Supporting Information

Simple synthesis of a swellable porous β-cyclodextrin-based polymer in aqueous phase for rapid removal of organic micro-pollutants from water

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Content

Text S1 Instrumental analysis

HPLC analysis for a single component solution

Micro-volumes of water samples were analyzed directly by an Agilent HPLC coupled with an Agilent XDB-C18 analytical column (5 μm, 4.6 × 250 mm) and a UV detector. Column temperature was set at 30°C, and the mobile phase was a mixture of methanol and water (70:30, V:V) with a flow rate of 1.0 mL/min. The detection wavelengths for BPA, BPS, 2-NO, 3-PH, E2, EE2 and E3 were 276, 258, 264, 250, 230, 230, and 230 nm, respectively. The injection volume was 10 μL. All the pollutants were quantified from external calibration standards based on the analyte responses by linear least-squares regression.

HPLC analysis for a mixture solution of different pollutants

In the adsorption experiments at environmental concentrations, the adsorbed T–E–CDP was eluted with methanol firstly to get a mixture of different pollutants and then concentrated to a suitable volume for HPLC analysis. In order to get a better response signal to all the pollutants, the detection wavelengths was set to 230 nm. Other analysis conditions were same to the analysis of single component solution as described above.

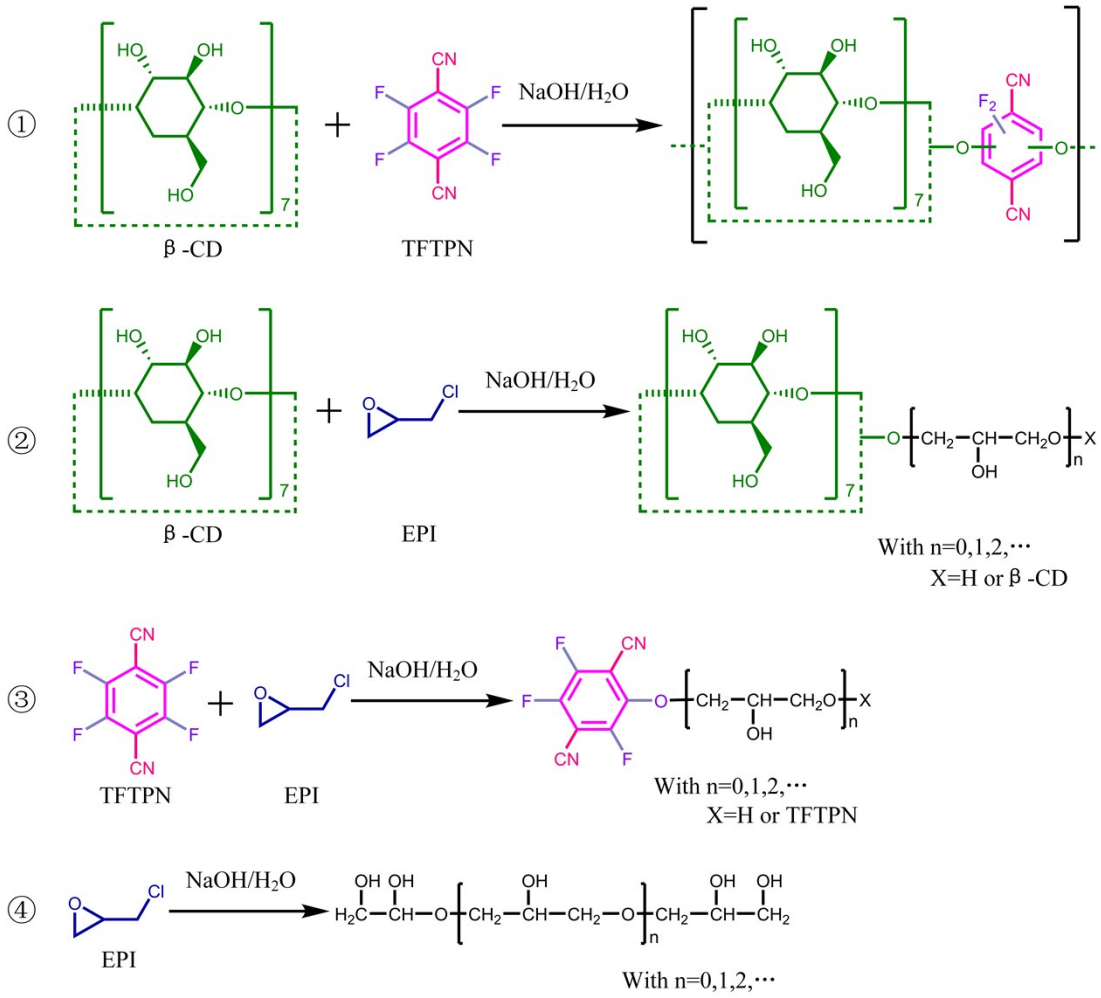

Fig. S1. Possible reactions may be involved during the synthesis of T-E-CDP.

