Porous Thienyl Cyclodextrin Polymer Synthesized in Homogeneous Ionic Liquid Catalyst System for Rapid Removal of Pharmaceuticals and Personal Care Products (PPCPs)

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Content

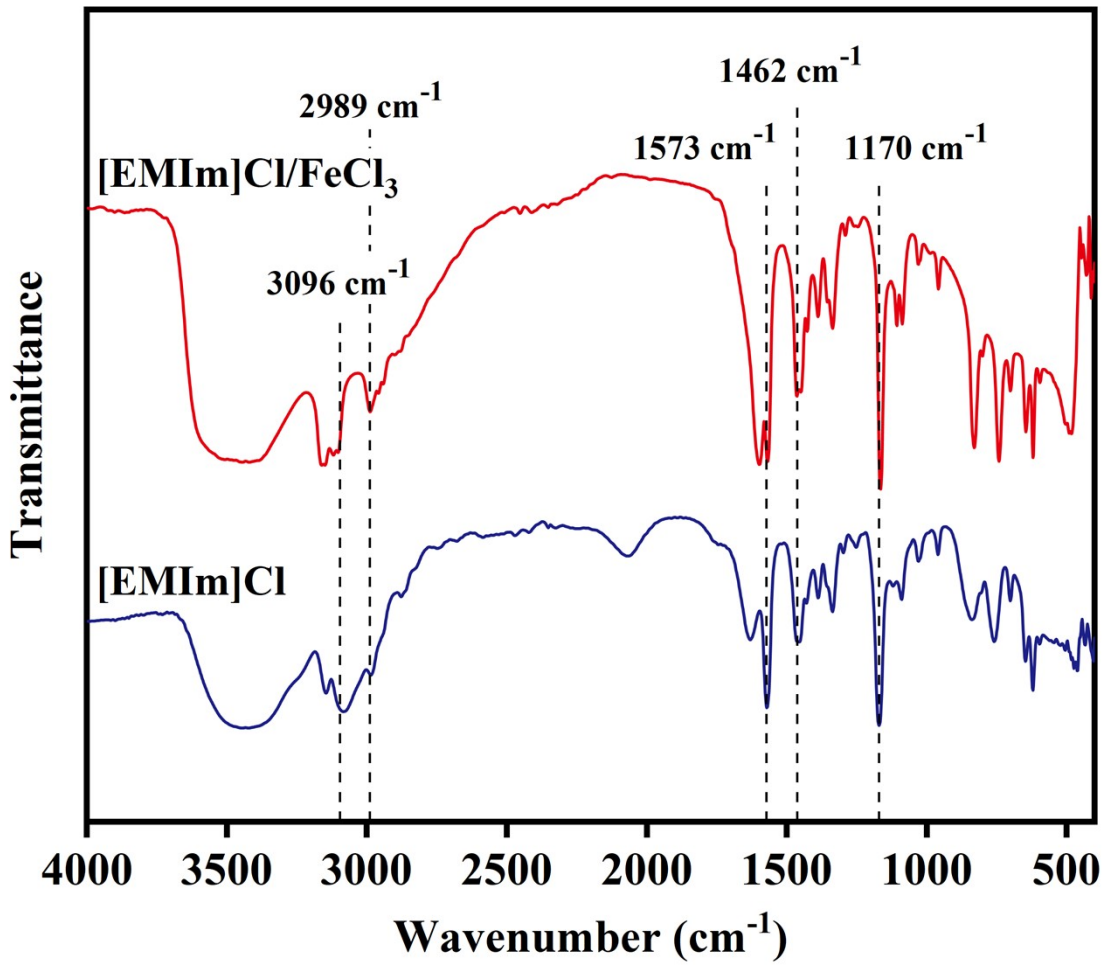


Fig. S1. IR spectra of [EMIm]Cl and [EMIm]Cl/$FeCl_3$ ionic liquids.

