Support information

$\Delta E = | E_{complex} - E_{C16mimBr} - E_{analyte} |$

TableS1 The energy of each molecule after minimization

Structures	E (kcal mol^{-1})
4-CP	-6.64
2,4-DCP	-7.63
2,4,6-TCP	-4.84
C_{16}mimBr	-61.46
C_{16}mimBr@C_{16}mimBr	-115.75
Complex of C_{16}mimBr and 4-CP	-61.44
Complex of C_{16}mimBr and 2,4-DCP	-75.72
Complex of C_{16}mimBr and 2,4,6-TCP	-73.59
Complex of C_{16}mimBr@C_{16}mimBr and 4-CP	-120.67
Complex of C_{16}mimBr@C_{16}mimBr and 2,4-DCP	-135.93
Complex of C_{16}mimBr@C_{16}mimBr and 2,4,6-TCP	-133.90

Table S2. Main factors, symbols, levels and design matrix for simultaneous optimization of amount of C_{16}mimBr and pH by CCD (MGO-C_{16}mimBr system).

Factor	Symbol	Level				
		-1.41	-1	0	1	1.41
amount of C_{16}mimBr (mg)	X_1	1.8	3.3	6.9	10.5	12
pH	X_2	2	3.4	7	10.5	12
Std	Run	X_1	X_2	Recovery/%		
				4-CP	DCP	TCP
1	4	-1	-1	3.34	26.82	29.34
2	5	1	-1	8.23	30.65	32.35
3	13	-1	1	12.56	61.25	71.36
4	3	1	1	22.75	82.31	90.15
5	7	-1.41	0	8.51	54.02	59.21
6	1	1.41	0	22.58	70.62	78.80
7	9	0	-1.41	2.35	11.73	15.35
8	10	0	1.41	13.64	67.23	78.23
9	2	0	0	20.67	55.20	74.35

10	6	0	0	20.89	54.31	75.69
11	12	0	0	20.21	55.87	76.23
12	11	0	0	21.57	53.73	77.56
13	8	0	0	18.68	55.56	74.89

Table S3. ANOVA table for optimization of amount of C_{16}mimBr and pH (MGO-C_{16}mimBr system).

Response	Recovery/% 4-CP					Recovery/% DCP					Recovery/% TCP				
Source	Sum of Squares	df	Mean Square	F-value	p-value	Sum of Squares	df	Mean Square	F-value	p-value	Sum of Squares	df	Mean Square	F-value	p-value
Model	644.74	5	128.95	59.63	<0.0001	4332.43	5	866.49	528.55	<0.0001	6413.77	5	1282.75	262.54	<0.0001
A-A	152.93	1	152.93	70.73	<0.0001	292.41	1	292.41	178.37	<0.0001	306.34	1	306.34	62.70	<0.0001
B-B	197.08	1	197.08	91.14	<0.0001	3385.77	1	3385.77	2065.31	<0.0001	4453.12	1	4453.12	911.41	<0.0001
AB	7.02	1	7.02	3.25	0.1145	74.22	1	74.22	45.27	0.0003	62.25	1	62.25	12.74	0.0091
A^2	41.48	1	41.48	19.18	0.0032	86.80	1	86.80	52.95	0.0002	105.48	1	105.48	21.59	0.0024
B^2	268.88	1	268.88	124.35	<0.0001	432.80	1	432.80	264.01	<0.0001	1565.50	1	1565.50	320.41	<0.0001
Residual	15.14	7	2.16			11.48	7	1.64			34.20	7	4.89		
Lack of Fit	10.46	3	3.49	2.98	0.1593	8.30	3	2.77	3.48	0.1297	27.99	3	9.33	6.01	0.0579
Pure Error	4.68	4	1.17			3.18	4	0.79			6.21	4	1.55		
Cor Total	659.87	12				4343.91	12				6447.97	12			
Standard deviation			1.47					1.28					2.21		
Coefficient of			9.75					2.45					3.45		

variation			
R^2	0.9771	0.9974	0.9947
Adjusted R^2	0.9607	0.9955	0.9909
Adequate precision	21.476	82.129	52.074

Table S4. Main factors, symbols, levels and design matrix for simultaneous optimization of amount of C_{16}mimBr and pH by CCD (Fe_3O_4NPs@C_{16}mimBr system).

