Supplementary Data

Reverse-phase high performance liquid chromatography separation of positional isomers on the MIL-53(Fe) packed column

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SUMMARY

This supporting information file includes additional results and informations as described in the text of the main article. Including:

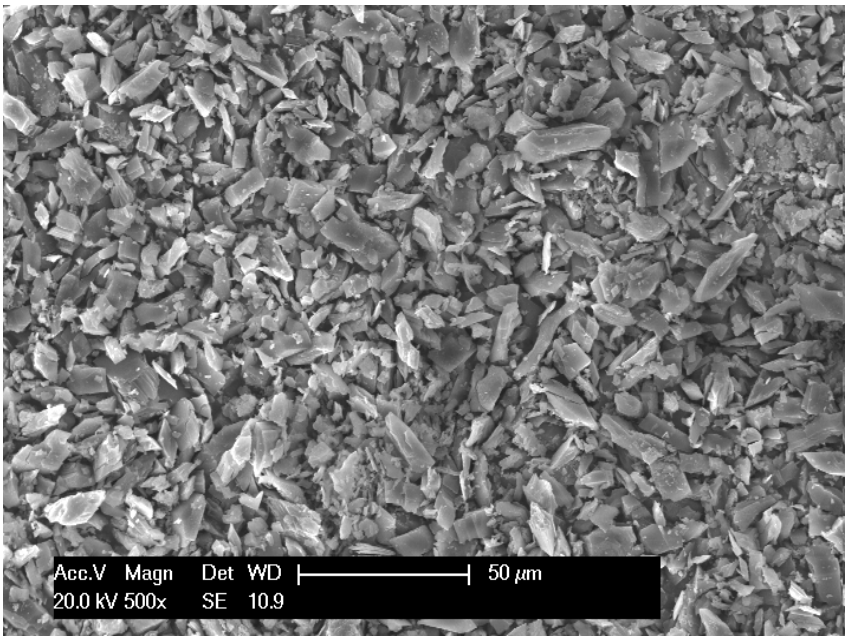

Fig. S1. SEM images of MIL-53(Fe) after HPLC analysis

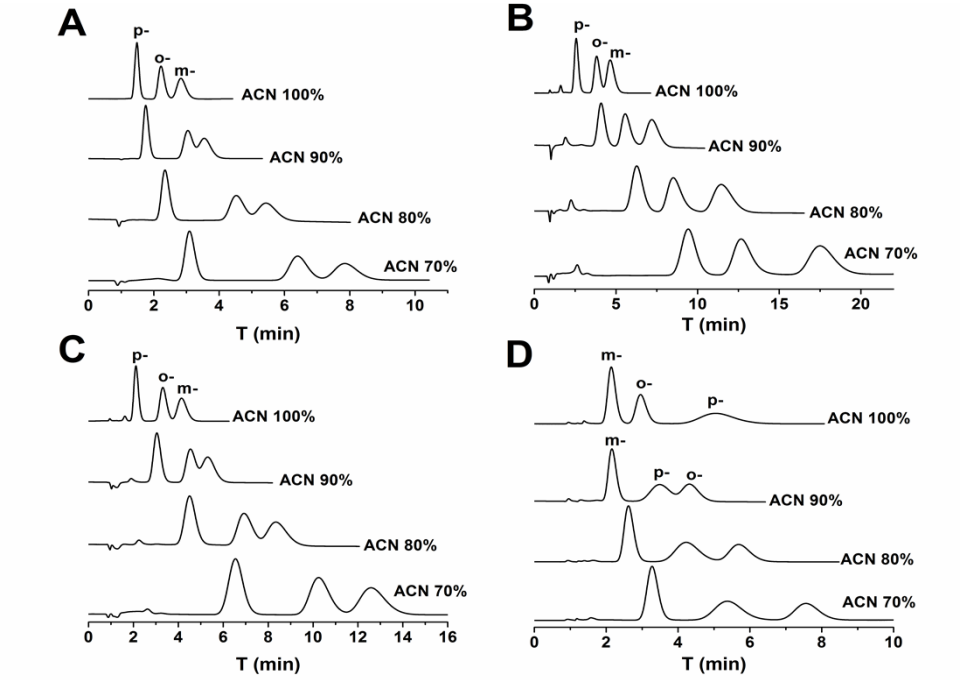

Fig. S2. HPLC chromatograms for the separation of : (A) xylene; (B) dichlorobenzene; (C) chlorotuluene; (D) nitroanline on the