

## **Supplementary Information for**

### **Elimination of pharmaceutical compounds from aqueous solution by novel functionalized pitch-based porous adsorbents: Kinetic, isotherm, thermodynamic studies and mechanism analysis**

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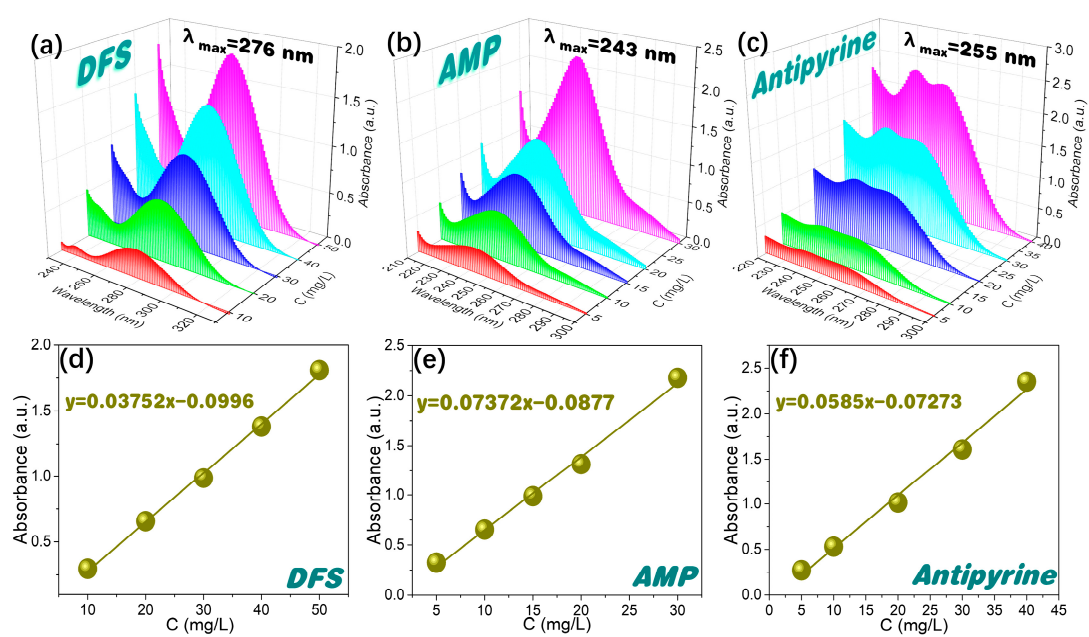


Fig. S1. Standard curves of DFS(a,d), AMP(b,e), and Antipyrine(c,f).

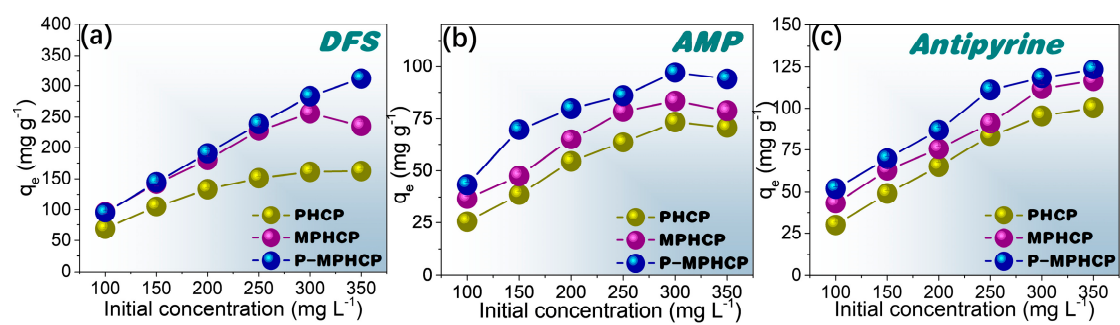


Fig. S2. Isotherm adsorption capacity for pitch-based HCP adsorbents toward PPCPs (a) DFS, (b) AMP, and (c) Antipyrine with different initial concentrations at 35 °C.