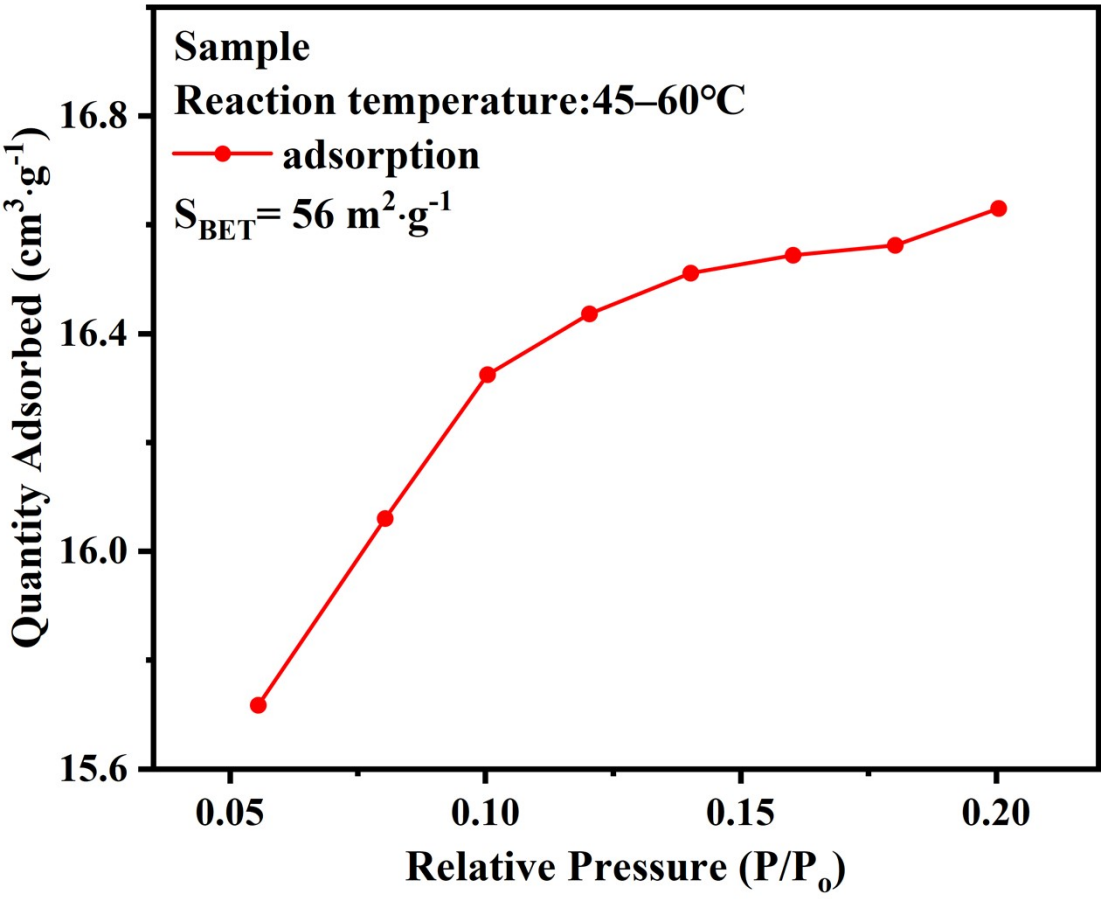


Fig. S2 Nitrogen adsorption isotherm of the sample with a final temperature of 60 °C measured at 77K (activated in vacuum at 170 °C for 12 h in advance).