Factor	Symbol	Level				
		-1.41	-1	0	1	1.41
amount of C_{16}mimBr (mg)	X_1	0.8	1.84	4.4	6.95	8
pH	X_2	2	3.4	7	10.5	12
Std	Run	X_1	X_2	Recovery/%		
				4-CP	DCP	TCP
1	3	-1	-1	2.56	22.78	28.89
2	7	1	-1	8.21	20.21	26.23
3	8	-1	1	11.89	45.23	56.35
4	1	1	1	20.92	50.51	65.56
5	5	-1.41	0	7.56	41.23	52.35
6	6	1.41	0	20.68	43.62	56.32
7	4	0	-1.41	1.64	10.56	15.74
8	12	0	1.41	14.50	46.30	60.59
9	10	0	0	18.69	64.93	71.38
10	9	0	0	16.79	63.85	73.68
11	13	0	0	18.32	63.72	72.23
12	2	0	0	20.43	63.81	72.51
13	11	0	0	18.68	64.29	71.85

Table S5. ANOVA table for optimization of amount of C_{16}mimBr and pH (Fe_3O_4NPs@C_{16}mimBr system).

Response	Recovery/% DCP					Recovery/% TCP								
Source	Sum of Squares	df	Mean Square	F-value	p-value	Sum of Squares	Df	Mean Square	F-value	p-value	Sum of Squares	df	Mean Square	F-Value	p-value
Model	559.13	5	111.83	75.11	<0.0001	4148.91	5	829.78	2083.04	<0.0001	4690.53	5	938.11	527.00	<0.0001
A-A	138.18	1	138.18	92.82	<0.0001	4.64	1	4.64	11.64	0.0113	18.50	1	18.50	10.39	0.0146
B-B	203.41	1	203.41	136.63	<0.0001	1337.71	1	1333.71	3348.06	<0.0001	2119.57	1	2119.57	1190.71	<0.0001
AB	2.86	1	2.86	1.92	0.2086	15.41	1	15.41	38.67	0.0004	35.22	1	35.22	19.79	0.0030
A^2	35.98	1	35.98	24.16	0.0017	846.91	1	846.91	2126.04	<0.0001	627.25	1	627.25	352.37	<0.0001
B^2	197.01	1	197.01	132.33	<0.0001	2261.75	1	2261.75	5677.75	<0.0001	2150.11	1	2150.11	1207.86	<0.0001
Residual	10.42	7	1.49			2.79	7	0.40			12.46	7	1.78		
Lack of Fit	3.71		1.24	0.74	0.5831	1.77	3	0.59	2.33	0.2155	9.46	3	3.15	4.21	0.0994
Pure Error	6.72		1.68			1.01	4	0.25			3.00	4	0.75		
Cor Total	569.55					4151.70	12				4702.99	12			
Standard deviation			1.22					0.63					1.33		
Coefficient of variation			6.77					1.37					2.40		
R^2			0.9617					0.9993					0.9974		
Adjusted R^2			0.9666					0.9988					0.9955		

