

Electronic Supplementary Material

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A Thorough Investigation of Photo-catalytic Degradation of ortho and para-Nitro Phenols in binary mixtures: New Insights into Evaluating Degradations Progress Using Chemometrics Approaches

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Table 1S. Experimental conditions for 2^{5-1} central composite design and experimental responses for the analytes in acidic condition

Independent variables		Levels				
		$-\alpha$	-1	0	1	$+\alpha$
A (Catalyst dosage(g))		0.002	0.003	0.003	0.004	0.005
B (H ₂ O ₂ volume(mL))		0.1	0.2	0.2	0.3	0.4
C (2-NP concentration)		3	19	25	30	38
D (4-NP concentration)		2	8	10	13	19
E (Temperature(°C))		15.0	22.9	32.5	42.1	50.0

Factor		Standard deviation of Profiles							
Run	A	B	C	D	E	YA-2-NP	YB-2-NP	YA-2-NP	YB-4-NP
1	0.003	0.2	25	2	32.5	9.514	1.698	0.8873	0
2	0.004	0.3	15	5	42.1	6.456	1.148	2.114	0.3177
3	0.003	0.2	22	13	32.5	5.911	1.518	5.194	2.65
4	0.003	0.4	19	8	32.5	6.302	2.114	3.483	0.3537
5	0.003	0.2	38	8	32.5	10.56	2.975	2.932	2.306
6	0.002	0.3	30	5	42.11	11.42	2.303	2.281	1.237
7	0.002	0.1	34	10	23.5	7.84	1.966	1.901	0.7429
8	0.002	0.1	30	10	42.11	11.33	1.698	3.707	2.513
9	0.003	0.2	25	5	15	11.29	0.3383	2.304	1.351
10	0.003	0.2	22	8	32.5	8.242	1.616	3.957	2.3
11	0.002	0.3	25	10	42.11	8.641	2.242	4.579	2.363
12	0.004	0.3	30	5	22.89	10.75	2.778	2.243	1.215
13	0.004	0.3	15	10	22.89	4.932	1.211	4.064	0.9863
14	0.003	0.2	22	8	50	8.417	1.092	3.754	2.382
15	0.005	0.2	30	8	32.5	11.54	1.211	3.835	2.219
16	0.003	0.2	22	8	32.5	7.433	1.411	3.438	1.515
17	0.004	0.1	25	5	42.11	11.29	0.3379	2.306	1.356
18	0.002	0.3	22	10	22.89	4.901	2.728	3.484	1.5
19	0.003	0.2	3	8	32.5	0.7608	0.3483	3.461	0.6933
20	0.004	0.1	25	10	42.11	7.754	1.79	3.711	2.868
21	0.002	0.1	15	5	32.1	5.369	0.9624	2.226	0.7142
22	0.003	0.2	15	0	32.5	4.765	1.593	0	0
23	0.003	0.2	0	19	32.5	0	0	6.71	2.223

Table 2S. The results of SVD analysis on the data of individual nitrophenols

Data SV*	S _{a-2NP}	S _{a-4NP}	S _{b-2NP}	S _{b-4NP}
1	14.09	17.76	14.54	45.79
2	3.15	6.86	2.30	11.66
3	0.47	0.47	0.42	0.94
4	0.13	0.26	0.15	0.30
5	0.09	0.12	0.02	0.19

*SV is the abbreviation of singular value.

Table 3S. Analysis of variance (ANOVA) for central composite design for 2-NP-A at acidic condition

Source	Sum of Squares	df	Mean Square	F Value	p-value Prob > F
Model	224	10	22.4	27.66	< 0.0001
C	6.964	1	6.964	8.598	0.01255
D	18.89	1	18.89	23.32	0.000412
E	8.945	1	8.945	11.05	0.006071
AE	1.381	1	1.381	1.705	0.2161
BC	3.757	1	3.757	4.639	0.05228
CD	18.48	1	18.48	22.82	0.000451
DE	5.211	1	5.211	6.434	0.02611
A ²	3.099	1	3.099	3.827	0.07413
C ²	5.341	1	5.341	6.595	0.02463
D ²	5.223	1	5.223	6.449	0.02597
Residual	9.719	12	0.8099		
Lack of Fit	9.391	11	0.8537	2.606	0.4518
Pure Error	0.3276	1	0.3276		
Cor Total	233.7	22			

Table 4S. Analysis of variance (ANOVA) for central composite design for 2-NP-B at acidic condition

Source	Sum of Squares	df	Mean Square	F Value	p-value Prob > F
Model	13.9	13	1.069	23.68	< 0.0001
B	3.078	1	3.078	68.15	< 0.0001
C	5.216	1	5.216	115.5	< 0.0001
E	0.8243	1	0.8243	18.25	0.002075
AB	0.2519	1	0.2519	5.577	0.04249
AC	1.123	1	1.123	24.85	0.000754
AD	2.387	1	2.387	52.84	< 0.0001
BD	0.2012	1	0.2012	4.454	0.06403
BE	2.827	1	2.827	62.58	< 0.0001
CE	2.279	1	2.279	50.45	< 0.0001
DE	0.424	1	0.424	9.388	0.01348
A ²	0.7599	1	0.7599	16.82	0.00267
B ²	0.745	1	0.745	16.49	0.002836
E ²	2.891	1	2.891	64	< 0.0001
Residual	0.4065	9	0.04517		
Lack of Fit	0.3855	8	0.04819	2.293	0.4725
Pure Error	0.02102	1	0.02102		
Cor Total	14.31	22			