MIL-53(Fe) packed column using different ratios of ACN/H_2O as the mobile phase at a flow rate of 0.6 mL min^{-1}. All the separations were performed at room temperature and monitored with a UV detector at 254 nm.

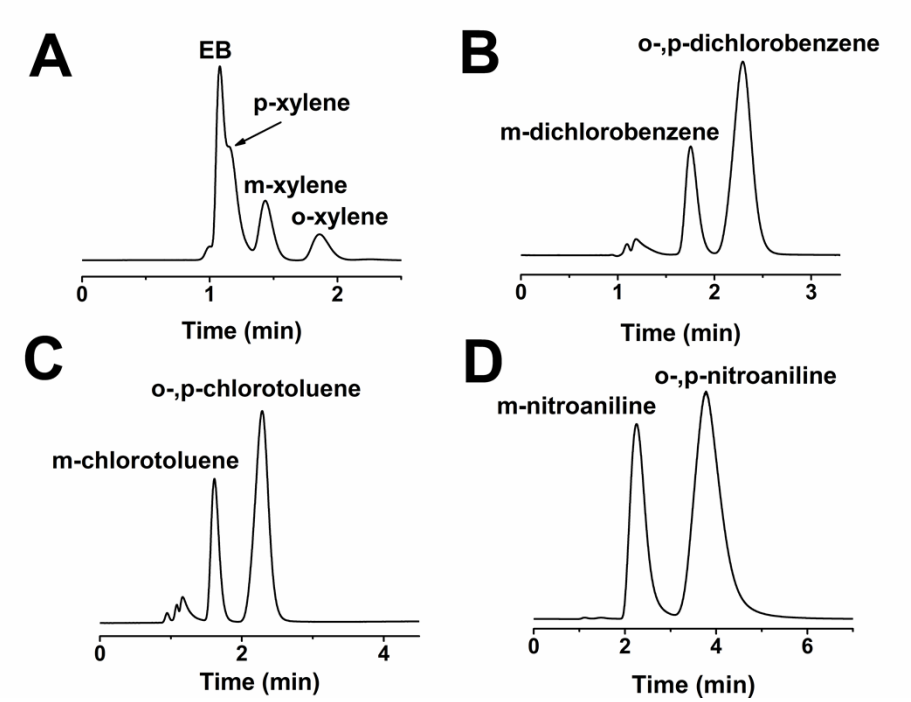

Fig. S3. HPLC chromatograms on the MIL-53(Al) packed column for the separation of (A) xylene isomers; (B) dichlorobenzene isomers; (C) chlorotuluene isomers; (D) nitroanline isomers using 100% ACN as the mobile phase at a flow rate of 0.6 mL min^{-1}. All the separations were performed at room temperature and monitored with a UV detector at 254 nm.

