

Supporting Information

Multiresponse optimization followed by multivariate calibration for simultaneous determination of carcinogenic polycyclic aromatic hydrocarbons in environmental samples using gold nanoparticles

Mahsa Rezaian, Hadi Parastar*, M. Reza Hormozi-Nezhad

Department of Chemistry, Sharif University of Technology, P.O. Box 11155-3516, Tehran,

Iran

* Author to whom correspondence should be addressed;

Tel.: +98- 21- 66165306; fax: +98- 21- 66005718 (Hadi Parastar)

E-mail: h.parastar@sharif.edu, h.parastar@gmail.com

Table S1 – ANOVA table for quadratic response surface for Aceny

Source	SS	df	MS	F	p-value	
Block	0.00046	1	0.00046	0.03511	0.8527	Not significant
Model	0.434502	6	0.072417	5.535891	0.0007	Significant
A	0.17512	1	0.17512	13.38701	0.0010	
D	0.055615	1	0.055615	4.251471	0.0486	
E	0.044719	1	0.044719	3.418508	0.0751	
AE	0.050971	1	0.050971	3.896472	0.0583	
CD	0.068927	1	0.068927	5.269141	0.0294	
A ²	0.039149	1	0.039149	2.992739	0.0946	
Residual	0.366278	28	0.013081			
Lack of Fit	0.26645	20	0.013322	1.067635	0.4910	Not significant
Pure Error	0.099828	8	0.012478			
Corrected Total	0.801239	35				

Table S2 - ANOVA table for quadratic response surface for Flu

Source	SS	df	MS	F	p-value	
Block	9.84E-03	1	9.84E-03	4.41	0.0460	Significant
Model	0.19	9	0.021	9.38	< 0.0001	Significant
A	9.54E-03	1	9.54E-03	4.27	0.0493	
C	0.043	1	0.043	19.06	0.0002	
AC	0.011	1	0.011	4.83	0.0374	
AD	9.70E-03	1	9.70E-03	4.34	0.0475	
BC	0.028	1	0.028	12.37	0.0017	
BD	0.016	1	0.016	7.37	0.0119	
CD	0.031	1	0.031	13.66	0.0011	
CE	0.034	1	0.034	15.29	0.0006	
DE	7.11E-03	1	7.11E-03	3.18	0.0866	
Residual	0.056	25	2.23E-03			
Lack of Fit	0.043	17	2.55E-03	1.62	0.2489	Not significant
Pure Error	0.013	8	1.57E-03			
Corrected Total	0.25	35				

Table S3- ANOVA table for quadratic response surface for Ant

Source	SS	df	MS	F	p-value	
Block	0.08	1	0.08	4.21	0.050	Significant
Model	0.51	7	0.072	3.85	0.005	significant
C	0.068	1	0.068	3.65	0.0668	
E	0.067	1	0.067	3.55	0.0705	
AB	0.097	1	0.097	5.15	0.0315	
CD	0.057	1	0.057	3.03	0.0931	
DE	0.078	1	0.078	4.18	0.0506	
B ²	0.061	1	0.061	3.25	0.0824	
C ²	0.078	1	0.078	4.17	0.0511	
Residual	0.51	27	0.019			
Lack of Fit	0.27	19	0.014	0.47	0.9182	not significant
Pure Error	0.24	8	0.03			
Corrected Total	1.09	35				

Table S4- ANOVA table for quadratic response surface for B[a]A

Source	SS	df	MS	F	P-value	
Block	0.023	1	0.023	0.621	0.4371	Not significant
Model	1.33E+00	5	0.27	7.27	0.0002	significant
C	4.10E-01	1	0.41	11.06	0.0024	
D	1.40E-01	1	0.14	3.94	0.0567	
AC	2.20E-01	1	0.22	5.94	0.0212	
A ²	0.34	1	0.34	9.3	0.0049	
E ²	0.22	1	0.22	6.09	0.0198	
Residual	1.06	29	0.037			
Lack of Fit	0.8	21	0.038	1.16	0.4365	not significant
Pure Error	0.26	8	0.033			
Corrected Total	2.42	35				

Table S5- ANOVA table for quadratic response surface for Chr

Source	SS	df	MS	F	p-value	
Block	0.21	1	0.21	28.79	0.0001	Significant
Model	0.75	7	0.11	14.72	< 0.0001	significant
A	0.19	1	0.19	25.82	< 0.0001	
C	0.033	1	0.033	4.53	0.0426	
D	0.04	1	0.04	5.55	0.026	
AC	0.084	1	0.084	11.51	0.0022	
BE	0.075	1	0.075	10.23	0.0035	
D ²	0.26	1	0.26	35.85	< 0.0001	
E ²	0.07	1	0.07	9.58	0.0045	
Residual	0.2	27	7.30E-03			
Lack of Fit	0.16	19	8.64E-03	2.1	0.1419	not significant
Pure Error	0.033	8	4.11E-03			
Corrected Total	1.16	35				

