

Supplementary Information

Application of a Zn(II) based metal-organic framework as an efficient solid-phase extraction sorbent for preconcentration of plasticizer compounds

Elham Tahmasebi, Mohammad Yaser Masoomi, Yadollah Yamini and Ali Morsali*

Department of Chemistry, Faculty of Sciences, Tarbiat Modares University, Tehran,
Islamic Republic of Iran

Email: Morsali_a@modares.ac.ir, Morsali_a@yahoo.com

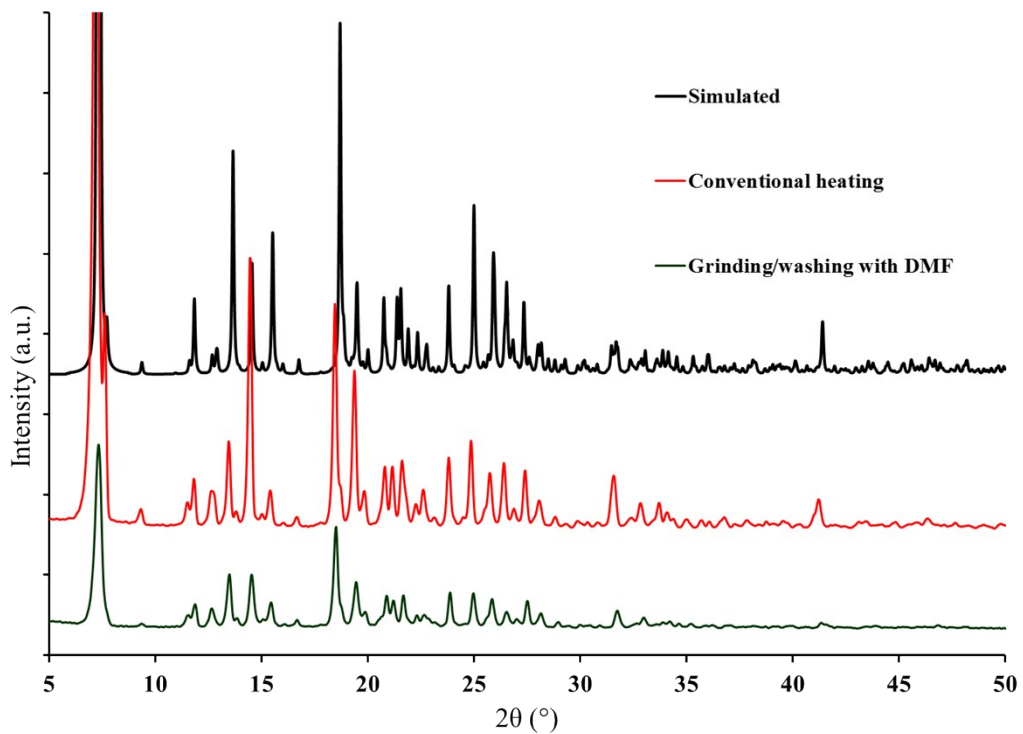


Fig. S1. Comparison of PXR D for TMU-6: simulated; solvothermal synthesis; mechanothesized after washing with DMF.

