Electronic Supplementary Information

Fabrication of dual-template molecularly imprinted mesoporous silica for simultaneous rapid and efficient detection bisphenol A and diethylstilbestrol in environmental water samples

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1. Equations

The pseudo-first-order rate equation is listed as follows:

$$\ln(Q_e - Q_t) = \ln Q_e - k_1 t \qquad (1)$$

where Q_e and Q_t (mg/g) are the amount of BPA or DES adsorbed on DMIMS at equilibrium and time t, respectively. k_1 (cm^{-1}) is the rate constant of pseudo-first-order model.

The pseudo-second-order rate equation is listed as follows:

$$\frac{t}{Q_t} = \frac{1}{k_2 Q_e^2} + (\frac{1}{Q_e})t \qquad (2)$$

where k_2 is the rate constant of pseudo-second-order model.

Scatchard analysis based on the equation as follows:

$$Q/C_e = Q_{max}/K_d - Q/K_d \qquad (3)$$

where Q and Q_{max} are the experimental binding capacity (mg/g) of BPA and DES and the theoretical maximum binding capacity of the DMIMS or NIMS (mg/g), respectively, and C_e is the concentration of BPA or DES in equilibrium solution (mg/L), K_d is the dissociation constant (mg/ L). The values of K_d and Q_{max} can be calculated from the slope and intercept of the linear equation plotted in Q versus -Q/C_e, respectively.

The non-linear form of Langmuir equation is as follows:

$$Q_e = \frac{K_L Q_m C_e}{1 + K_L C_e} \qquad (4)$$

The non-linear form of Freundlich equation is as follows:

$$Q_e = K_F C_e^{1/n} \qquad (5)$$

The non-linear form of Langmuir-Freundlich equation is as follows:

where K_L (L/mg) is the Langmuir constant, and Q_m (mg/g) is the maximum adsorption capacity for monolayer formation on the sorbents, C_e (mmol/L) is the free analytical concentration at equilibrium, and n and K_F are the Freundlich constants.

