	165.00	400.00	6.50	79.10
1.5Ag_0.5Pt	1.50	0.50	0.00	5.12	259.34	291.05	1531.50	911.28	620.23	-1152.89	164.00	400.00	11.00	71.10
2.5Ag_0.5Pt	2.50	0.50	0.00	13.87	367.21	416.65	2262.50	1339.58	922.93	-1152.78	181.00	400.00	14.00	80.30
4.5Ag_0.5Pt	4.50	0.50	0.00	7.70	582.95	667.85	3724.50	2196.18	1528.33	-1152.58	166.00	400.00	10.90	94.30
6.5Ag_0.5Pt	6.50	0.50	0.00	15.00	798.68	919.05	5186.50	3052.78	2133.73	-1152.38	134.00	400.00	7.40	94.40
0.1Pt	0.00	0.10	0.00	6.38	19.51	20.53	87.00	53.77	33.24	-1153.07	134.60	400.00	4.80	89.40
0.25Pt	0.00	0.25	0.00	6.39	48.77	51.33	217.50	134.41	83.09	-1153.06	163.38	400.00	6.70	98.10
0.5Pt	0.00	0.50	0.00	6.62	97.54	102.65	435.00	268.83	166.18	-1153.04	129.20	400.00	25.70	93.00
1.25Pt	0.00	1.25	0.00	5.65	243.86	256.63	1087.50	672.06	415.44	-1152.99	152.10	400.00	12.50	97.00
0.1Au	0.00	0.00	0.10	6.47	19.70	22.28	89.01	55.65	33.37	-1153.06	187.80	400.00	4.00	56.10
0.25Au	0.00	0.00	0.25	6.21	49.24	55.70	222.53	139.11	83.41	-1153.05	168.10	400.00	6.80	54.10
0.5Au_0.1Pt	0.00	0.10	0.50	6.02	117.99	131.93	532.05	331.99	200.06	-1153.02	196.40	400.00	10.70	83.10
0.1Au_0.1Pt	0.00	0.10	0.10	5.97	39.21	42.81	176.01	109.41	66.60	-1153.06	190.59	400.00	8.00	71.80
0.25Au_0.25Pt	0.00	0.25	0.25	6.22	98.01	107.03	440.03	273.53	166.50	-1153.03	154.10	400.00	6.40	83.70
0.5Au_0.5Pt	0.00	0.50	0.50	6.34	196.03	214.05	880.05	547.05	333.00	-1152.99	151.07	400.00	12.60	76.00
0.5Au_0.25Pt	0.00	0.25	0.50	5.11	147.25	162.73	662.55	412.64	249.91	-1153.01	153.48	400.00	12.70	71.70
0.1Au_0.25Pt	0.00	0.25	0.10	4.97	68.47	73.61	306.51	190.06	116.45	-1153.05	105.00	400.00	9.90	90.60
0.25Au_0.1Pt	0.00	0.10	0.25	4.54	68.75	76.23	309.53	192.88	116.65	-1153.04	150.45	400.00	6.10	77.60
0.05Au_0.05Pt	0.00	0.05	0.05	6.48	19.60	21.41	88.01	54.71	33.30	-1153.07	164.97	400.00	11.20	64.10

Table S7. Williams plot describing applicability domains of MLR-GA models presented in eq. 6 (a) and eq. 7 (b), respectively.

a)



b)