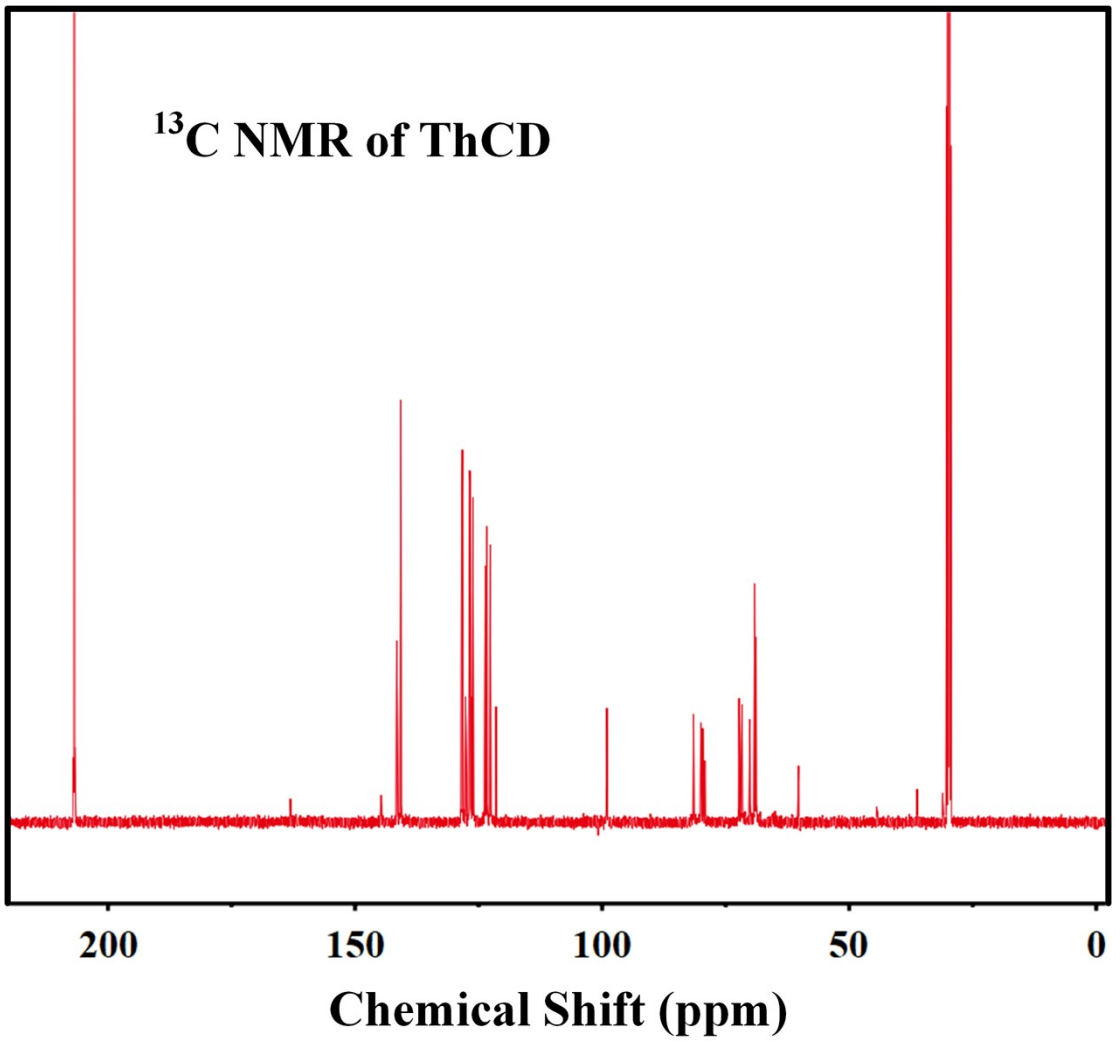


Fig. S3 ^{13}C NMR spectrum of ThCD (dissolve with deuterated acetone).