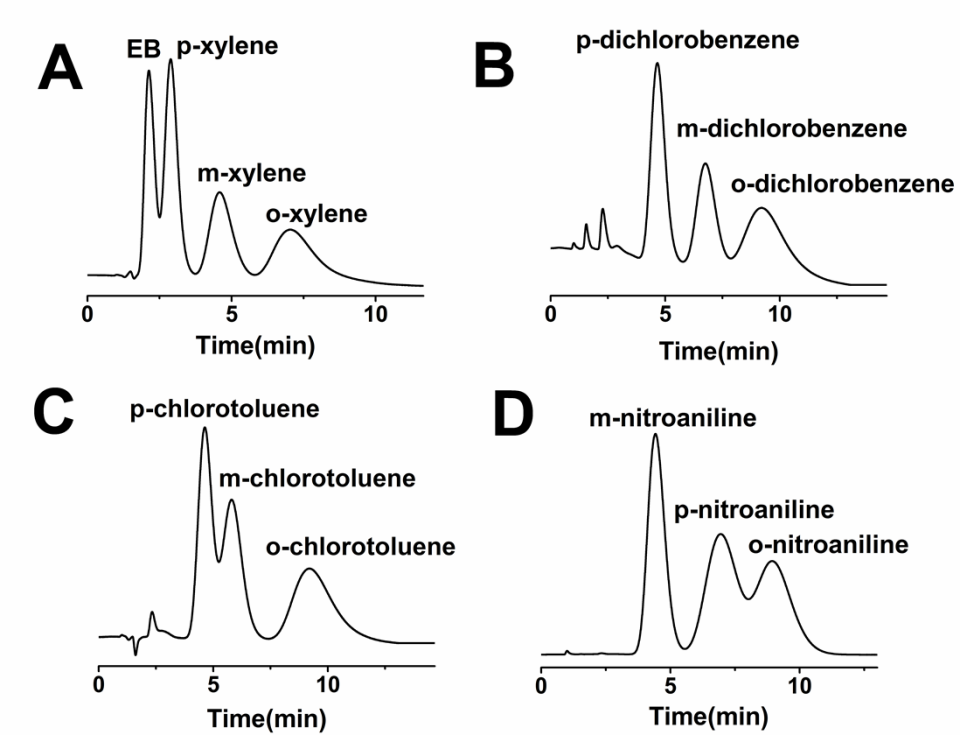

Fig. S4. HPLC chromatograms on the MIL-53(Cr) packed column for the separation of (A) xylene isomers; (B) dichlorobenzene isomers; (C) chlorotuluene isomers; (D) nitroanline isomers using 100% ACN as the mobile phase at a flow rate of 0.6 mL min^{-1}. All the separations were performed at room temperature and monitored with a UV detector at 254 nm.