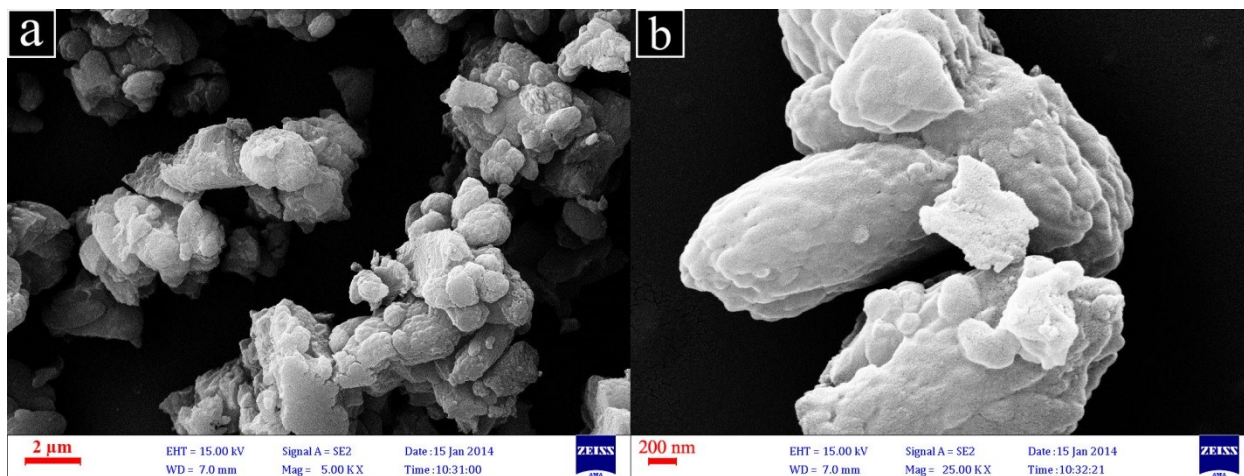


Fig. S2. (a) and (b), FE-SEM images of TMU-6 synthesized by mechanochemical reaction.

