

Supplementary Materials

Nanostructured metal-organic frameworks, TMU-4, TMU-5, and TMU-6 as a novel adsorbents for solid phase microextraction of polycyclic aromatic hydrocarbons

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Table S1. _____

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Design matrix of central composite design (CCD) for optimization of HS-SPME parameters.

Std	Run	Extraction temperature (°C)	Extraction time (min)	Ionic strength (%w/v)	Stirring rate (rpm)
7	1	50	35	27	300
27	2	60	25	18	600
4	3	70	35	9	300
1	4	50	15	9	300
26	5	60	25	18	600
13	6	50	15	27	900
9	7	50	15	9	900
12	8	70	35	9	900
20	9	60	45	18	600
5	10	50	15	27	300
24	11	60	25	18	1200
19	12	60	5	18	600
16	13	70	35	27	900
11	14	50	35	9	900
29	15	60	25	18	600
23	16	60	25	18	0
25	17	60	25	18	600
15	18	50	35	27	900
22	19	60	25	36	600
30	20	60	25	18	600
17	21	40	25	18	600
14	22	70	15	27	900
3	23	50	35	9	300
8	24	70	35	27	300
21	25	60	25	0	600
18	26	80	25	18	600
10	27	70	15	9	900
28	28	60	25	18	600
2	29	70	15	9	300
6	30	70	15	27	300

Table S2.

Factors and levels of the experimental design.

Factors	Unit	Levels			Star point $\alpha = 2.0$	
		Lower	Central	Upper	$-\alpha$	$+\alpha$
Extraction temperature	°C	50	60	70	40	80
Extraction time	min	15	25	35	5	45
Ionic strength	%w/v	9	18	27	0	36
Stirring rate	rpm	300	600	900	0	1200

Table S3.

ANOVA results for the optimization of HS-SPME of PAHs.

Source	Sum of Squares	Degree of Freedom	Mean Square	F-value	p-value Prob > F	
Model	6.94×10^7	14	4.96×10^6	11.77	< 0.0001	Significant
A-Extraction temperature	8.58×10^6	1	8.58×10^6	20.37	0.0004	
B-Extraction time	1.28×10^7	1	1.28×10^7	30.34	< 0.0001	
C-Ionic strength	4.21×10^6	1	4.21×10^6	10.00	0.0064	
D-Stirring rate	8.94×10^5	1	8.94×10^5	2.12	0.1657	
AB	19951.56	1	19951.56	0.047	0.8307	
AC	7.67×10^5	1	7.67×10^5	1.82	0.1973	
AD	96565.56	1	96565.56	0.23	0.6390	
BC	1.80×10^5	1	1.80×10^5	0.43	0.5237	
BD	64643.06	1	64643.06	0.15	0.7008	
CD	19951.56	1	19951.56	0.047	0.8307	
A ²	3.90×10^7	1	3.90×10^7	92.56	< 0.0001	
B ²	3.26×10^6	1	3.26×10^6	7.74	0.0139	
C ²	10982.86	1	10982.86	0.026	0.8739	
D ²	13719.07	1	13719.07	0.033	0.8592	
Residual	6.32×10^6	15	4.21×10^5			
Lack of Fit	5.43×10^6	10	5.43×10^5	3.06	0.1144	Not significant
Pure Error	8.87×10^5	5	1.77×10^5			
Cor Total	7.57×10^7	29				