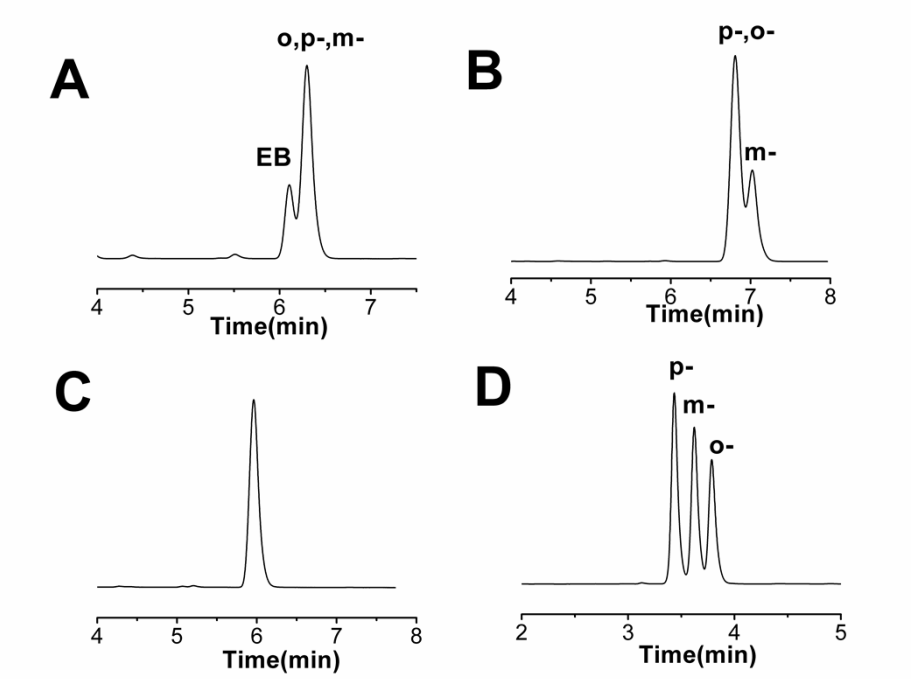

Fig. S5. HPLC chromatograms on the C8 column (25-cm long × 4.0-mm i.d., 5 μm): (A) EB and xylene using CH_3CN/H_2O (50:50) as the mobile phase (B) Dichlorobenzene isomers using CH_3CN/H_2O (70:30) as the mobile phase. (C) Chlorotoluene isomers using CH_3CN/H_2O (60:40) as the mobile phase; (D) Nitroanline isomers using CH_3CN/H_2O (60:40) as the mobile phase. Flow rate: 1.0 mL min^{-1}. All the separations were performed at room temperature and monitored with a UV detector at 254 nm.

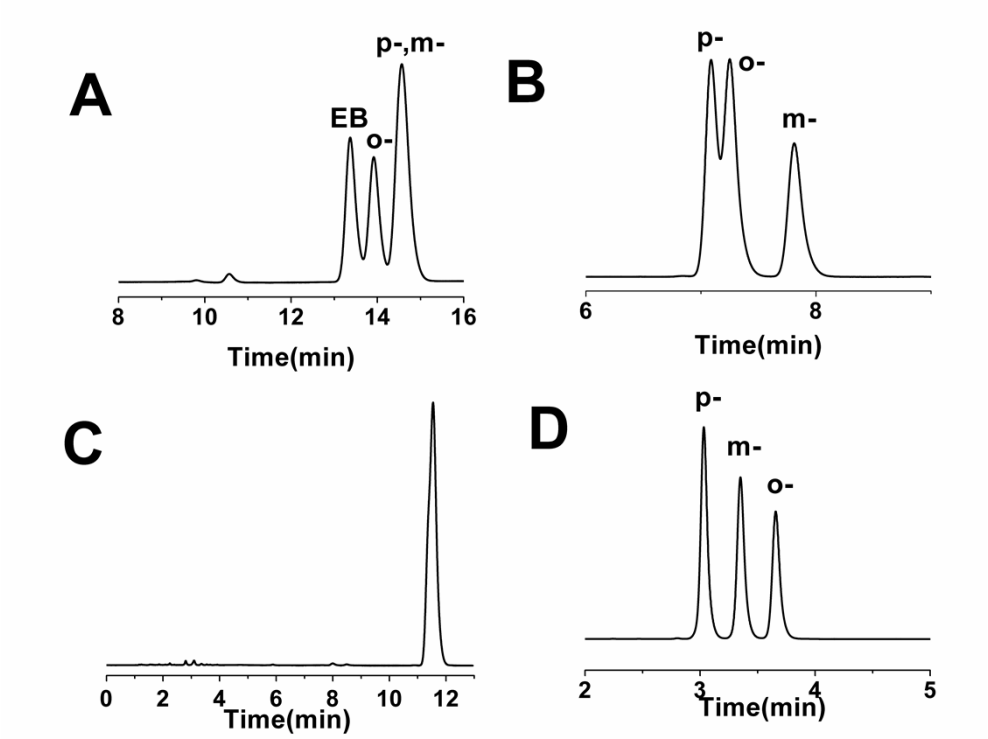

Fig. S6. HPLC chromatograms on the C18 column (25-cm long × 4.0-mm i.d., 5 μm): (A) EB and xylene using CH_3CN/H_2O (70:30) as the mobile phase (B) Dichlorobenzene isomers using CH_3CN/H_2O (70:30) as the mobile phase. (C) Chlorotoluene isomers using CH_3CN/H_2O (70:30) as the mobile phase; (D) Nitroanline isomers using CH_3CN/H_2O (70:30) as the mobile phase. Flow rate: 1.0 mL min^{-1}. All the separations were performed at room temperature and monitored with a UV detector at 254 nm.