In basic medium, the hydroxyl groups on β-cyclodextrin can undergo a nucleophilic substitution reaction with TFTPNF. Similarly, the hydroxyl groups on β-cyclodextrin can react with epichlorohydrin to form a polymer. In addition, EPI also undergoes self-polymerization and TFTPN can also react with hydroxyl groups on the EPI segments.

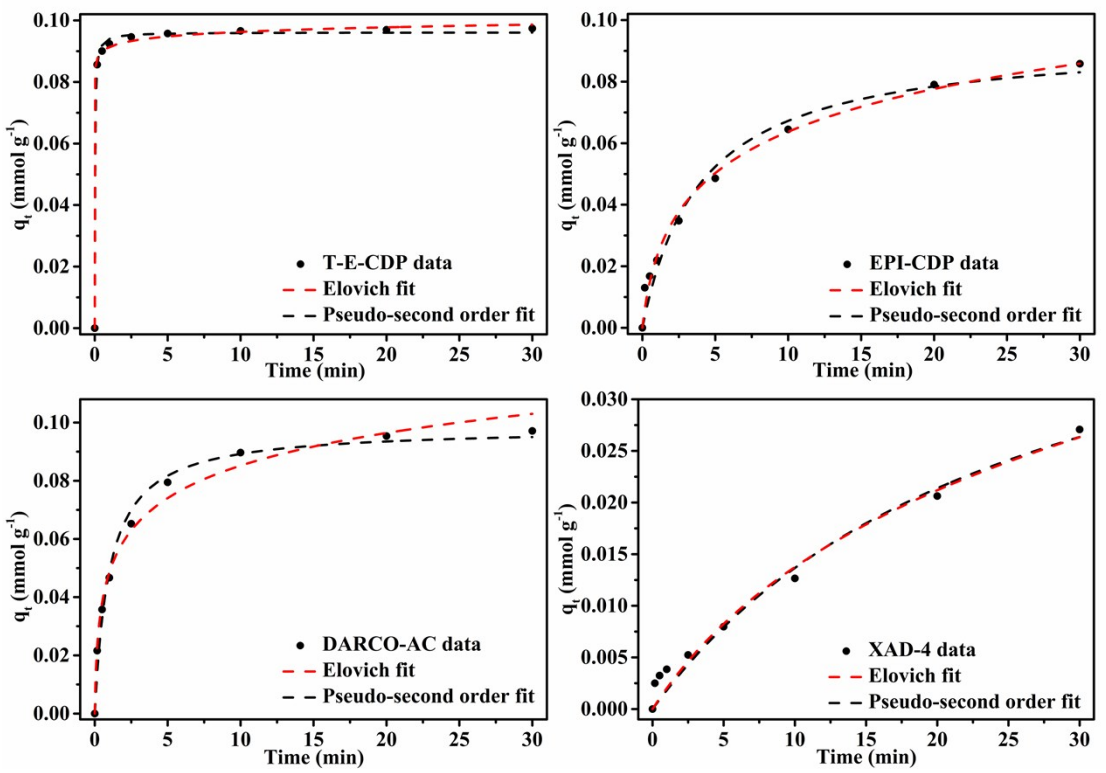

Fig. S2. Adsorption kinetics data and modeling by Pseudo-second order and Elovich equations for BPA onto different adsorbents. Symbols are experimental data and lines are model results.