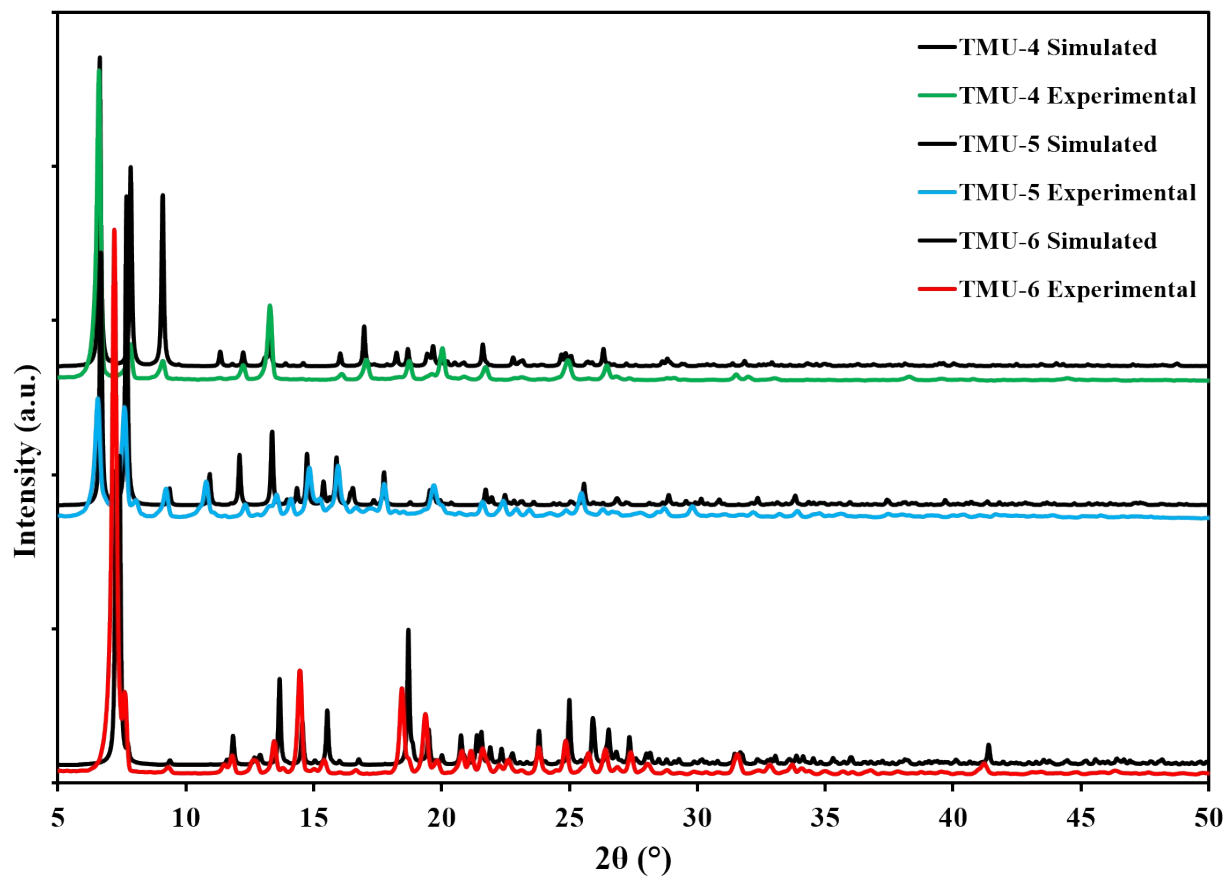


Fig. S1: Comparison of XRD patterns for TMU-4, TMU-5 and TMU-6.