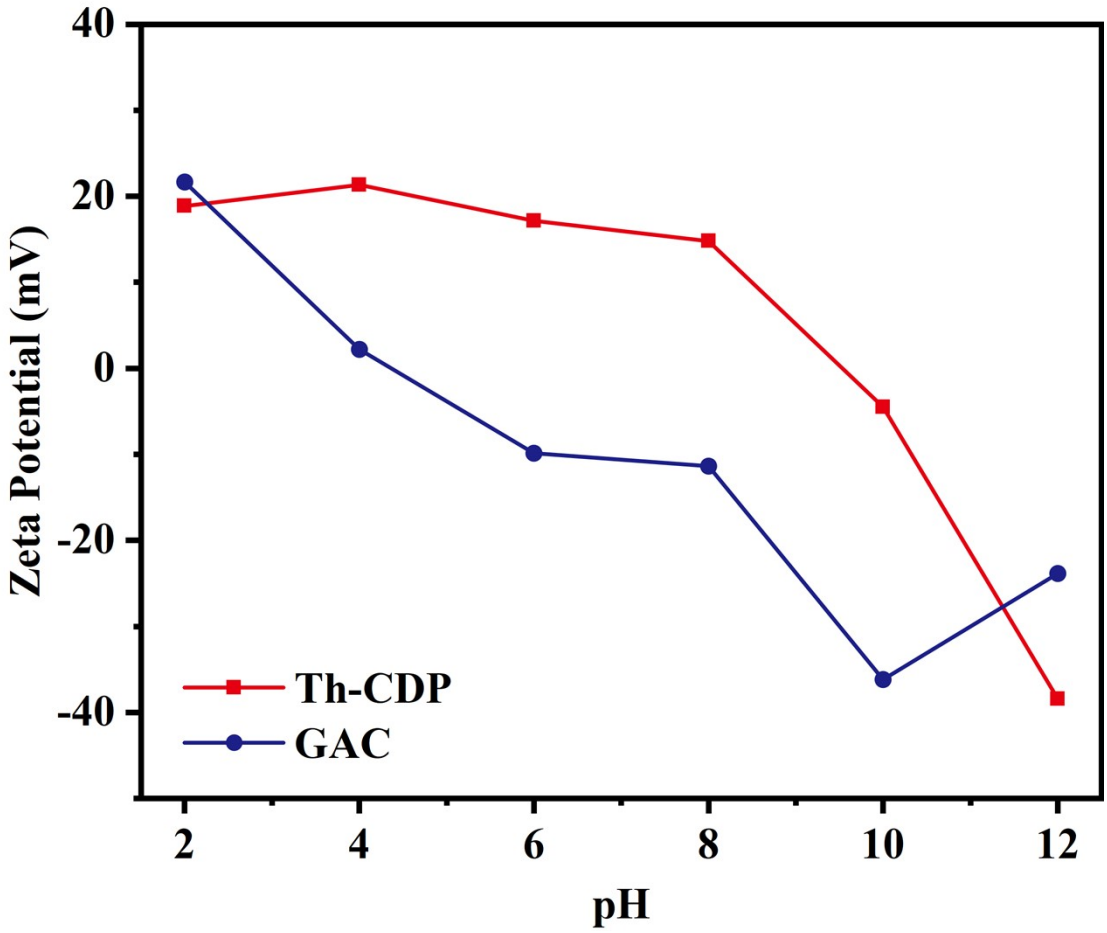


Fig. S4 The Zeta potential diagram of Th-CDP and GAC in the range of pH 2–12.