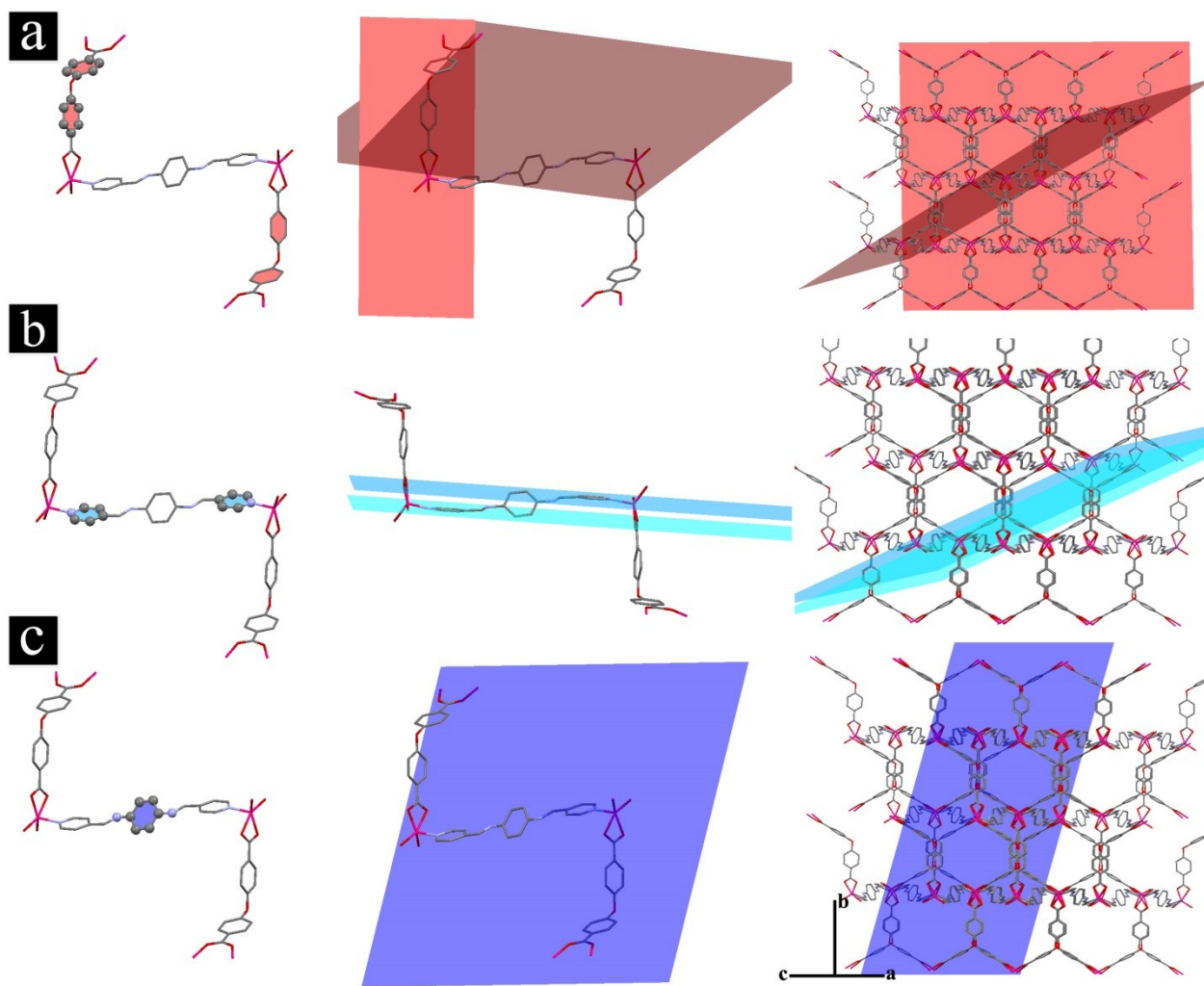


Fig. S3. Representation of phenyl rings of (a) oba and (b and c) 4-bpmb ligands in the pore walls of TMU-6.

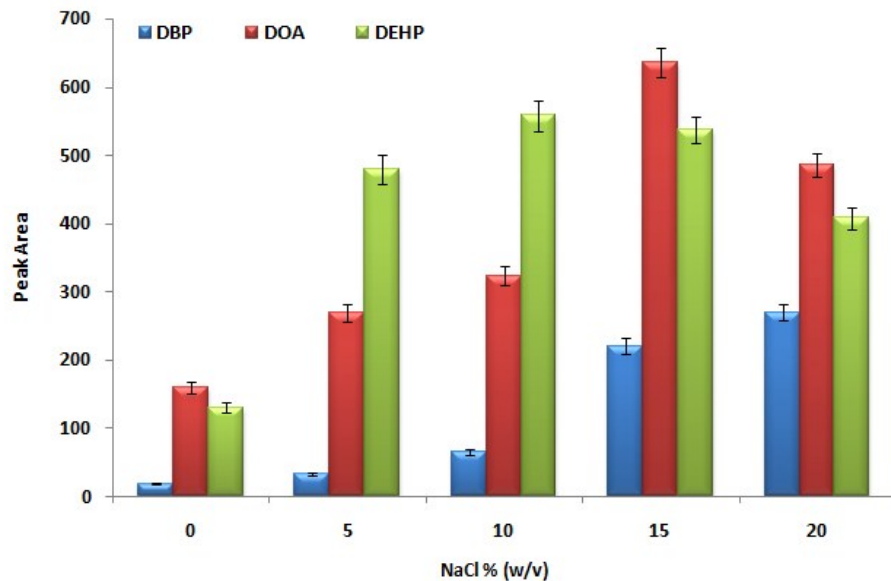


Fig.S4. Effect of NaCl concentration on extraction efficiency. Extraction conditions: sample solution, 30 mL of 100 $\mu\text{g L}^{-1}$ of target analytes; MOF, 4 mg; eluent, 100 μL of ethyl acetate; extraction time, 5 min; desorption time, 1 min.