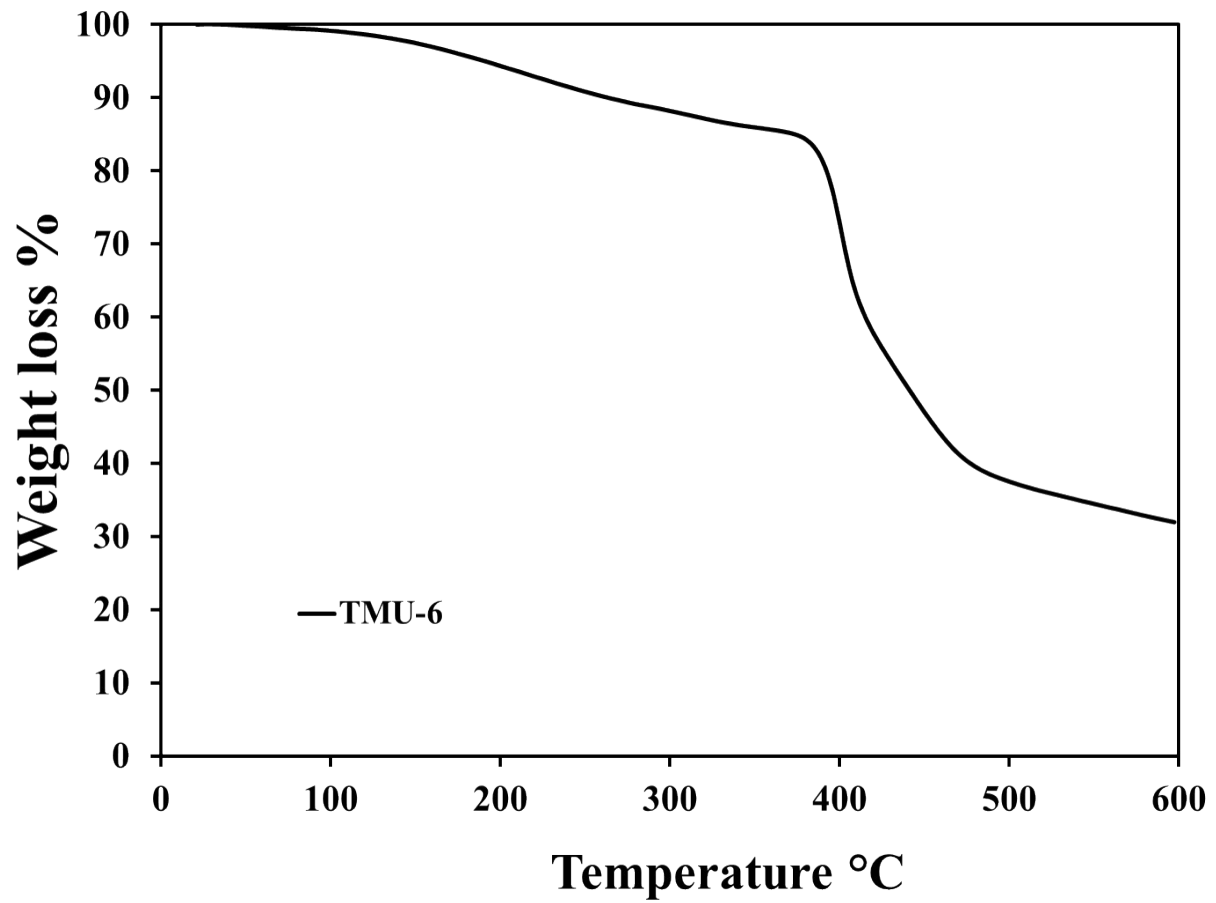


Fig. S2: Thermogravimetric profile of TMU-6.