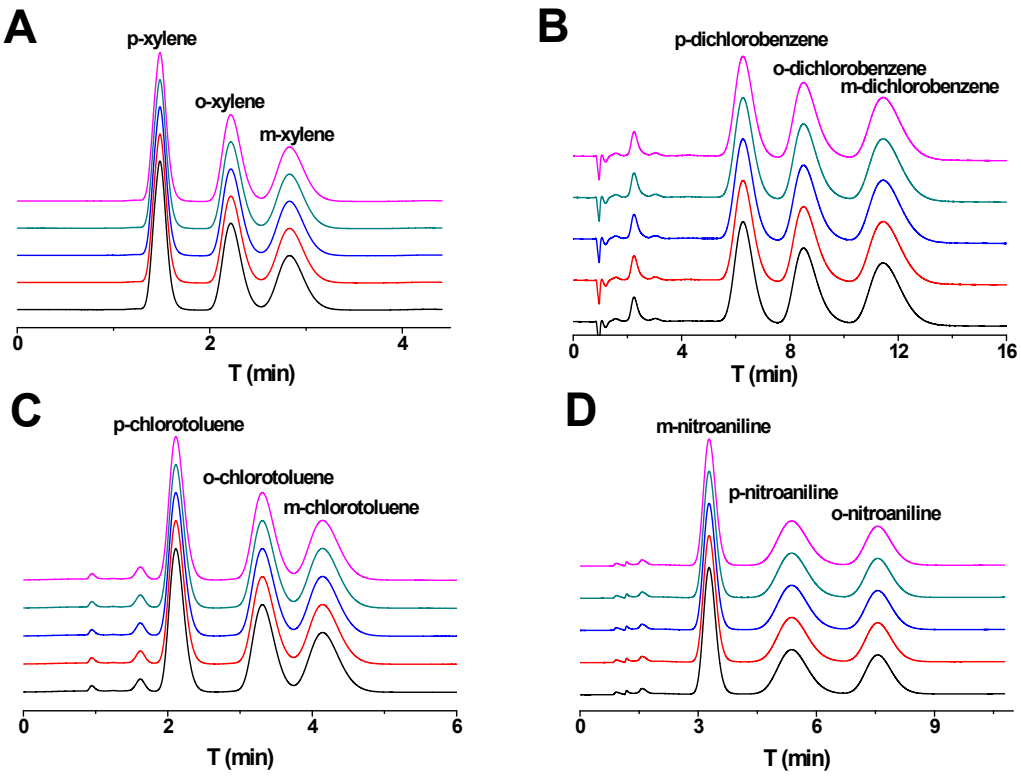

Fig.S7. Reproducibility of the chromatograms for HPLC on MIL-53(Fe) packed column: (A) xylene isomers using ACN/H_2O (100:0) as the mobile phase; (B) dichlorobenzene isomers using ACN/H_2O (80:20) as the mobile phase; (C) chlorotuluene isomers using ACN/H_2O (100:0) as the mobile phase; (D) nitroanline isomers using ACN/H_2O (70:30) as the mobile phase at a flow rate of 0.6 mL min^{-1}. All the separations were performed at room temperature and monitored with a UV detector at 254 nm.