Table 5S. Analysis of variance (ANOVA) for central composite design for 4-NP-A at acidic condition

Source	Sum of Squares	df	Mean Square	F Value	p-value Prob > F
Model	43.56	11	3.96	167.3	< 0.0001
D	20.45	1	20.45	864	< 0.0001
AB	0.2753	1	0.2753	11.63	0.005825
AC	1.156	1	1.156	48.84	< 0.0001
AD	1.101	1	1.101	46.5	< 0.0001
BC	0.4451	1	0.4451	18.8	0.001182
BE	1.034	1	1.034	43.67	< 0.0001
CE	2.118	1	2.118	89.48	< 0.0001
A ²	0.7488	1	0.7488	31.63	0.000155
C ²	0.2432	1	0.2432	10.27	0.008378
D ²	0.6543	1	0.6543	27.64	0.000269
E ²	0.2625	1	0.2625	11.09	0.006708
Residual	0.2604	11	0.02367		
Lack of Fit	0.126	10	0.0126	0.09378	0.9915
Pure Error	0.1344	1	0.1344		
Cor Total	43.82	22			

Table 6S. Analysis of variance (ANOVA) for central composite design for 4-NP-B at acidic condition

Source	Sum of Squares	df	Mean Square	F Value	p-value Prob > F
Model	16.56	10	1.656	19.93	< 0.0001
B	0.8916	1	0.8916	10.73	0.006635
C	2.425	1	2.425	29.18	0.00016
D	7.33	1	7.33	88.21	< 0.0001
E	1.18	1	1.18	14.2	0.002679
AB	0.2937	1	0.2937	3.535	0.08458
BC	0.3473	1	0.3473	4.179	0.06351
BE	0.3936	1	0.3936	4.736	0.05023
CD	0.4583	1	0.4583	5.515	0.03681
DE	0.8533	1	0.8533	10.27	0.007569
B ²	0.7431	1	0.7431	8.942	0.01127
Residual	0.9972	12	0.0831		
Lack of Fit	0.6892	11	0.06265	0.2034	0.9514
Pure Error	0.308	1	0.308		
Cor Total	17.56	22			

Table 7S. Analysis of variance (ANOVA) for central composite design for 2-NP-A at basic condition

Source	Sum of Squares	df	Mean Square	F Value	p-value Prob > F
Model	452.6	6	75.43	52.69	< 0.0001
B	11.54	1	11.54	8.063	0.01393
C	328.1	1	328.1	229.2	< 0.0001
D	1.941	1	1.941	1.356	0.2652
E	10.57	1	10.57	7.386	0.01759
CE	5.742	1	5.742	4.011	0.06652
E ²	1.758	1	1.758	1.228	0.2878
Residual	18.61	13	1.432		
Lack of Fit	12.82	12	1.068	0.1846	0.9618
Pure Error	5.789	1	5.789		
Cor Total	471.2	19			

Table 8S. Analysis of variance (ANOVA) for central composite design for 2-NP-B at basic condition

Source	Sum of Squares	df	Mean Square	F Value	p-value Prob > F
Model	141	12	11.75	15.83	0.000629
A	5.238	1	5.238	7.06	0.0326
B	23.34	1	23.34	31.46	0.000808
C	32.55	1	32.55	43.87	0.000298
D	12.65	1	12.65	17.04	0.004412
E	23.55	1	23.55	31.74	0.000788
AB	7.688	1	7.688	10.36	0.01467
AC	3.958	1	3.958	5.334	0.05422
AD	4.155	1	4.155	5.6	0.04987
AE	25.69	1	25.69	34.62	0.000609
BC	1.585	1	1.585	2.136	0.1872
BD	14.25	1	14.25	19.21	0.003224
DE	20.06	1	20.06	27.04	0.001253
Residual	5.194	7	0.7419		
Lack of Fit	3.418	6	0.5697	0.3209	0.872
Pure Error	1.775	1	1.775		
Cor Total	146.1	19			

Table 9S. Analysis of variance (ANOVA) for central composite design for 2-NP-C at basic condition

Source	Sum of Squares	df	Mean Square	F Value	p-value Prob > F
Model	557.9	8	69.74	30.66	< 0.0001
C	203.6	1	203.6	89.52	< 0.0001
E	7.271	1	7.271	3.197	0.1013
AB	45.14	1	45.14	19.85	0.000971
AC	4.661	1	4.661	2.049	0.1801
AE	113.9	1	113.9	50.06	< 0.0001
BE	76.38	1	76.38	33.58	0.00012
CE	16.59	1	16.59	7.294	0.02063
DE	15.25	1	15.25	6.703	0.02518
Residual	25.02	11	2.275		
Lack of Fit	12.97	10	1.297	0.1076	0.9877
Pure Error	12.05	1	12.05		
Cor Total	582.9	19			

Table 10S. Analysis of variance (ANOVA) for central composite design for 4-NP-A at basic condition

Source	Sum of Squares	df	Mean Square	F Value	p-value Prob > F
Model	26.69	3	8.897	109.5	< 0.0001
D	8.517	1	8.517	104.8	< 0.0001
DE	0.3572	1	0.3572	4.397	0.05226
D ²	1.474	1	1.474	18.14	0.000599
Residual	1.3	16	0.08123		
Lack of Fit	1.297	15	0.08649	36.18	0.1298
Pure Error	0.002391	1	0.002391		
Cor Total	27.99	19			