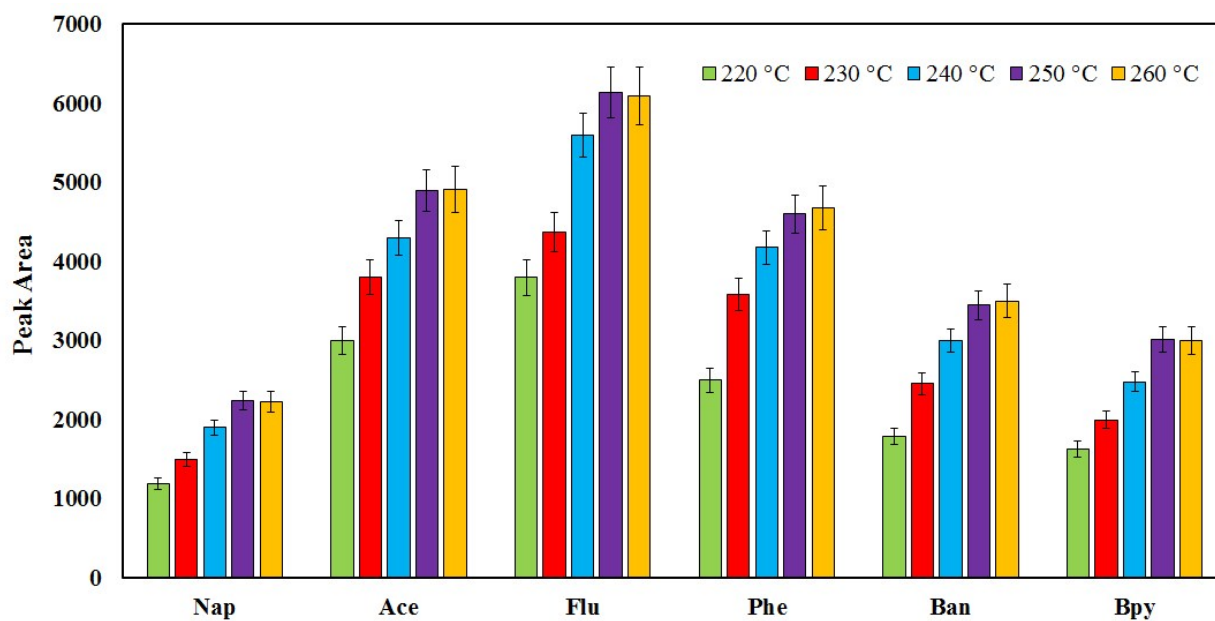


Fig. S3. Effect of desorption temperature on the extraction efficiency. Conditions: Extraction temperature, 60 °C; extraction time, 20 min; salt, 20 %w/v; stirring rate 600 rpm.

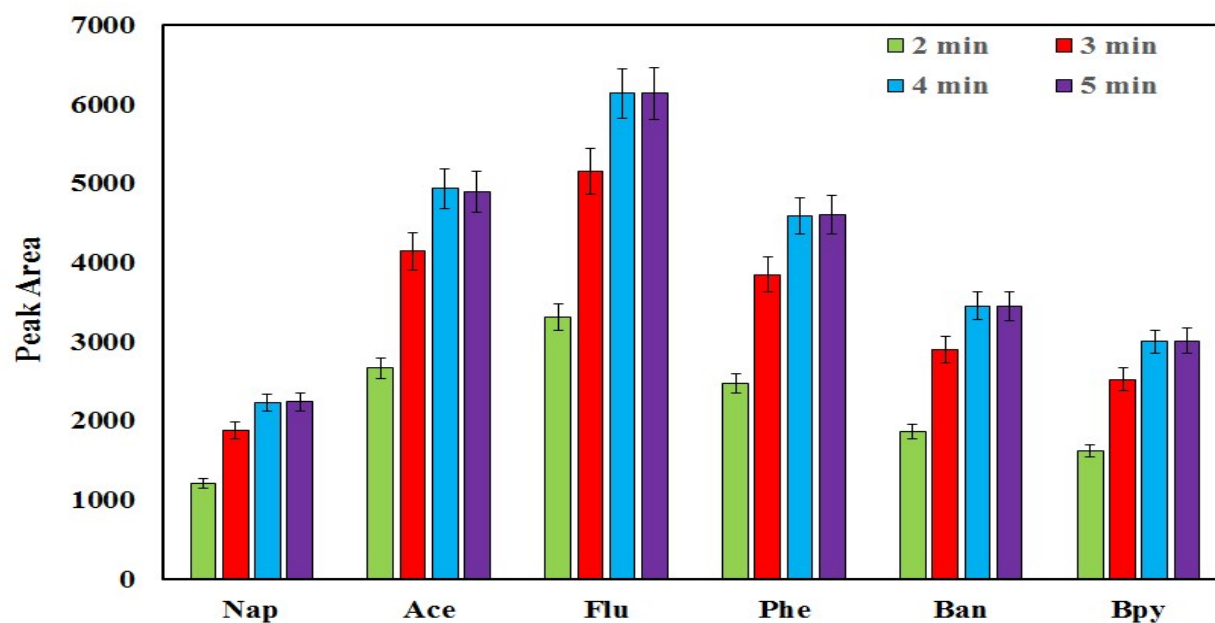


Fig. S4. Effect of desorption time on the extraction efficiency. Conditions: Extraction temperature, 60 °C; extraction time, 20 min; salt, 20 %w/v; stirring rate 600 rpm; desorption temperature, 250 °C.