2. Supporting data

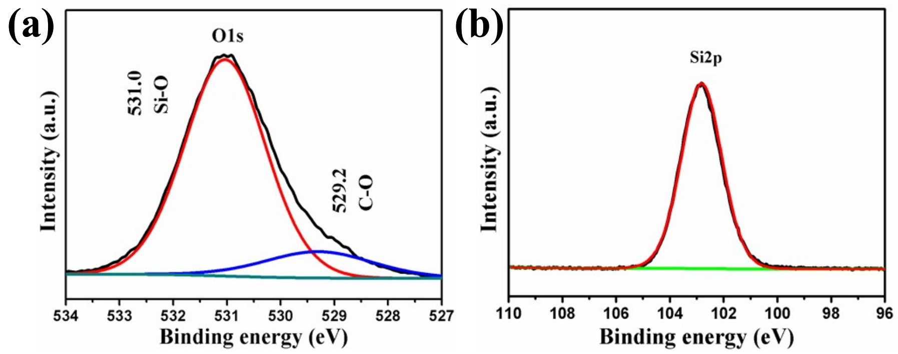

Figure S1 High-resolution XPS spectra of (a) O1s and (b) Si2p of DMIMS

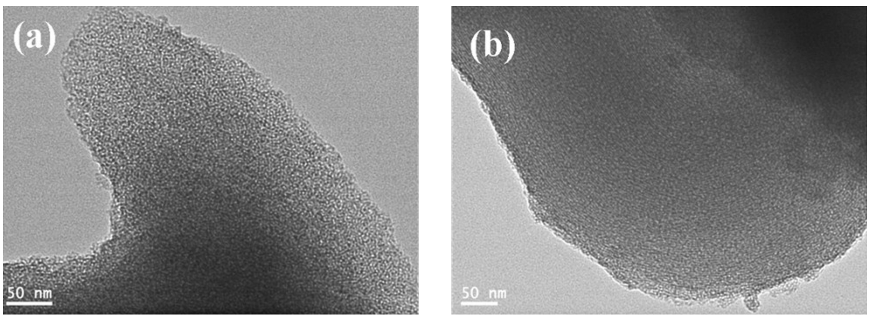

Figure S2 TEM (a, b) images of DMIMS

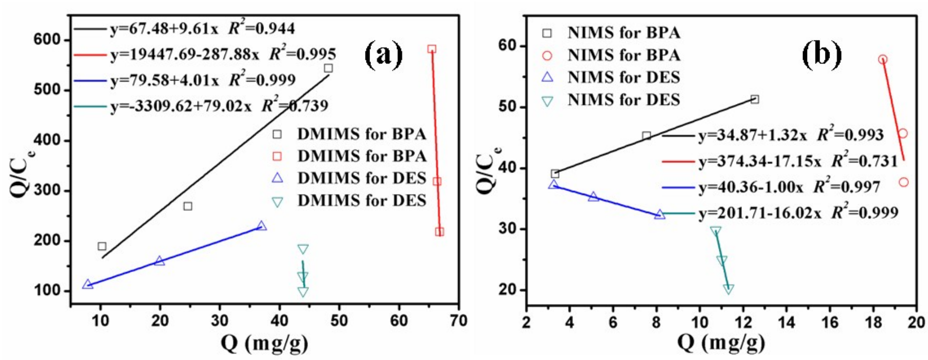

Figure S3. Scatchard plots of DMIMS (a) and NIMS (b)

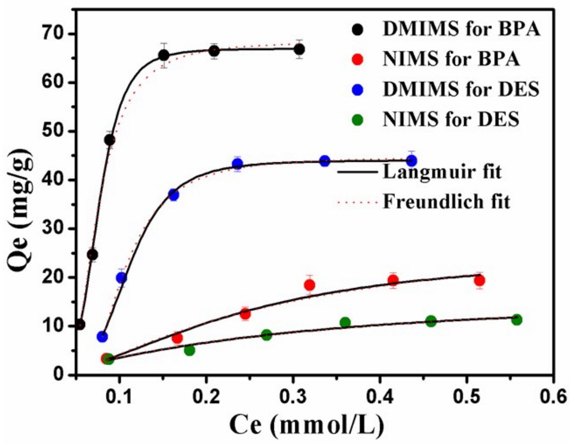

Figure S4. Langmuir and Freundlich plots of DMIMS and NIMS for BPA and DES

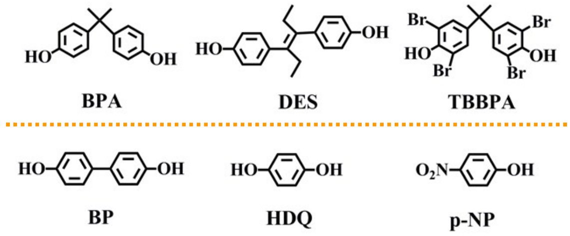

Figure S5. Molecular structure of analogs used in this work

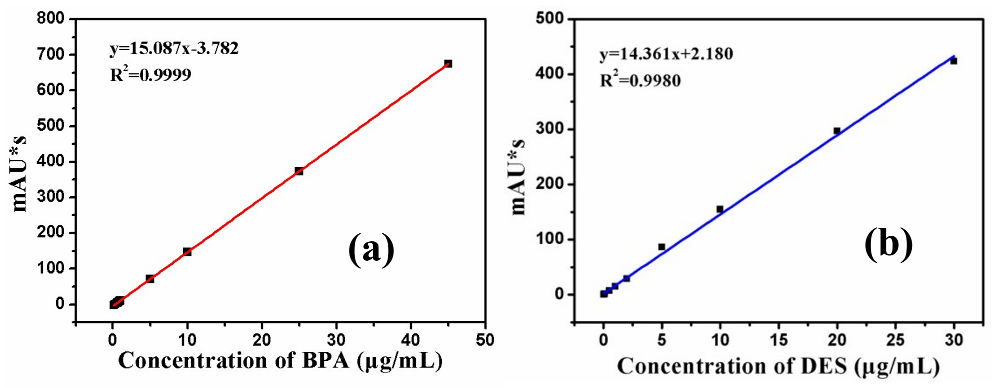

Figure S6 Calibration curve for the determination of BPA (a) and DES (b) by HPLC/UV