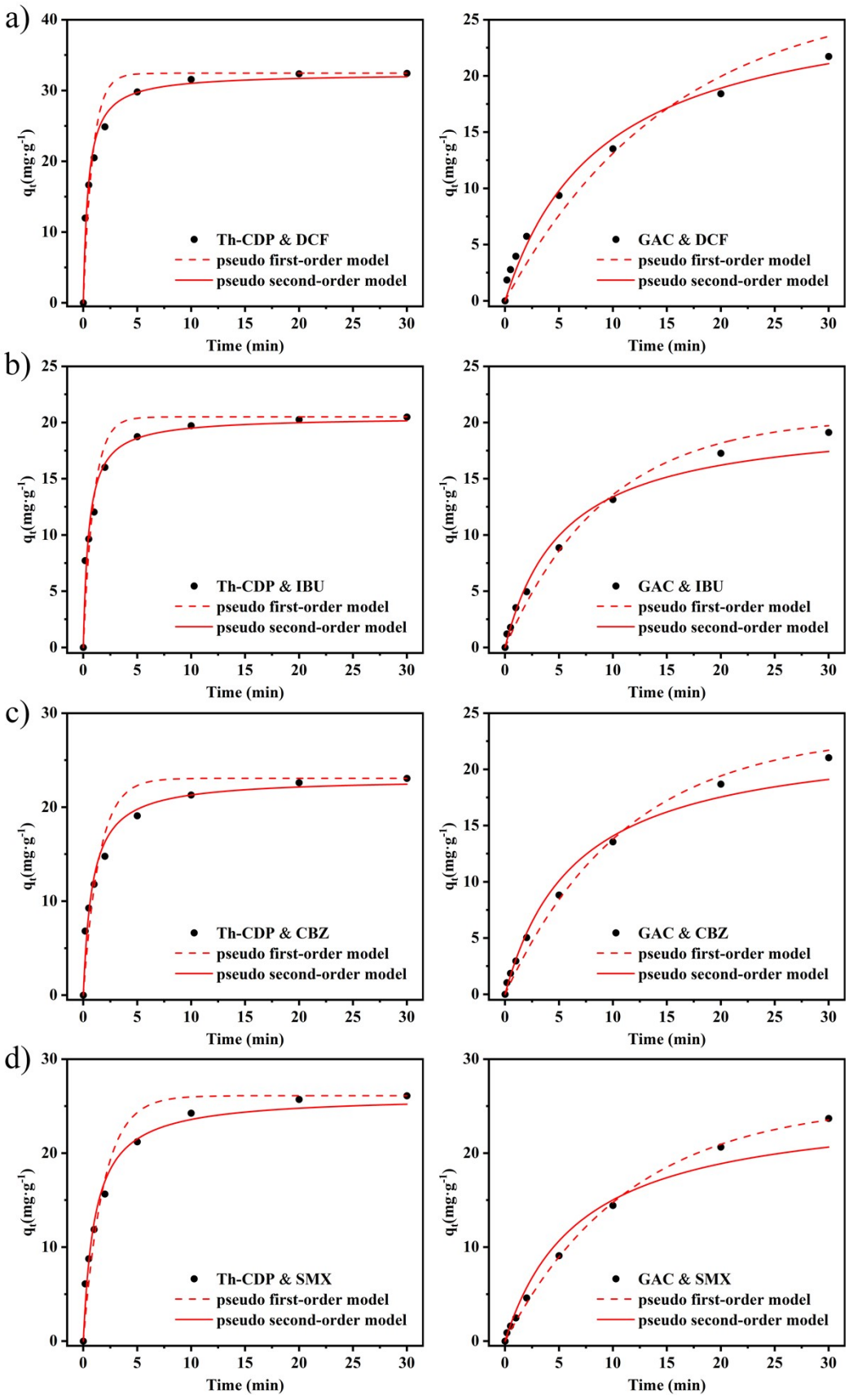


Fig. S5 Model fitting results of adsorption kinetic for four PPCPs by Th-CDP and GAC.