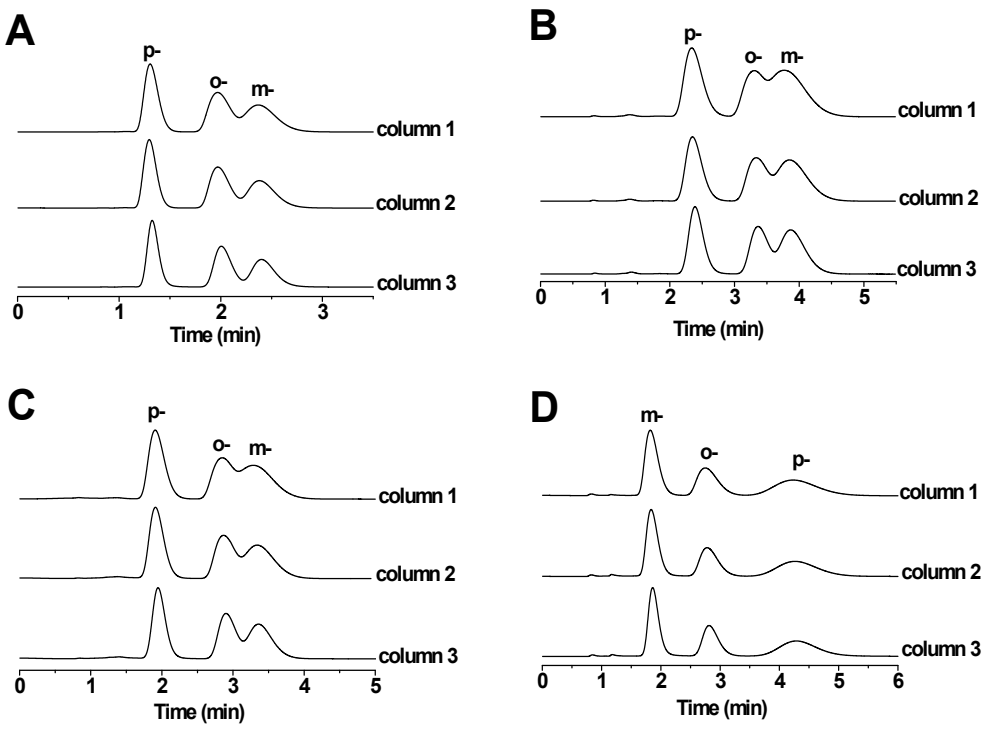

Fig.S8. Column-to-column reproducibility of the chromatograms for HPLC on MIL-53(Fe) packed columns: (A) xylene isomers, (B) dichlorobenzene isomers, (C) chlorotuluene isomers and (D) nitroanline isomers at 25°C using 100% ACN as the mobile phase at a flow rate of 0.6 mL min^{-1}. All the signals were monitored with a UV detector at 254nm.

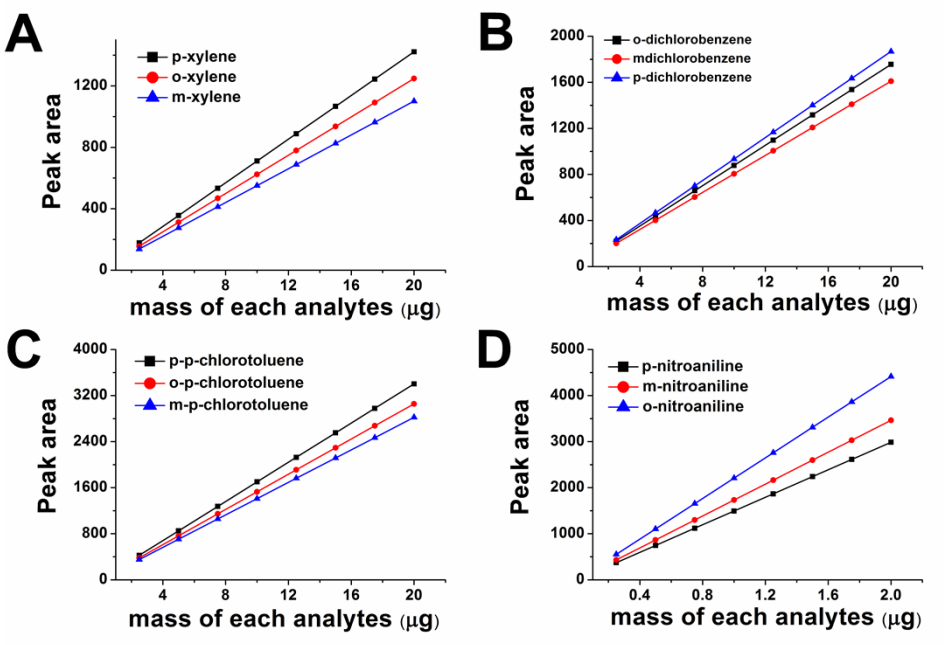

Fig.S9. Effects of mass on the peak area: (A) EB and p-, m- and o-xylene; (B) p-, m- and o-dichlorobenzene; (C) p-, m- and o- chlorotuluene; (D) p-, m- and o- nitroanline. Condition see Fig. S7.