Adequate precision	24.395	126.690	64.188

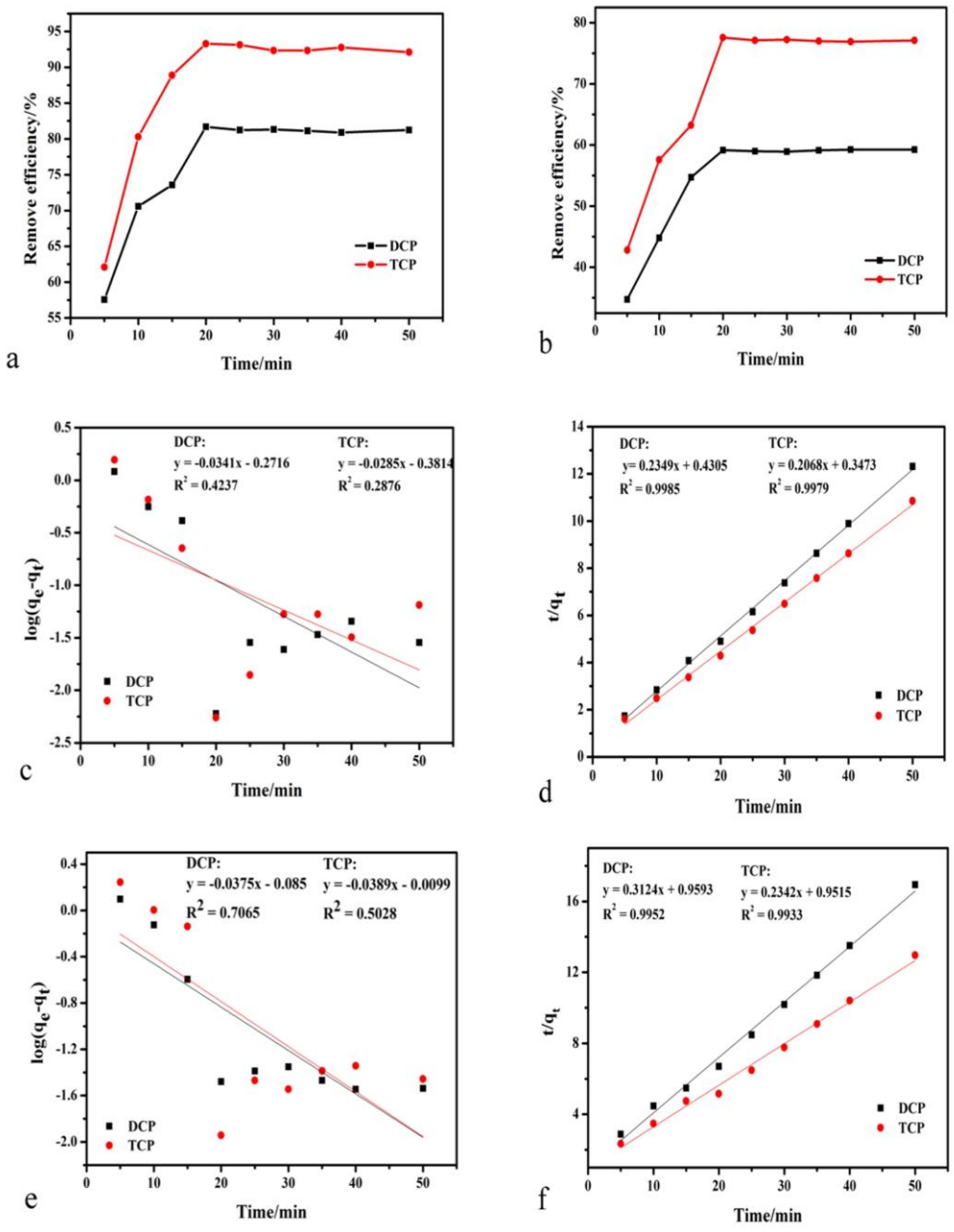

Fig. S1 adsorption kinetic studies: Influence of contact time on removal efficiency of CPs for MGO sorbent (a); influence of contact time on removal efficiency of CPs for magnetic sorbent (b); pseudo-first order model for CPs of MGO sorbent (c); pseudo-second order model for CPs of MGO sorbent (d); pseudo-first order model for CPs of magnetic sorbent (e); pseudo-second order model for CPs of magnetic sorbent (f).

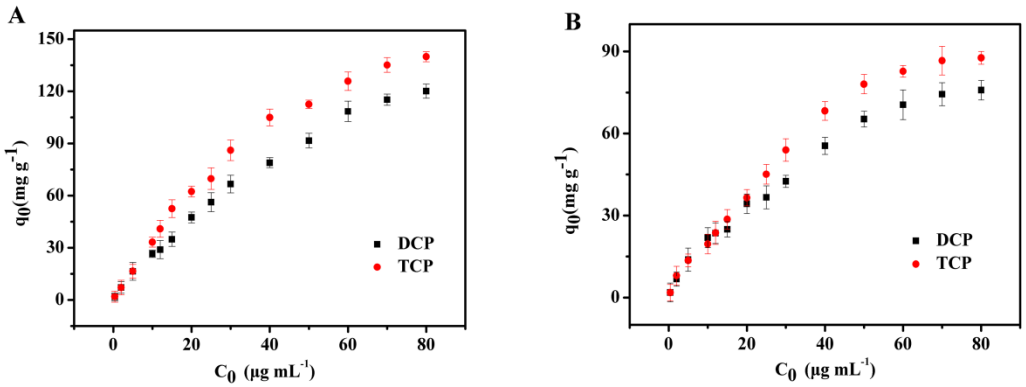

Fig. S2 Adsorption isotherm of CPs on MGONPs(A) and Fe_3O_4NPs(B).