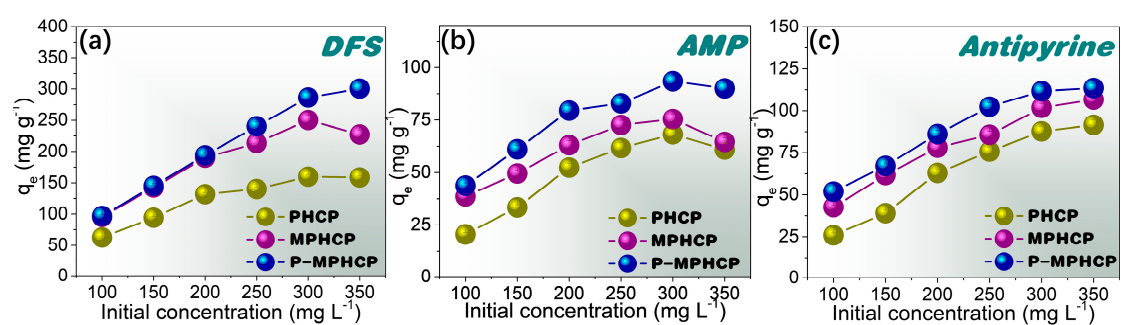


Fig. S3. Isotherm adsorption capacity for pitch-based HCP adsorbents toward PPCPs (a) DFS, (b) AMP, and (c) Antipyrine with different initial concentrations at 45 °C.

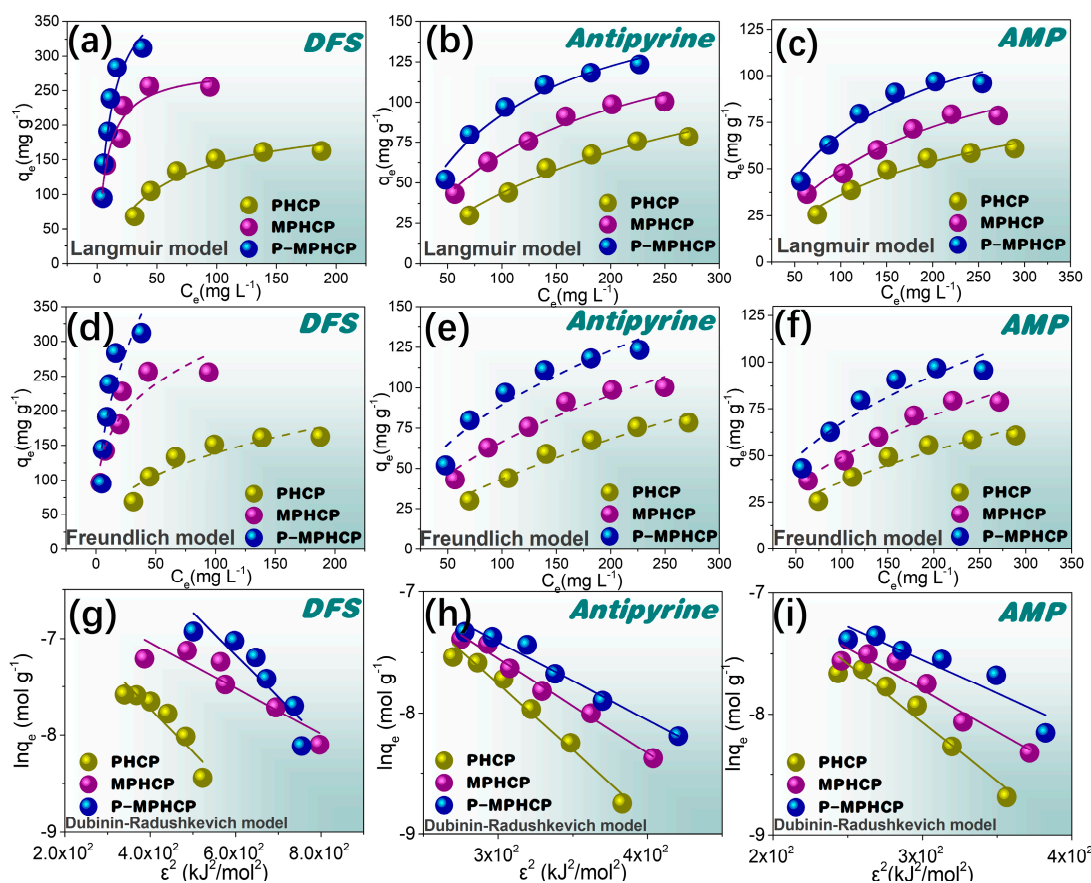


Fig. S4. Langmuir (a-c), Freundlich (d-f), and D-R (g-i) isotherms for the adsorption of pitch-based HCP adsorbents toward DFS, AMP, and antipyrine at 35 °C.