Table S1 Resolutions of xylene, dichlorobenzene, chlorotoluene and nitroaniline isomers on the MIL-53(Fe) packed column in different mobile phase. Conditions see Fig. S2.

Composition of mobile phase (ACN/H_2O)	Resolution *(Rs)*							
	xylene		dichlorobenzene		chlorotoluene		nitroaniline	
	o/p	*m/o*	*o/p*	*m/o*	*o/p*	*m/o*	*p/m*	*o/p*
100:0	2.5	1.45	2.22	1.2	2.45	1.4	-	-
90:10	3.0	0.86	1.37	1.32	1.9	0.8	1.45	0.91
80:20	3.33	1.01	1.86	2.04	2.1	1.07	1.93	1.34
70:30	4.24	1.44	2.22	2.6	2.89	1.55	2.26	1.8
60:40	5.16	1.84	2.3	2.94	3.58	1.9	2.69	2.37

Table S2 Selectivity of xylene, dichlorobenzene, chlorotoluene and nitroaniline isomers on the MIL-53(Fe) packed column in the temperature range of 25–75°C. Separation conditions as shown in Fig. 4.

T/°C	Selectivity (α)							
	xylene		dichlorobenzene		chlorotoluene		nitroaniline	
	o/p	*m/o*	*o/p*	*m/o*	*o/p*	*m/o*	*p/m*	*o/p*
25	2.33	1.33	1.86	1.22	1.63	1.20	1.81	1.91
35	2.28	1.15	1.75	1.10	1.53	1.11	1.84	1.80
45	2.27	1.08	1.67	1.03	1.45	1.04	1.89	1.64
55	2.29	0.98	1.64	0.94	1.38	0.98	1.91	1.50
65	2.20	0.91	1.60	0.88	1.34	0.94	1.95	1.35
75	2.20	0.85	1.59	0.82	1.32	0.89	1.96	1.21

Table S3 Selectivities of xylene, dichlorobenzene, chlorotoluene and nitroaniline isomers on the C8 and C18 columns.

column	Selectivity (α)							
	xylene		dichlorobenzene		chlorotoluene		nitroaniline	
	p/o	*m/o*	*o/p*	*m/o*	*o/p*	*m/o*	*m/p*	*o/m*
C8 column	1.0	1.0	1.0	1.07	1.0	1.06	1.8	1.4
C18 column	1.3	1.0	1.2	1.7	1.0	1.0	1.60	1.58

Table S4 Column efficiency of MIL-53(Fe) packed column and C18 column for nitroanline isomers. Separation conditions see Fig.S7 and Fig.S6 respectively.

Analytes	Column efficiency (plates m^{-1})	
	MIL-53(Fe)	C18
m-nitroanline	2331	50464
p-nitroanline	1480	48665
o-nitroanilie	3272	55158

Table S5 Column-to-column reproducibility of the MIL-53(Fe) packed columns.

analytes	RSD (%) (n=3)			
	retention time	peak area	Peak high	half peak width
p-xylene	1.13	1.50	10.49	8.18
o-xylene	1.02	0.75	11.11	10.91
m-xylene	0.68	2.66	12.54	10.52
p-dichlorobenzene	1.13	2.42	11.91	10.43
o-dichlorobenzene	0.87	6.26	6.69	13.3
m-dichlorobenzene	1.39	6.90	14.36	9.67
p-chlorotoluene	1.15	1.97	10.83	9.88
o-chlorotoluene	0.90	4.14	9.20	13.17
m-chlorotoluene	1.13	4.14	13.93	9.98
m-nitroaniline	1.09	5.37	11.69	14.44
p- nitroaniline	1.15	5.64	12.97	17.01
o- nitroaniline	1.31	4.87	5.53	10.62