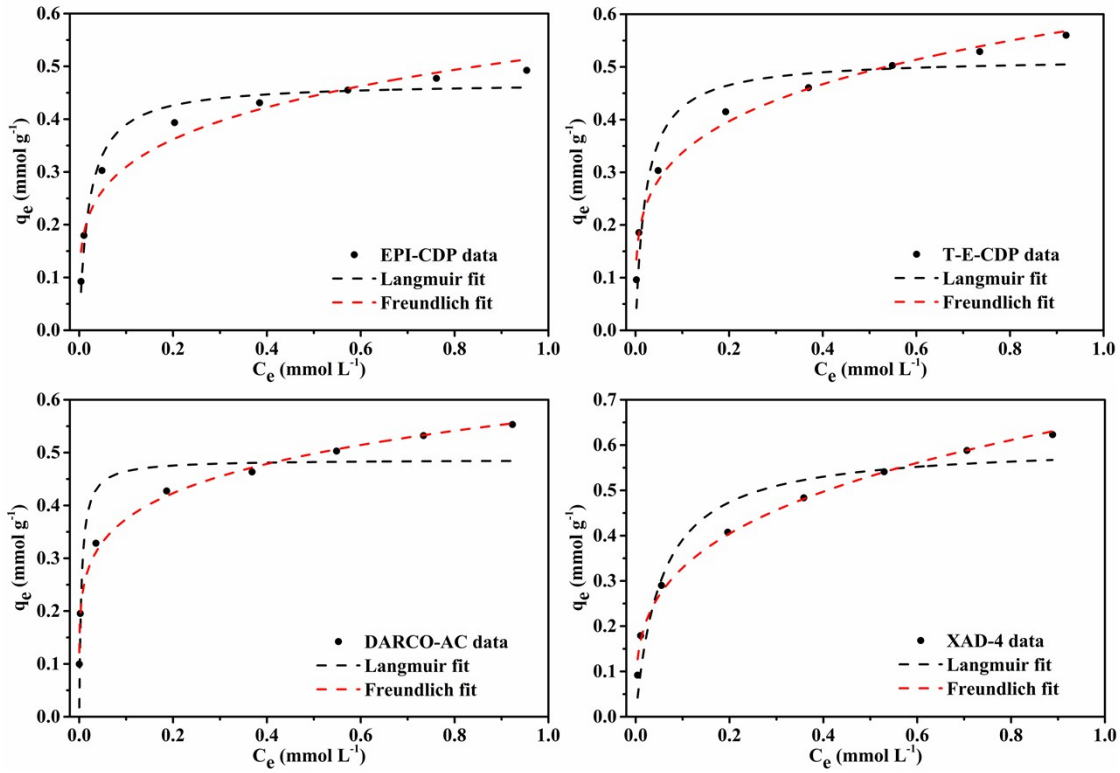

Fig. S3. Adsorption isotherms data and modeling by Langmuir model and Freundlich model for BPA onto different adsorbents. Symbols are experimental data and lines are model results.

Table S1

Elemental composition, water regain, pore volume and surface area of different adsorbents.

Adsorbent	C (wt%)	H (wt%)	N (wt%)	F (wt%)	TFTPN content (wt%)	Substitution of F	H_2O regain (wt%)	Volumetric H_2O regain ($cm^3\ g^{-1}$)	Dry pore volume[a] ($cm^3\ g^{-1}$)	S_L[b] ($m^2\ g^{-1}$)	S_{BET}[c] ($m^2\ g^{-1}$)
EPI–CDP	46.71	7.23	--	--	--	--	346	3.46	0.0018	1.2	0.005
T–E–CDP	43.27	5.87	1.72	0.79	8.41	3.32	263	2.63	0.0339	103	0.31
DARCO-AC	--	--	--	--	--	--	--	--	--		525[d]
XAD-4	--	--	--	--	--	--	--	--	--		725[d]

[a] Pore volume obtained from CO_2 adsorption-desorption isotherms.

[b] Langmuir surface area obtained from CO_2 adsorption-desorption isotherms.

[c] BET surface area obtained from N_2 adsorption-desorption isotherms.

[d] Surface area obtained from supplier on sigma.

Table S2

Kinetics parameters for the removal of BPA by different adsorbents based on the Pseudo-second order model and Elovich model.

Adsorbent	Pseudo-second order			Elovich		
	k_2 (g mmol^{-1} min^{-1})	q_e (mmol g^{-1})	R^2	α (mmol g^{-1} min^{-1})	β (g mmol^{-1})	R^2
EPI–CDP	2.67	0.094	0.978	4.28 E^{-2}	48	0.991
T–E–CDP	456.56	0.096	0.999	6.62 E^{15}	466	0.999
DARCO-AC	10.08	0.098	0.989	0.307	62	0.990
XAD-4	0.78	0.049	0.974	2.13 E^{-3}	60	0.977

Table S3

Isotherms parameters for sorption of BPA on different adsorbents fitted by Langmuir model and Freundlich model.

Adsorbent	Langmuir fit			Freundlich fit		
	Q_{max} (mg g^{-1})	K_L (L $mmol^{-1}$)	R^2	K_F ($mmol^{1-1/n}$ g^{-1} $L^{1/n}$)	n	R^2
EPI–CDP	107	48.61	0.971	0.5188	4.46	0.959
T–E–CDP	118	45.50	0.921	0.5793	4.26	0.988
DARCO-AC	111	211.0	0.852	0.5632	5.64	0.995
XAD-4	137	18.61	0.929	0.6530	3.36	0.994

Table S4

Physiochemical properties of organic micro-pollutants studied in this work.

Pollutants	M_W (g mol^{-1})	$logK_{OW}$[a]	pKa[b]	C_S (g L^{-1})[b]
BPA	228.29	3.6	10.3	0.071
BPS	250.27	2.1	7	0.38
EE2	296.40	4.1	10.2	0.004
2-NO	144.17	2.7	9.6	0.49
3-PH	170.21	3.5	9.7	0.14
E2	272.38	4.1	10.3	0.003
E3	288.38	2.5	10.2	0.029

[a] Log octanol-water partition coefficient. Predicted using KOWWIN v1.67 software implemented in ChemSpider Database.

[b] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02, as implemented in the SciFinder CAS Database.

Table S5

The removal efficiency of different pollutants by PTFE-Q membrane filter. The data are reported as the average of triplicate experiments.

Pollutants	Concentration (mmol L^{-1})	Removal efficiency by PTFE-Q (%)
BPA	0.1	0.996
BPS	0.1	0.005
2-NO	0.1	0.394
3-PH	0.1	0.984
E2	0.05	0.943
EE2	0.05	**2.321**
E3	0.1	0.274