Table 11S. Analysis of variance (ANOVA) for central composite design for 4-NP-B at basic condition

Source	Sum of Squares	df	Mean Square	F Value	p-value Prob > F
Model	11.85	9	1.316	24.99	< 0.0001
C	0.9622	1	0.9622	18.27	0.001626
D	6.993	1	6.993	132.8	< 0.0001
E	0.1444	1	0.1444	2.742	0.1287
AB	0.8151	1	0.8151	15.48	0.002803
AC	1.055	1	1.055	20.02	0.001189
BC	1.326	1	1.326	25.18	0.000524
BE	0.312	1	0.312	5.924	0.03521
C ²	1.198	1	1.198	22.74	0.000759
E ²	0.1231	1	0.1231	2.336	0.1574
Residual	0.5267	10	0.05267		
Lack of Fit	0.4426	9	0.04918	0.5845	0.7767
Pure Error	0.08414	1	0.08414		
Cor Total	12.37	19			

Equations:

Acidic status: The relationship between the responses and experimental factors in acidic condition is as follows:

$$YA_{2-NP} = 6.114 + 1.310 C - 2.408 D + 1.351 E - 0.4840 AE - 0.8032 BC - 1.709 CD + 1.286 DE + 0.5571 A^2 - 0.5100 C^2 - 0.6589 D^2 \quad \text{Eq. 1S}$$

$$YB_{2-NP} = 1.946 + 0.6367 B + 0.6211 C + 0.6183 E - 0.1837 AB - 0.8600 AC + 1.143 AD + 0.1846 BD - 0.9865 BE - 1.736 CE + 0.4973 DE + 0.4707 A^2 - 0.2004 B^2 - 0.5499 E^2 \quad \text{Eq. 2S}$$

$$YA_{4-NP} = 4.504 + 1.615 D + 0.1785 AB + 0.6915 AC - 0.6415 AD + 0.2288 BC + 0.4611 BE + 1.163 CE - 0.3635 A^2 - 0.1078 C^2 - 0.1748 D^2 + 0.1329 E^2 \quad \text{Eq. 3S}$$

$$YB_{4-NP} = 2.060 - 0.2480 B + 0.6013 C + 0.9481 D + 0.5258 E - 0.1537 AB + 0.2577 BC - 0.1902 BE + 0.1866 CD + 0.5135 DE - 0.1820 B^2 \quad \text{Eq. 4S}$$

Figures:

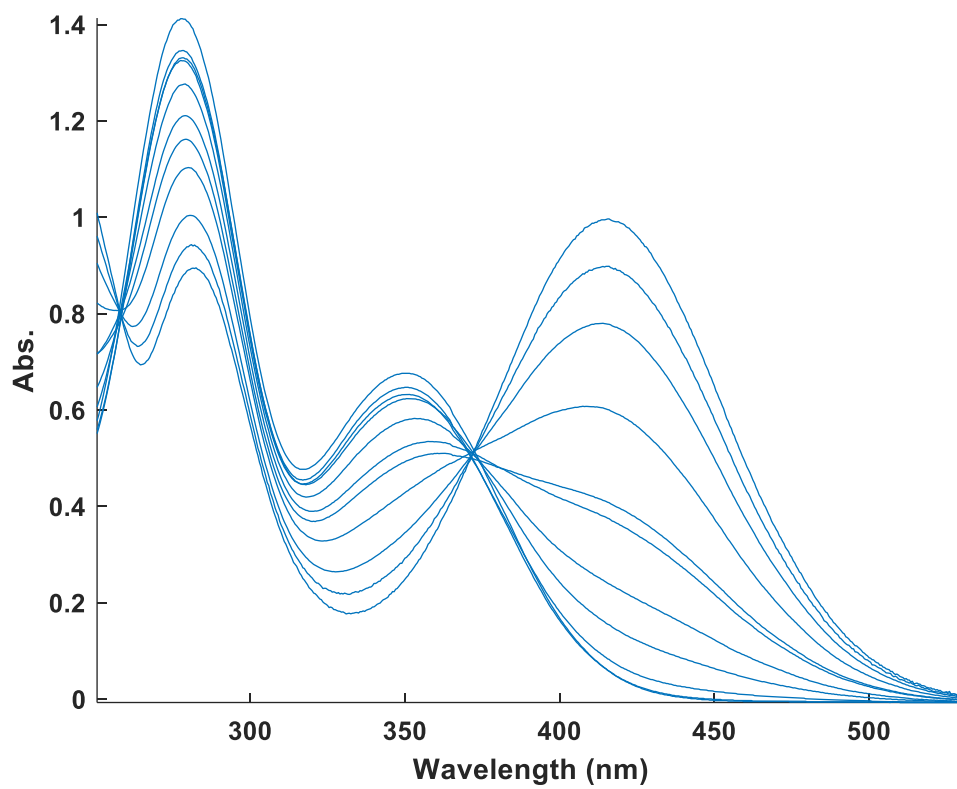


Fig. S1. pH titration data of 2-NP

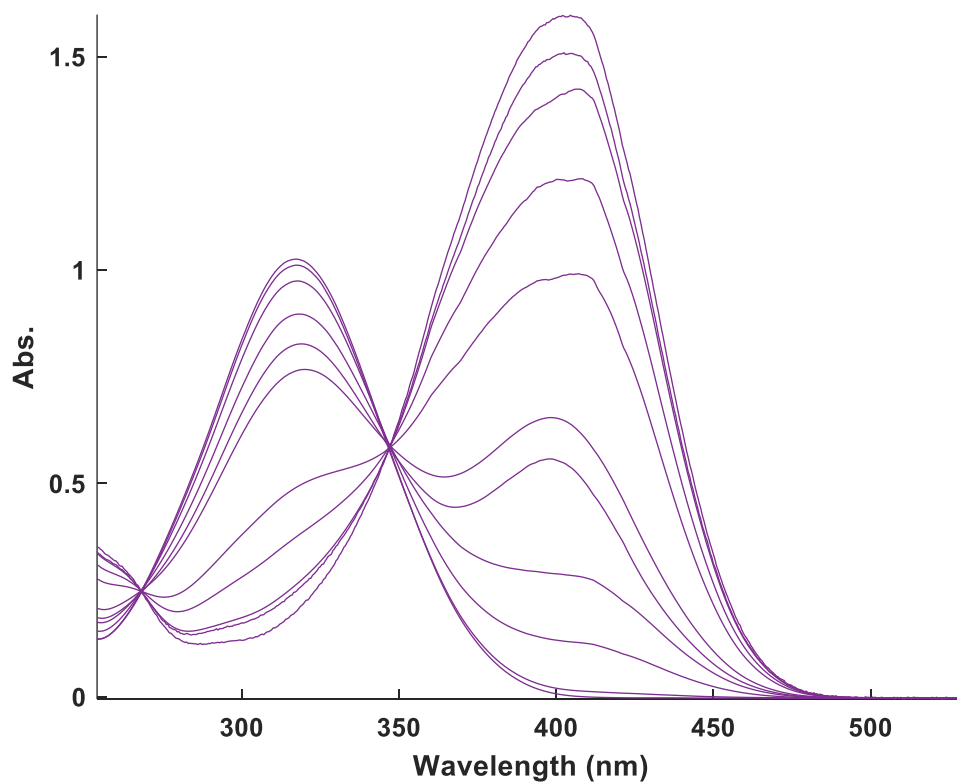


Fig. S2. pH titration data of 4-NP

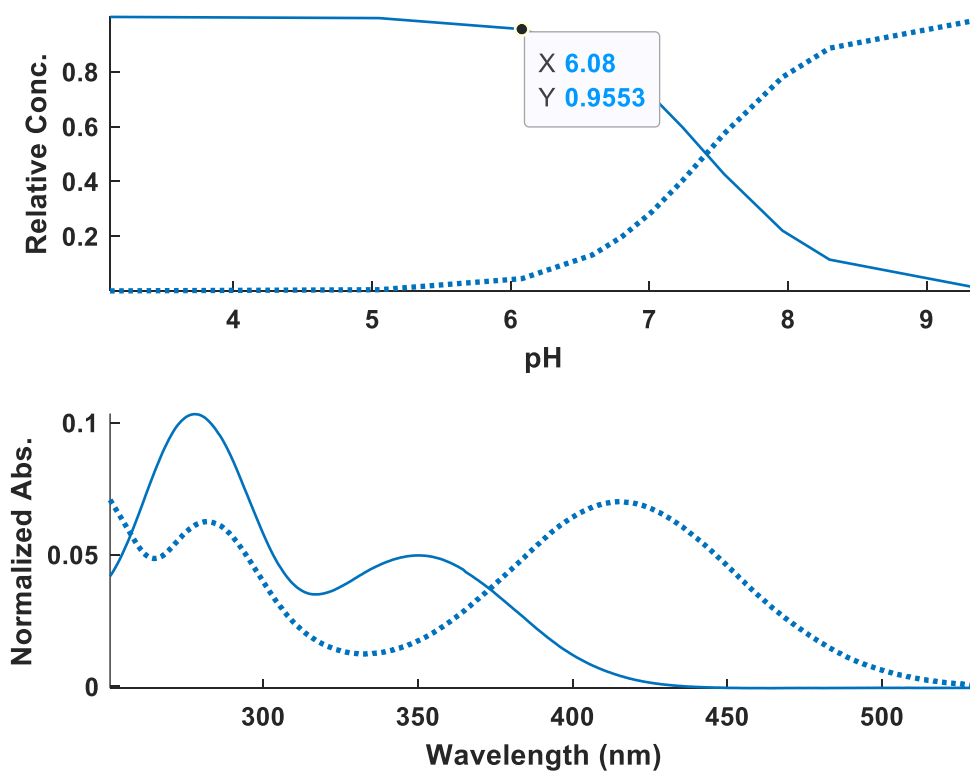


Fig. S3. The spectral and pH profiles of 2-NP

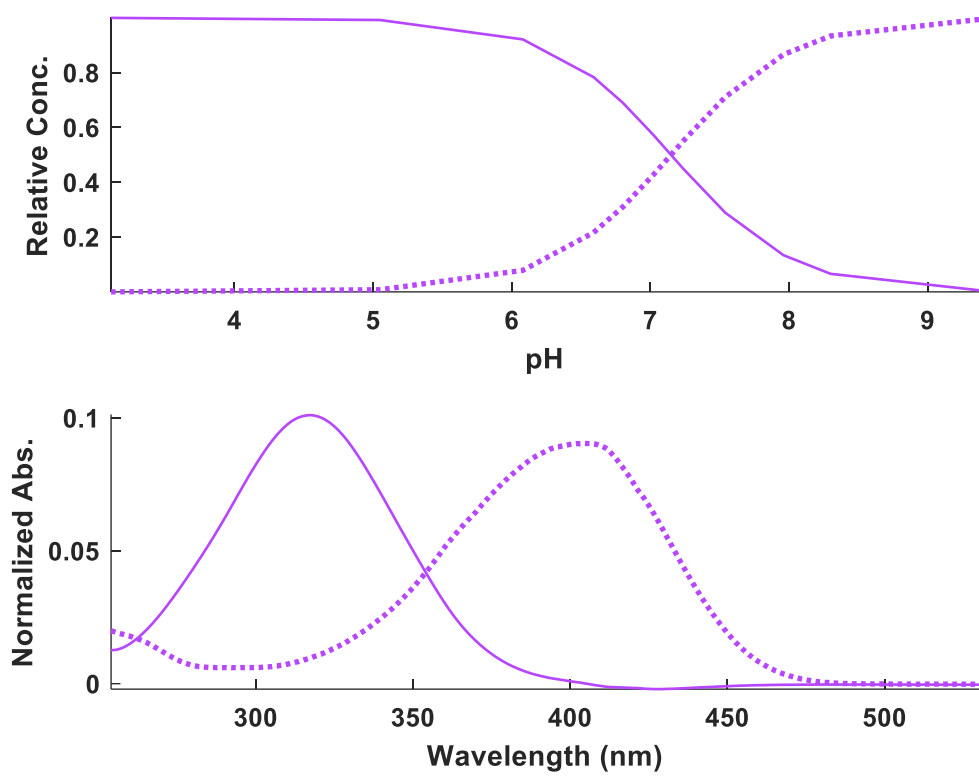


