

Supporting Information

Ordered mesoporous polymer in-situ coated on stainless steel wire for highly sensitive solid phase microextraction fiber

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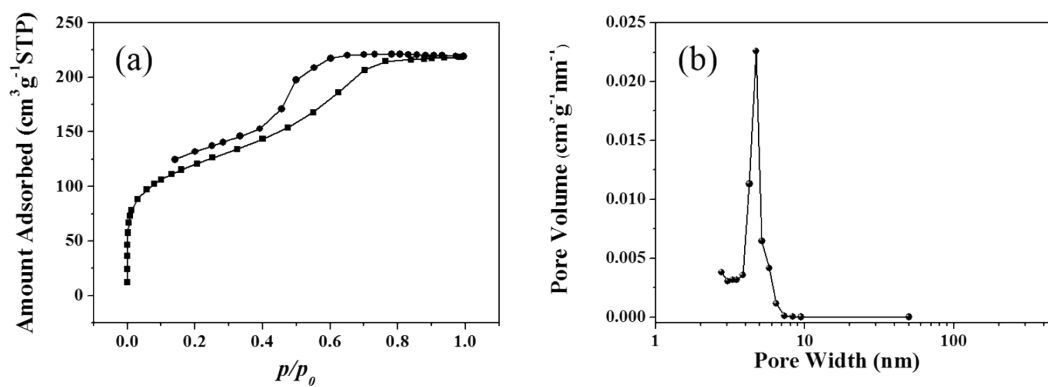


Fig.S1. N₂ adsorption-desorption isotherm (a) and BJH pore size distribution (b) for the OMP sample.

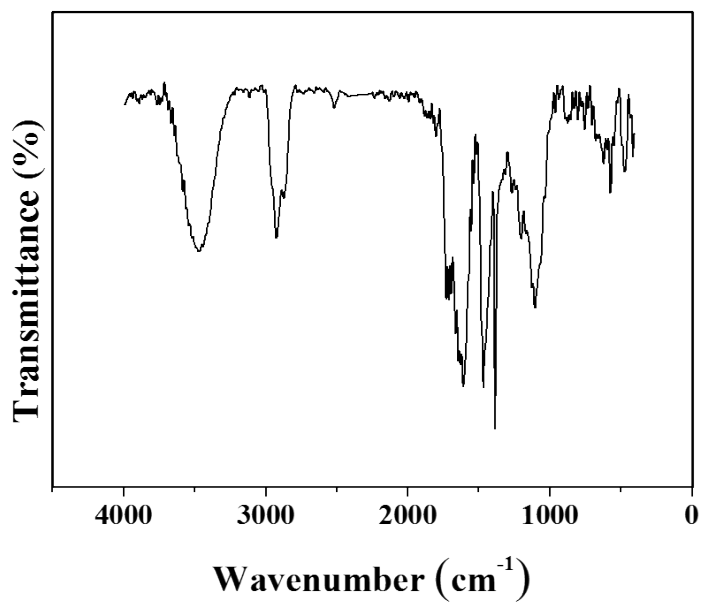


Fig. S2 FTIR spectroscopy of the OMP coating.

Optimization of SPME Parameters. In order to obtain the best extraction performance, SPME parameters, including extraction time, extraction temperature, desorption time and desorption temperature, were optimized. The central composite design (CCD), which can provide the information about the interactions between pairs of variables, was employed to determine the optimal conditions of the four factors.

The response surfaces for all analytes were shown in Fig. S1. The experiments were conducted at the concentration of $200 \mu\text{g}\cdot\text{L}^{-1}$ for PAHs and $1 \text{ mg}\cdot\text{L}^{-1}$ for BTEX. According to the results, the desorption temperature and desorption time didn't significantly affect the responses of all the analytes (data not shown). For BTEX, the desirability score was achieved under the following conditions: extraction time 12 min, extraction temperature $40 \text{ }^\circ\text{C}$, desorption time 2.5 min, desorption temperature $214 \text{ }^\circ\text{C}$. For PAHs, the optimal conditions were as follows: extraction time 35 min, extraction temperature $47 \text{ }^\circ\text{C}$, desorption time 4 min, desorption temperature $235 \text{ }^\circ\text{C}$.