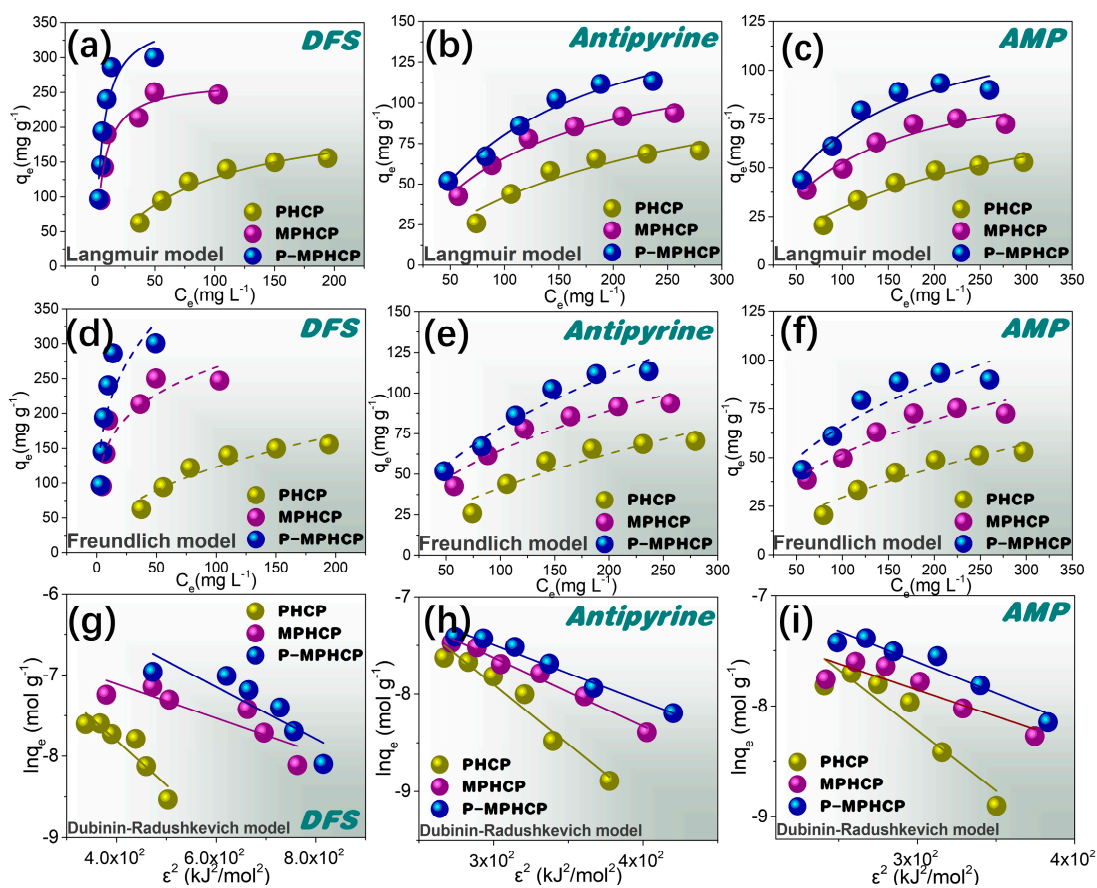


Fig. S5. Langmuir (a-c), Freundlich (d-f), and D-R (g-i) isotherms for the adsorption of pitch-based HCP adsorbents toward DFS, AMP, and antipyrine at 45 °C.

Table S1. Correlation coefficient and isotherm parameters for the adsorption of pitch-based HCP adsorbents at 35 °C.

Sample	PPCP	Langmuir isotherm			Freundlich isotherm			Dubinin-Redushkevich isotherm			
		$q_{\max}$	$K_L$	$R^2$	$n$	$K_F$	$R^2$	$q_{DR}$	$B$	$E_a$	$R^2$
PHCP	DFS	217.3	0.0198	0.9339	2.658	24.55	0.8512	0.0027	0.0045	10.55	0.8697
	AMP	105.4	0.0052	0.9595	1.828	2.908	0.9223	0.0057	0.0097	7.19	0.9495
	Antipyrine	163.9	0.0037	0.9757	1.555	2.260	0.9538	0.0115	0.0110	6.75	0.9751
MPHCP	DFS	283.8	0.1329	0.9418	3.888	87.38	0.8454	0.0022	0.0024	14.56	0.8475
	AMP	134.8	0.00581	0.9713	1.863	4.159	0.9513	0.0033	0.0069	8.49	0.9172
	Antipyrine	165.1	0.0069	0.9768	1.919	6.025	0.9455	0.0055	0.0079	7.98	0.9876
P-MPHCP	DFS	424.0	0.1062	0.9142	2.909	82.57	0.8080	0.0106	0.0044	10.70	0.8317
	AMP	155.1	0.0064	0.9734	1.878	5.126	0.9414	0.0027	0.0055	9.53	0.8630
	Antipyrine	210.3	0.0059	0.9860	1.738	5.404	0.9632	0.0042	0.0065	8.79	0.9726