Fig. S4. The spectral and pH profiles of 4-NP

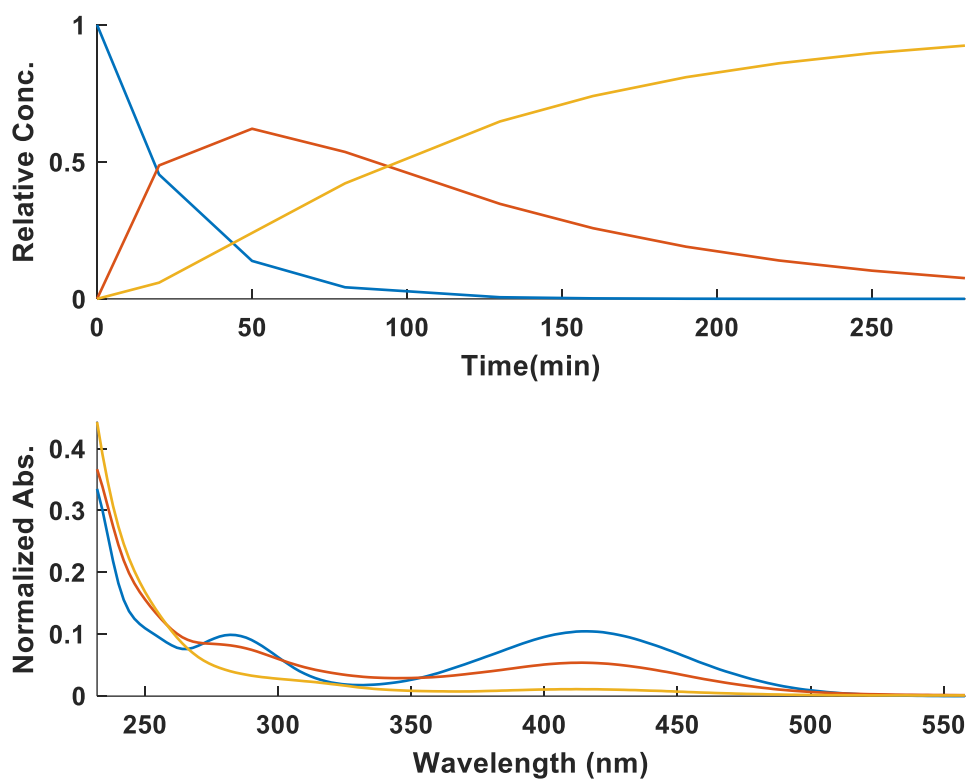


Fig. S5. Resolved profiles for 2-NP in basic media

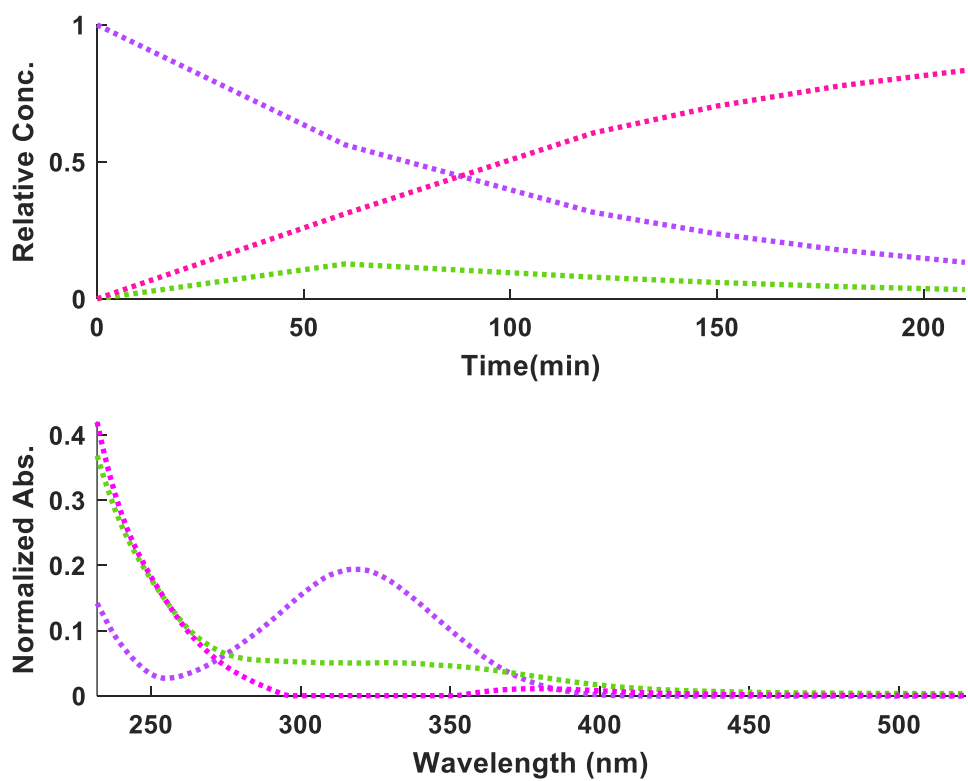


Fig. S6. Resolved profiles for 4-NP in acidic media