Table S6- ANOVA table for quadratic response surface for B[b]F

Source	SS	df	MS	F	p-value	
Block	0.027	1	0.027	1.59	0.2164	Not significant
Model	0.26	2	0.13	7.69	0.0019	significant
A	0.19	1	0.19	11.26	0.0021	
AE	0.07	1	0.07	4.13	0.0506	
Residual	0.55	32	0.017			
Lack of Fit	0.32	24	0.013	0.48	0.9187	not significant
Pure Error	0.22	8	0.028			
Corrected Total	0.84	35				

Table S7- ANOVA table for quadratic response surface for B[k]F

Source	SS	df	MS	F	p-value	
Block	3.45E-03	1	3.45E-03	1.92	0.1761	Not significant
Model	0.54	4	0.13	7.47	0.0003	significant
A	0.21	1	0.21	11.92	0.0017	
B	0.079	1	0.079	4.41	0.0442	
A ²	0.12	1	0.12	6.69	0.0148	
E ²	0.12	1	0.12	6.88	0.0136	
Residual	0.54	30	0.018			
Lack of Fit	0.43	22	0.02	1.5	0.2846	not significant
Pure Error	0.1	8	0.013			
Corrected Total	1.08	35				

Table S8- ANOVA table for quadratic response surface for B[a]P

Source	SS	df	MS	F	p-value	
Block	0.023	1	0.023	2.09	0.1598	Not significant
Model	0.75	7	0.11	9.85	< 0.0001	significant
A	0.37	1	0.37	33.61	< 0.0001	
B	0.044	1	0.044	4.04	0.0546	
AC	0.054	1	0.054	4.97	0.0343	
AE	0.037	1	0.037	3.41	0.0758	
CE	0.047	1	0.047	4.34	0.0468	
DE	0.045	1	0.045	4.17	0.0509	
A ²	0.16	1	0.16	14.37	0.0008	
Residual	0.29	27	0.011			
Lack of Fit	0.23	19	0.012	1.47	0.2963	not significant
Pure Error	0.065	8	8.18E-03			
Corrected Total	1.07	35				

Table S9 - ANOVA table for quadratic response surface for I[123-cd]P

Source	SS	df	MS	F	p-value	
Block	0.33	1	0.33	8.25	0.0073	significant
Model	0.81	3	0.27	6.75	0.0012	significant
A	0.35	1	0.35	8.82	0.0057	
AE	0.27	1	0.27	6.64	0.015	
B ²	0.19	1	0.19	4.79	0.0362	
Residual	1.24	31	0.04			
Lack of Fit	0.71	23	0.031	0.46	0.9298	not significant
Pure Error	0.53	8	0.067			
Corrected Total	2.37	35				

Table S10- ANOVA table for quadratic response surface for D[ah]A

Source	SS	df	MS	F	p-value	
Block	2.74E-03	1	2.74E-03	2.98	0.0957	Not significant
Model	0.059	7	8.41E-03	9.15	< 0.0001	significant
A	0.016	1	0.016	16.93	0.0003	
B	8.72E-03	1	8.72E-03	9.49	0.0047	
AE	0.012	1	0.012	12.72	0.0014	
DE	4.63E-03	1	4.63E-03	5.04	0.0331	
A ²	4.70E-03	1	4.70E-03	5.11	0.032	
B ²	0.01	1	0.01	11.14	0.0025	
E ²	3.30E-03	1	3.30E-03	3.59	0.0689	
Residual	0.025	27	9.19E-04			
Lack of Fit	0.019	19	1.01E-03	1.46	0.3017	not significant
Pure Error	5.57E-03	8	6.96E-04			
Corrected Total	0.086	35				

Table S11- ANOVA table for quadratic response surface for B[ghi]P

Source	SS	df	MS	F	p-value	
Block	0.12	1	0.12	6.00	0.0206	significant
Model	0.86	5	0.17	8.44	< 0.0001	significant
A	0.36	1	0.36	17.89	0.0002	
B	0.074	1	0.074	3.62	0.0669	
AE	0.21	1	0.21	10.44	0.0031	
A ²	0.098	1	0.098	4.8	0.0367	
B ²	0.11	1	0.11	5.43	0.0269	
Residual	0.59	29	0.02			
Lack of Fit	0.48	21	0.023	1.57	0.2628	not significant
Pure Error	0.12	8	0.014			
Corrected Total	1.57	35				