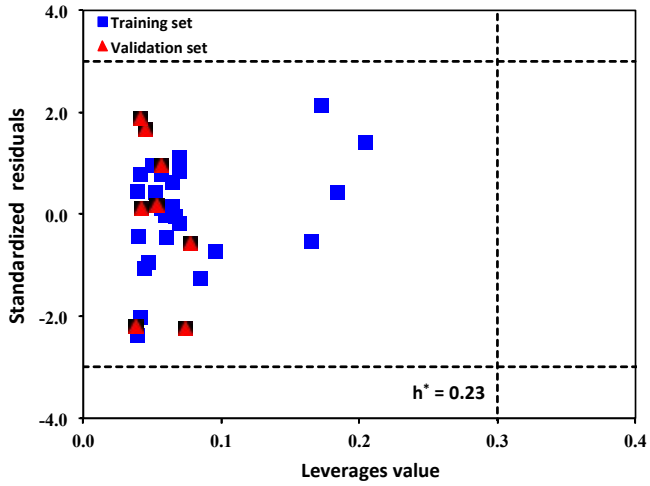


Table S8. Double Cross-Validation data for developer MLR Nano-QSAR models.*

MLR equation	**LogEC50 = 4.6897(±0.0305) +0.1833(±0.0101) %mol$_{Ag}$**	**LogEC50 = 4.6100(±0.0333) +0.0004(±0) μ_{mix}**
INTERNAL Validation Parameters 100% data; TRAINING SET):		
R^2	0.9274	0.928
R^2_{Adj}	0.9247	0.9253
SEE	0.1247	0.1242
Q^2	0.9153	0.9149
SDEP	0.1299	0.1302
Scaled Average $r_m^2{}_{LOO}$	0.8852	0.8849
Scaled Delta $r_m^2{}_{LOO}$	0.0454	0.0427
MAE	0.0986	0.0981
SD	0.086	0.0871
For 95% Training Data :		
MAE	0.0828	0.0851
SD	0.0658	0.0755
MAE+3*SD	0.2802	0.3117
Prediction Quality):	**MODERATE**	**MODERATE**
EXTERNAL Validation Parameters (100% data; TEST SET):		
Q^2_{F1}	0.8947	0.8745
Q^2_{F2}	0.8936	0.8732
Scaled Average r_m^2	0.9408	0.8567
Scaled Delta r r_m^2	0.0284	0.0613
CCC	0.9374	0.9237
MAE	0.0979	0.1086
SD	0.078	0.0825
For 95% Test Data :		
Q^2_{F1}	0.9364	0.9551
Q^2_{F2}	0.9311	0.9513
Scaled Average r_m^2	0.9523	0.8769
Scaled Delta r_m^2	0.0155	0.0271
CCC	0.9603	0.9723
MAE	0.0771	0.0769
SD	0.066	0.0307
MAE+3*SD	0.2751	0.1689
Prediction Quality	**MODERATE**	**GOOD**

*K. Roy, P. Ambure, *Chemometrics and Intelligent Laboratory Systems*, 2016, **159**, 108-126 (Please see, MS, References section, position 45); K. Roy, S. Kar and P. Ambure, *Chemometrics and Intelligent Laboratory Systems,* 2015, ***145***, 22-29 (Please see, MS, References section, position 61)

Table S9. The external validation criteria and results analysis based on Golbraikh and Tropsha method.*

The external validation criteria	For model from eq.6	For model from eq.7
R^2_{Ext} >0.6	0.90	0.90
Q^2_{F1}/ Q^2_{F2}/ Q^2_{F3} >0.6	0.88/0.88/0.90	/0.83/0.83/0.87/
Rcvext2 >0.5	0.92	0.93
$(R^2_{Ext} - R_0^2)/ R^2_{Ext} < 0.1$	0.01	0.07
abs(R_0^2 - R'$_0^2$) < 0.3	0.06	0.28
r^2_m >0.5	0.74	0.56
$0.85 \le k \le 1.15$	1.01	1
$0.85 \le k' \le 1.15$	0.99	1

* A. Golbraikh, A. Tropsha, *Journal of Molecular Graphics and Modelling*, 2002, **20**, 269-276. (Please see, MS, References section, position 22); G. Melagraki and A. Afantitis, *RSC Advances,* 2014, **4**, 50713-50725. (Please see, MS, References section, position 43)

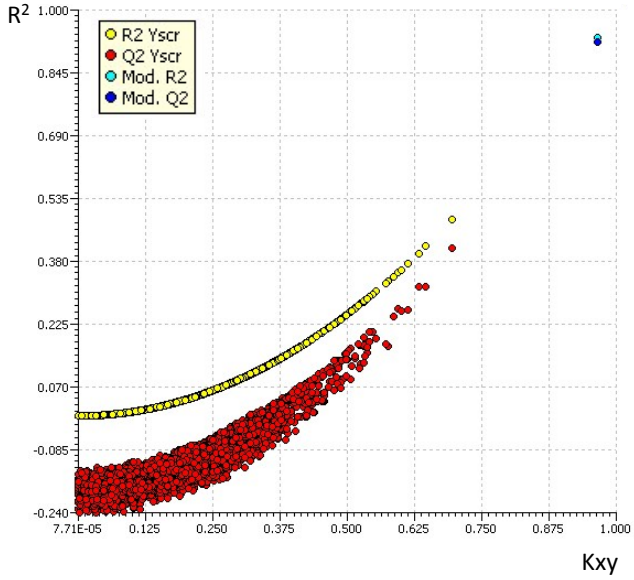
Where:
R_{Ext}^2)(simply called R^2 by the authors): Correlation coefficient between the predicted and observed activities
Rcv^2: External cross validation
R_0^2: Coefficient of determination: predicted versus observed activities
R'_0^2: Coefficient of determination: observed versus predicted activities
k = slope: predicted versus observed activities regression lines through the origin
k'= slope: observed versus predicted activities regression lines through the origin
$r^2_m = r^2 (1-\sqrt{r^2 - r_0^2})$ (proposed by Roy group) similar to to the Golbraikh and Tropsha concept where r^2, r^2_0 correspond to R^2 and R_0^2 in the Golbraikh and Tropsha method.

Table S10. The external validation criteria and results analysis based on Golbraikh and Tropsha method.*

Obtained random models parameters for model from eq. 6:	Value of selected parameters
Average R^2Y_{scr} :	0.04
Average Q^2Y_{scr} :	-0.13
The y-rand R^2 range	-0.24-0.51
Obtained random models parameters for model from eq. 7:	**Value of selected parameters**
Average R^2Y_{scr} :	0.04
Average Q^2Y_{scr} :	-0.13
The y-rand R^2 range	-0.25-0.53

Figure S1. The results of the Y-scrambling test (blue circle is the original model).

a) Y-scrambling for model described in eq.6



b) Y-scrambling for model described in eq.7