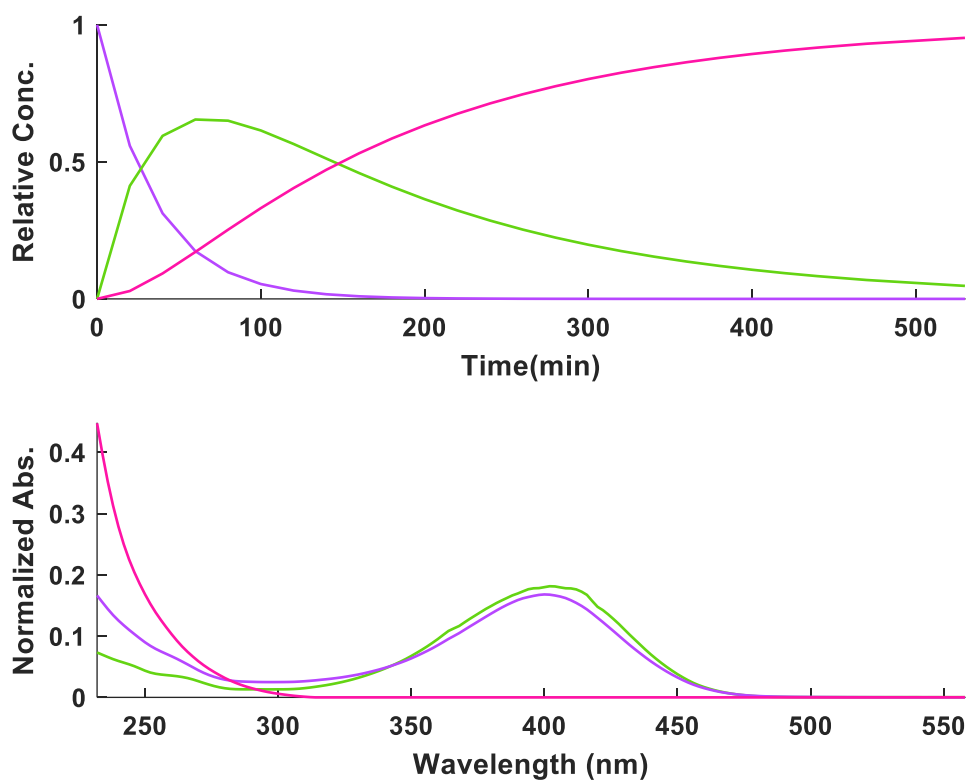


Fig. S7. Resolved profiles for 4-NP in basic media

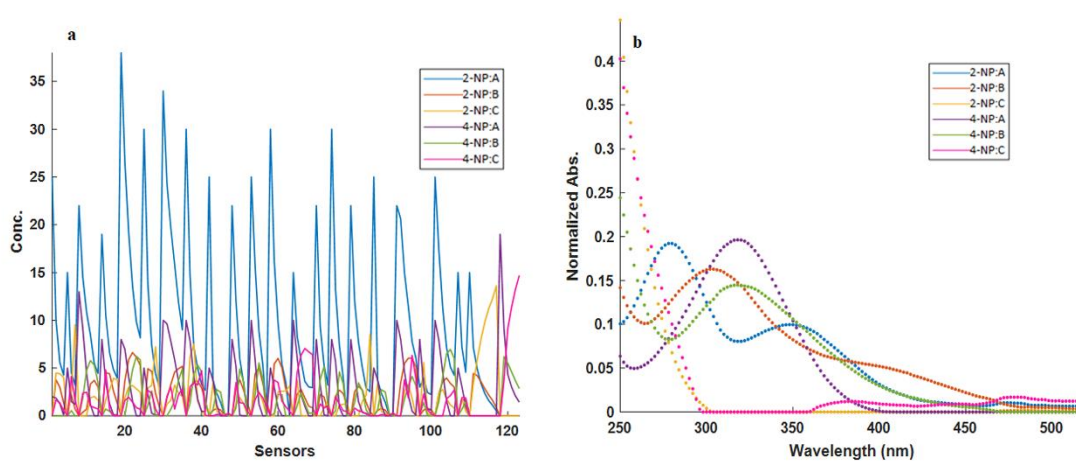


Fig. S8. The acquired profiles in (a) time and (b) wavelength mode by MA-MCR-ALS method for the mixtures of nitrophenols at acidic condition

