Supplementary for:

Asymmetric Schiff Base Functionalized Gold Nanoparticles based

colorimetric sensor for Hg²⁺ ions Determination: Experimental and DFT

Study

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Figure 1 Parity plot showing the correlation between the observed and predicted values

Table S1. Instruments

Instrument	Model	Company	Country
Field emission			
scanning electron	Zeiss Jena	Sigma	Germany
microscopy			
Ultraviolet-Visible	Т80+	PG	England
spectrophotometer	100	10	England
Fourier Transform			
Infrared	FT-IR 6300	Jasco	Japan
Spectroscopy			
Dynamic light	V1 04	LS Instruments	Switzerland
scattering	V 1.04	Lo mortumento	Switzerlund

Table S2. Chemicals

Chemical formula	Company	Country
Hydrogen tetrachloroaurate	Merck	Germany
hydrate	WORK	Germany
3,4-diaminotoloene	Merck	Germany
Benzaldehyde	Merck	Germany
Polyvinyl alcohol	Merck	Germany
Trisodium citrate	Merck	Germany
Mercury(II) nitrate	Merck	Germany

Factor	Name	Units	Minimum	Maximum	Coded	Values	Mean
A	GNPs volume	mL	500.00	1500.00	750.00	1250.00	1000.00
В	Schiff base volume	mL	100.00	300.00	150.00	250.00	200.00
C	pH	-	2.00	8.00	3.50	6.50	5.00
D	Response Time	S	20.00	100.00	40.00	80.00	60.00

Table S3. Experimental range and level of independent variables

Source	Sequential	Lack of Fit	Adjusted	Predicted	
	p-value		R-Squared	R-Squared	
Linear	0.0073	0.0003	0.4535	0.2172	
2FI	0.5849	0.0002	0.4117	-0.4534	
<u>Quadratic</u>	<u>< 0.0001</u>	<u>0.9196</u>	<u>0.9938</u>	<u>0.9879</u>	Suggested
Cubic	0.9196		0.9911		Aliased

 Table S4. The sequential model sum of squares for CCD analysis

Source	Sum of Squares	df	Mean Square	F Value	p-value Prob > F	
Linear	0.35	12	0.029	81.13	0.0003	
2FI	0.23	6	0.039	108.95	0.0002	
Quadratic	<u>6.120E-005</u>	2	<u>3.060E-005</u>	0.086	<u>0.9196</u>	Suggested
Cubic	0.000	0				Aliased
Pure Error	1.431E-003	4	3.577E-004			

Table S5. Lack of fit tests for CCD analysis

Source	Std. Dev.	R- Squared	Adjusted R- Squared	Predicted R- Squared	PRESS	
Linear	0.15	0.5628	0.4535	0.2172	0.63	
2FI	0.15	0.7058	0.4117	-0.4534	1.16	
Quadratic	<u>0.016</u>	<u>0.9981</u>	<u>0.9938</u>	<u>0.9879</u>	<u>9.665E-003</u>	Suggested
Cubic	0.019	0.9982	0.9911		+	Aliased

Table S6. Model summary statistics for CCD analysis

Table S7. Model summary statics

Std. Dev.	0.016	R-Squared	0.9981
Mean	0.65	Adj R-Squared	0.9938
C.V. %	2.43	Pred R-Squared	0.9879
PRESS	9.665E-003	Adeq Precision	49.137
-2 Log Likelihood	-141.00	BIC	-95.33
		AICc	-15.00

Source	Sum of Squares	df	Mean Square	F Value	p-value
Model	0.80	14	0.057	229.31	< 0.0001
A-Au Concentration	0.15	1	0.15	586.26	< 0.0001
B-Ligand Concentration	0.080	1	0.080	321.89	< 0.0001
C-pH	0.043	1	0.043	171.90	< 0.0001
D-Response Time	0.10	1	0.10	407.18	< 0.0001
AB	0.078	1	0.078	313.72	< 0.0001
AC	3.647E-003	1	3.647E-003	14.66	0.0087
AD	3.056E-003	1	3.056E-003	12.29	0.0127
BC	3.495E-003	1	3.495E-003	14.05	0.0095
BD	9.433E-004	1	9.433E-004	3.79	0.0994
CD	0.025	1	0.025	101.49	< 0.0001
A ²	0.015	1	0.015	60.58	0.0002
B ²	8.145E-003	1	8.145E-003	32.76	0.0012
C^2	0.23	1	0.23	908.49	< 0.0001
D ²	0.034	1	0.034	136.34	< 0.0001
Residual	1.492E-003	6	2.487E-004		
Lack of Fit	6.120E-005	2	3.060E-005	0.086	0.9196
Pure Error	1.431E-003	4	3.577E-004		
Cor Total	0.80	20			

Table S8. The results of ANOVA for the response surface quadratic model by the proposed colorimetric sensor