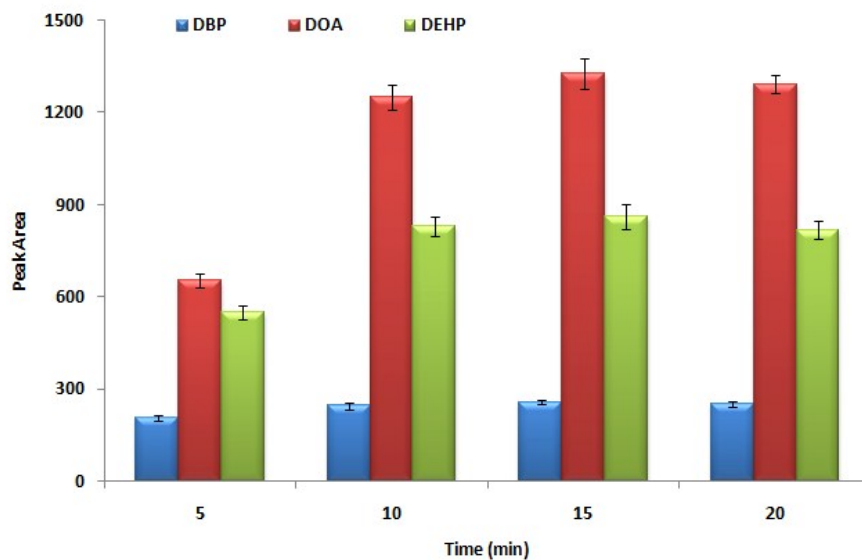


Fig.S5. Effect of extraction time on extraction efficiency. Extraction conditions: sample solution, 30 mL of $100 \mu\text{g L}^{-1}$ of target analytes and 15% (w/v) NaCl; MOF, 4 mg; eluent, 100 μL of ethyl acetate; desorption time, 1 min.

Table S1. Experimental factors, levels and matrix of the orthogonal and rotatable centered central composite design for determination of plasticizers by the proposed SPE method.

Factors	Symbol	Levels				
		$-\alpha$	-1	0	+1	$+\alpha$
Adsorbent amount (mg)	A	3.0	4.0	5.5	7.0	8.0
Sample volume (mL)	B	50	70	100	130	150
Eluent volume (μ L)	C	99	140	200	260	301

Run	A	B	C	Response
1	5.5	50	200	48.4
2	4.0	70	260	12.6
3	5.5	100	200	32.5
4	5.5	100	200	30.0
5	5.5	100	200	28.5
6	5.5	100	200	30.9
7	5.5	100	200	35.7
8	5.5	100	200	27.4
9	8.0	100	200	51.6
10	5.5	100	301	29.5
11	5.5	150	200	4.0
12	3.0	100	200	19.9
13	4.0	130	140	13.2
14	7.0	70	260	39.9
15	7.0	130	140	26.2
16	4.0	70	140	45.7
17	5.5	100	200	36.9
18	7.0	70	140	62.5
19	5.5	100	200	34.7
20	5.5	100	99	57.8
21	5.5	100	200	27.5
22	7.0	130	260	21.9
23	4.0	130	260	5.4

Table S2. Analysis of variance table (ANOVA) for response surface model.

Source	Sum of squares	d.f. ^a	Mean square	F-value	p-value Prob> F	Effect ^b
Model	4832.622	9	536.958	25.6135	< 0.0001	S
A-A : Adsorbent amount	1179.963	1	1179.96	56.2855	< 0.0001	S (+)
B-B : Sample volume	2086.285	1	2086.29	99.5179	< 0.0001	S (-)
C-C: Eluent volume	969.8208	1	969.821	46.2615	< 0.0001	S (-)
AB	26.43665	1	26.4367	1.26106	0.2818	NS
AC	24.42486	1	24.4249	1.16509	0.3000	NS
BC	238.268	1	238.268	11.3656	0.0050	S (+)
A ²	0.013958	1	0.01396	0.00067	0.9798	NS
B ²	178.2485	1	178.248	8.50264	0.0120	S (-)
C ²	127.0623	1	127.062	6.061	0.0286	S (+)
Residual	272.5308	13	20.9639			
Lack of Fit	170.6215	5	34.1243	2.6788	0.1038	NS
Pure Error	101.9093	8	12.7387			
Total Corr.	5105.153	22				

^a Degree of freedom

^b S(+): significant with positive effect, S(-): significant with negative effect, NS: not significant

F-value of the model ($F_{\text{model}} = 25.6135$) was much greater than the critical F-value with the same number of degrees of freedom ($F_{0.05 (9,13)} = 2.71$), indicating that the treatment differences are highly significant.