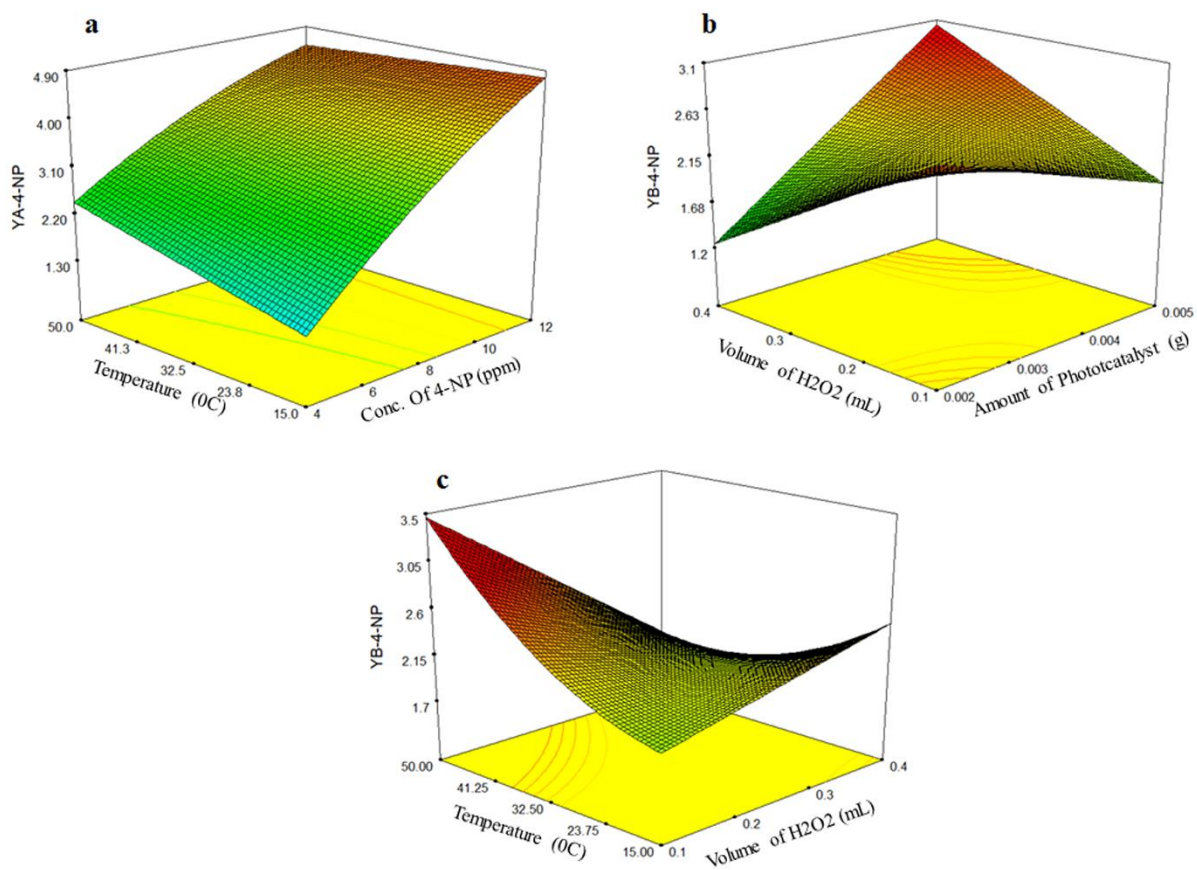


Fig. S9. Response surface for some components of 4-NP in basic condition

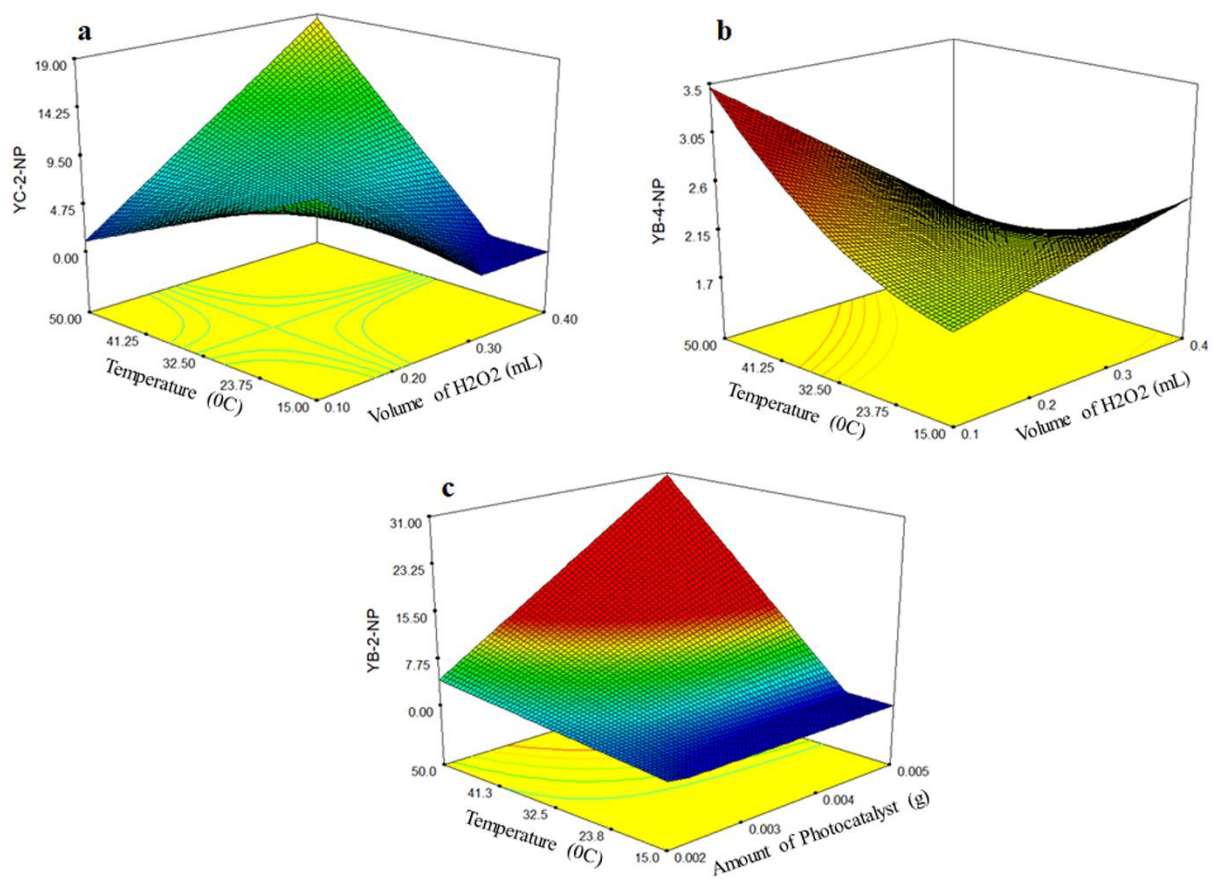