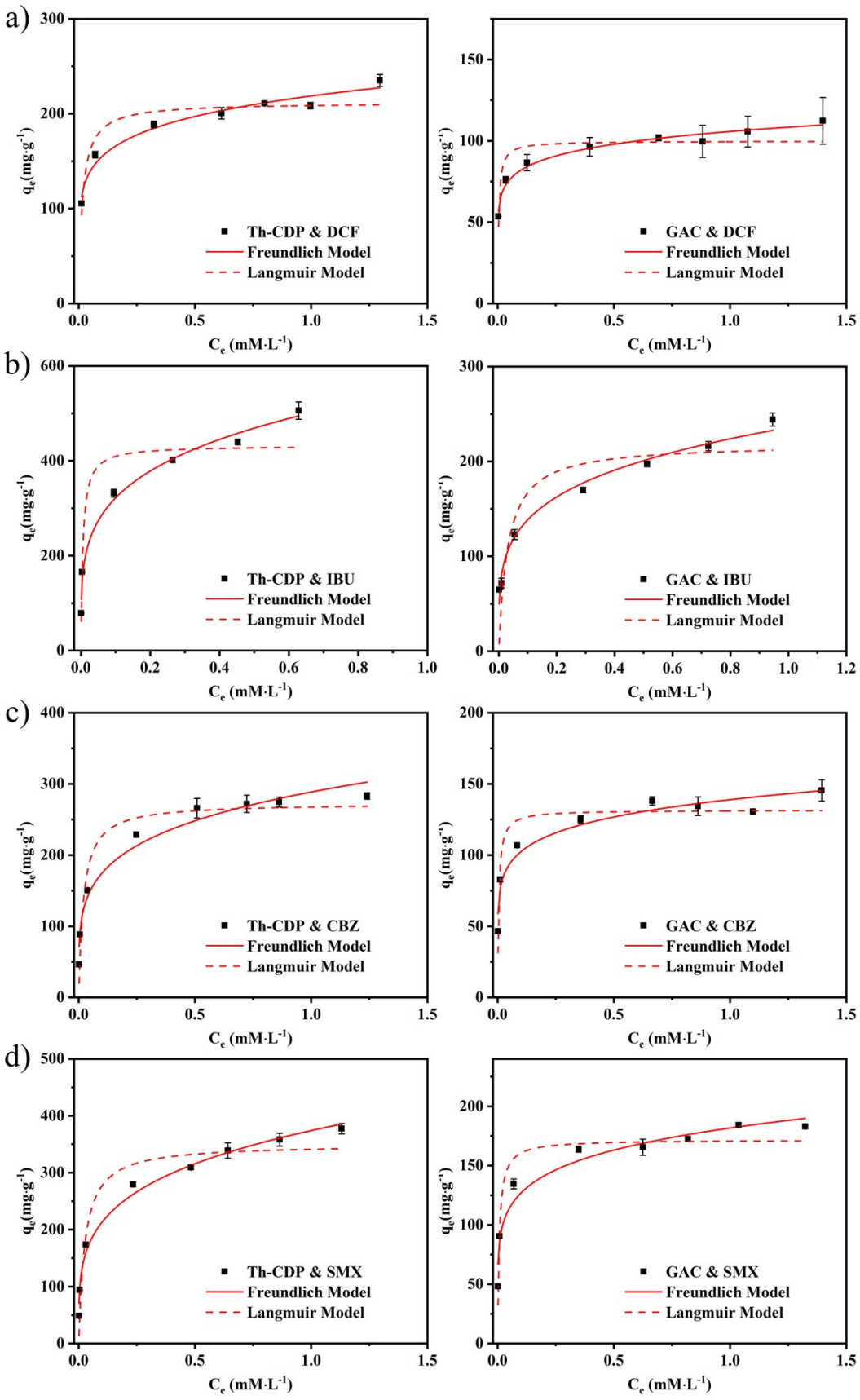


Fig. S6 Model fitting results of adsorption isotherm for four PPCPs by Th-CDP and GAC.

Table S1 The MRM (multiple reaction monitoring) parameters of the four PPCPs in mass spectrometry.

Compound	Polarity	Precursor	Product ion	CE	DP
DCF	Negative	294.1	249.9	–15.8	–49.7
			213.9	–27.7	–43.4
IBU	Negative	205.1	161.0	–10.8	–42.0
CBZ	Positive	237.0	194.0	26.0	81.0
			179.1	48.0	77.0
SMX	Positive	254.1	155.9	22.0	69.0
			108.0	34.0	71.0

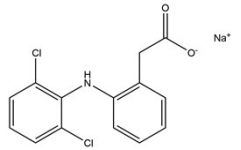
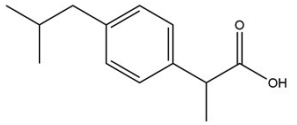
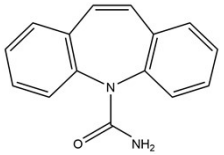
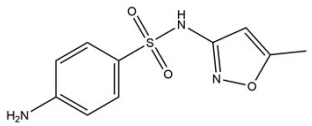
Table S2 Mass spectrometry methods of the four PPCPs.

Parameters	Negative	Positive
Collision Gas	4	4
Curtain Gas	20	35
Ion Source Gas 1	45	45
Ion Source Gas 2	55	55
IonSpray Voltage	–4500	5500
Temperature	600	550
Interface Heater	On	On

Table S3 Elemental analysis results of Th-CDP.

Sample	C (wt%)	H (wt%)	O (wt%)	N (wt%)	S (wt%)
Th-CDP	55.76	2.989	12.740	0.55	24.797

Table S4 Physicochemical properties and structure diagram of PPCPs studied in this work.

Pollutants	M_w (g mol^{-1})	logK_{ow}[a]	C_s (mg L^{-1})[b]	pK_a[c]	Diagram
DCF	318.13	4.02	15906.5	4.18	
IBU	206.28	3.79	21	4.41	
CBZ	236.27	2.25	38	13.94	
SMX	253.28	0.48	610	5.81	

[a] Log K_{ow} (KOWWIN v1.67 estimate) implemented in the ChemSpider database;

[b] Water Solubility obtained by the ChemSpider database;

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