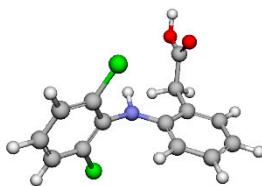
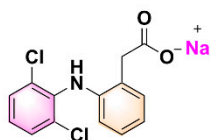
Table S2. Correlation coefficient and isotherm parameters for the adsorption of pitch-based HCP adsorbents at 45 °C.

Sample	PPCP	Langmuir isotherm			Freundlich isotherm			Dubinin-Redushkevich isotherm			
		$q_{\max}$	$K_L$	$R^2$	$n$	$K_F$	$R^2$	$q_{DR}$	$B$	$E_a$	$R^2$
PHCP	DFS	227.7	0.0127	0.9573	2.2011	15.18	0.9004	0.0036	0.00548	9.55	0.8536
	AMP	100.9	0.0041	0.9476	1.6811	1.915	0.9126	0.0071	0.0109	6.77	0.8714
	Antipyrine	133.7	0.0046	0.9125	1.6978	2.766	0.8699	0.0143	0.0122	6.40	0.9539
MPHCP	DFS	267.7	0.1597	0.9217	4.3657	92.74	0.8149	0.0019	0.0021	15.43	0.7543
	AMP	106.2	0.0098	0.9317	2.4176	7.748	0.8778	0.0016	0.00475	10.26	0.8090
	Antipyrine	139.8	0.0090	0.9652	2.1889	7.904	0.9168	0.0040	0.007	8.45	0.9826
P-MPHCP	DFS	361.1	0.1711	0.9469	4.0110	95.21	0.8232	0.0053	0.00319	12.52	0.7770
	AMP	133.8	0.0102	0.9198	2.3731	8.149	0.8708	0.0027	0.00561	9.44	0.9182
	Antipyrine	196.0	0.0058	0.9767	1.7488	5.073	0.9486	0.0032	0.00582	9.27	0.9748

Table S3. DFS adsorption performance of P-MPHCP compared to other reported adsorbents.

Adsorbent	pH	$q_{\max}$ (mg/g) (Langmuir model)	Stabilization time (h)	Reference
P-MPHCP	5	444	1	This work
Expanded Graphite	-	330	-	[1]
OAC(2.0)	4.2	487	3	[2]
Commercial AC	4.2	76	5	[2]
PCDM-1000	-	400	12	[3]
ZIF-8	-	100	12	[3]
OH-MCOF	5	203	0.5	[4]
CTAB-ZIF-67	8	43.9	1	[5]
P-POP-1	4	166	2	[6]
P-POP-2	4	217	1	[6]
PONF	4	380.8	0.5	[7]
ZCPC-10	7.4	70	-	[8]
ZCPC-20	7.4	134	-	[8]
ZCPC-30	7.4	159	-	[8]
CNT/Al <sub>2</sub> O <sub>3</sub>	4	27	-	[9]
Fe <sub>3</sub> O <sub>4</sub> @MOF-100(Fe)	5	377	2	[10]

**( a ) Diclofenac ( DFS )**

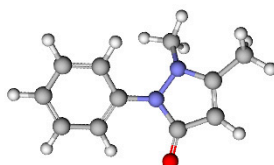


Molecular weight: 318.13;

$\lambda_{\max}(\text{nm})=276 \text{ nm}$ ;

$\text{pK}_{\text{a}}=4.15$  <sup>[7]</sup>;

**( b ) Antipyrine**

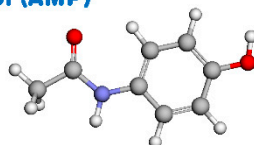
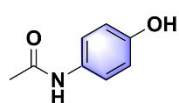


Molecular weight: 188.22;

$\lambda_{\max}(\text{nm})=255 \text{ nm}$ ;

$\text{pK}_{\text{a}}=1.4$  <sup>[11]</sup>;

**( c ) 4-acetylaminophenol ( AMP )**



Molecular weight: 151.26;

$\lambda_{\max}(\text{nm})=243 \text{ nm}$ ;

$\text{pK}_{\text{a}}=9.38$  <sup>[12]</sup>;

Fig. S6. Chemical and structural characteristics of three PPCPs [7, 11, 12].

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