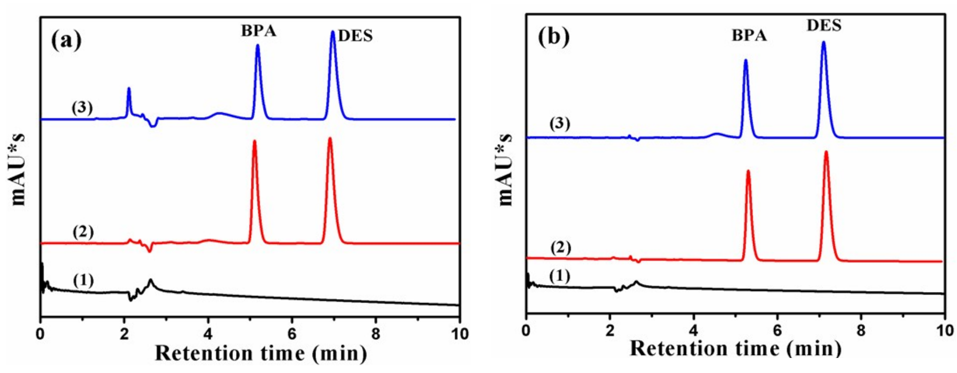

Figure S7 HPLC chromatograms of lake river (a) and river water (b): (1) water sample without spiked, (2) water sample spiked with 0.5 mg L^{-1} BPA and DES, 3) elution from DMIMS

Table S1 The Langmuir and Freundlich isotherm parameters obtained by the adsorption of BPA and DES onto DMIMS and NIMS

Adsorbents	$Q_e(exp)$ (mg/g)	Langmuir			Freundlich		
		Q_m(mg/g)	K_L(L/mg)	R^2	K_F	$1/n$	R^2
DMIMS for BPA	66.8	66.9	0.52	0.999	69.4	0.35	0.995
NIMS for BPA	19.4	19.6	0.017	0.980	20.4	1.29	0.973
DMIMS for DES	43.9	44.1	0.26	0.997	45.4	0.36	0.992
NIMS for DES	12.3	12.4	0.014	0.964	12.0	1.68	0.959

Table S2 Comparison of the present method for determination of BPA and DES

Sorbents	Target molecule	Binding capacity (mg/g)	Real samples	Recovery (%)	Refs.
SiO_2@MIP	BPA	3.6	Tap water, lake water, drinking water	97.0-106.0	1
P-MIPs	BPA	6.2	Tap water, river water	100.4-102.4	2
T-MIPs	BPA	7.9	Seawater, yogurt	94.8-98.5	3
MWNTs@MMIPs	BPA	11.3	Tap water, rain water, lake water	87.3-95.4	4
MIMIO-ir	BPA	15.0	Tap water, lake water	99.5-105.2	5
MI-SBA-15	BPA	27.9	Tap water, river water, well water, wastewater	87-110.2	6
m-MINPs	DES	9.7	Milk	90.7-105.2	7
Fe_3O_4@SiO_2@APBA/MIP	DES	18.9	Lake water	97.1-103.2	8
MIP-QDs	DES	32.5	Seawater and river water	95.5-107.5	9
m-TiMIF	BPA/DES	15.8/13.2	Pork and chicken samples	81.6-102.4	10
DMIMS	BPA/DES	66.8/43.9	Tap water, river water, lake water	95.0-107.1	This work

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