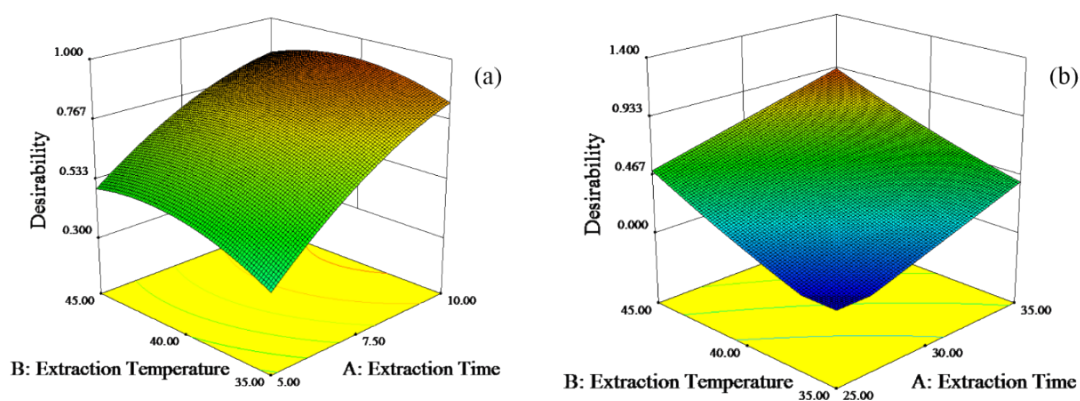


Fig. S3. The response surfaces estimated from CCD. (a) BTEX; (b) PAHs.

Table S1. Physical-chemical properties and EFs of the selected polar compounds.

	Compounds	Log K_{ow} ^a	EFs	Dipole ^b	Molecule volume ^c ($\text{cm}^3 \cdot \text{mol}^{-1}$)
OCPs	HCB	5.73	618.5	0.0000	127.5
	cis-chlordane	6.16	517.0	1.5	241.3
	o,p-DDT	6.79	399.6	2.7	239.5
	p,p-DDT	6.91	596.0	1.0	175.8
Musk	AHTN	5.70	486.0	1.2	205.2
	MK	4.30	116.5	2.3	219.7
Phenols	2-chlorophenol	2.15	96.20	0.93	78.99
	p-cresol	1.94	18.40	1.4	101.9
	2, 4 - dichlorophenol	3.06	247.1	3.1	118.5

^a K_{ow} : n-octanol-water partition coefficients calculated by the Epiweb.

^{b,c} Calculated with B3LYP density functional theory (DFT) by the Gaussian.

Table S2. Analytical performance of the OMP-coated fiber.

Compound	Linear Range($\text{ng}\cdot\text{L}^{-1}$)	Correlation Coefficient (R)	LODs ($\text{ng}\cdot\text{L}^{-1}$)	Single fiber (n=6, RSD %)	Fiber-to-fiber (n=3, RSD %)
Naphthalene	20-1000	0.9999	3.9	7.0	11
Acenaphthylene	10-1000	0.9988	1.4	10	7.2
Acenaphthene	10-1000	0.9991	0.30	6.5	3.9
Fluorene	10-1000	0.9995	0.90	5.9	3.9
Anthracene	10-1000	0.9949	2.1	5.2	6.8
Phenanthrene	10-1000	0.9991	2.4	6.7	3.0
Fluoranthene	10-1000	0.9944	1.7	7.4	3.7
Pyrene	10-1000	0.9913	2.2	8.1	4.4
Benzene	20-1000	0.9990	5.4	4.5	5.5
Toluene	20-1000	0.9996	5.5	5.2	1.4
Ethylbenzene	20-1000	0.9999	3.2	8.3	5.8
m-xylene	20-1000	0.9999	6.6	8.1	7.8

Table S3. The comparison of LODs between the OMP-coated fiber and the reported methods.

Compounds	LODs (ng·L ⁻¹)					
	OMP-coated fiber	Ref.1	Ref.2	Ref.3	Ref.4	Ref.5 ^a
Naphthalene	3.9	2.70	8.0		3	1.05 × 10 ³
Acenaphthylene	1.4				2	
Acenaphthene	0.30	1.64	8.1	100	1	0.11 × 10 ³
Fluorene	0.90	2.15	4.2	50	1	0.07 × 10 ³
Anthracene	2.1	1.92	4.0	50		0.07 × 10 ³
Phenathrene	3.4	2.14		50		0.06 × 10 ³
Fluoranthene	1.7	1.52	5.0			0.04 × 10 ³
Pyrene	2.2	2.32	4.0	10		0.05 × 10 ³

^a The unit of LODs in the Ref.5 was µg·L⁻¹ and converted to ng·L⁻¹.

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