Fig. S10. Response surface for some components of 2-NP and 4-NP in basic condition

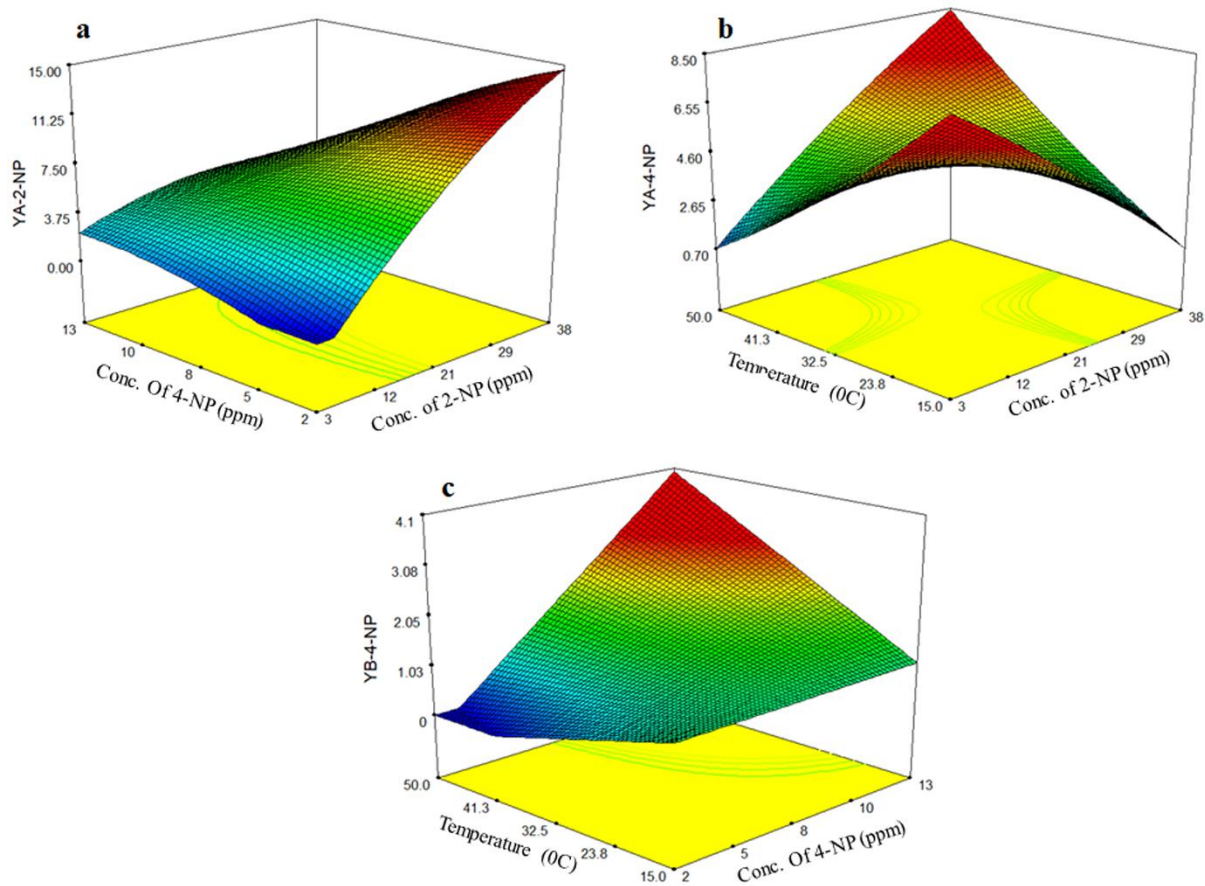


Fig. S11. Response surface for some components of 2-NP and 4-NP in acidic