

Supporting Information

Micro- and nanoplastics-mediated phototransformation and bioaccessibility of fluorinated liquid crystal monomer in aquatic environments

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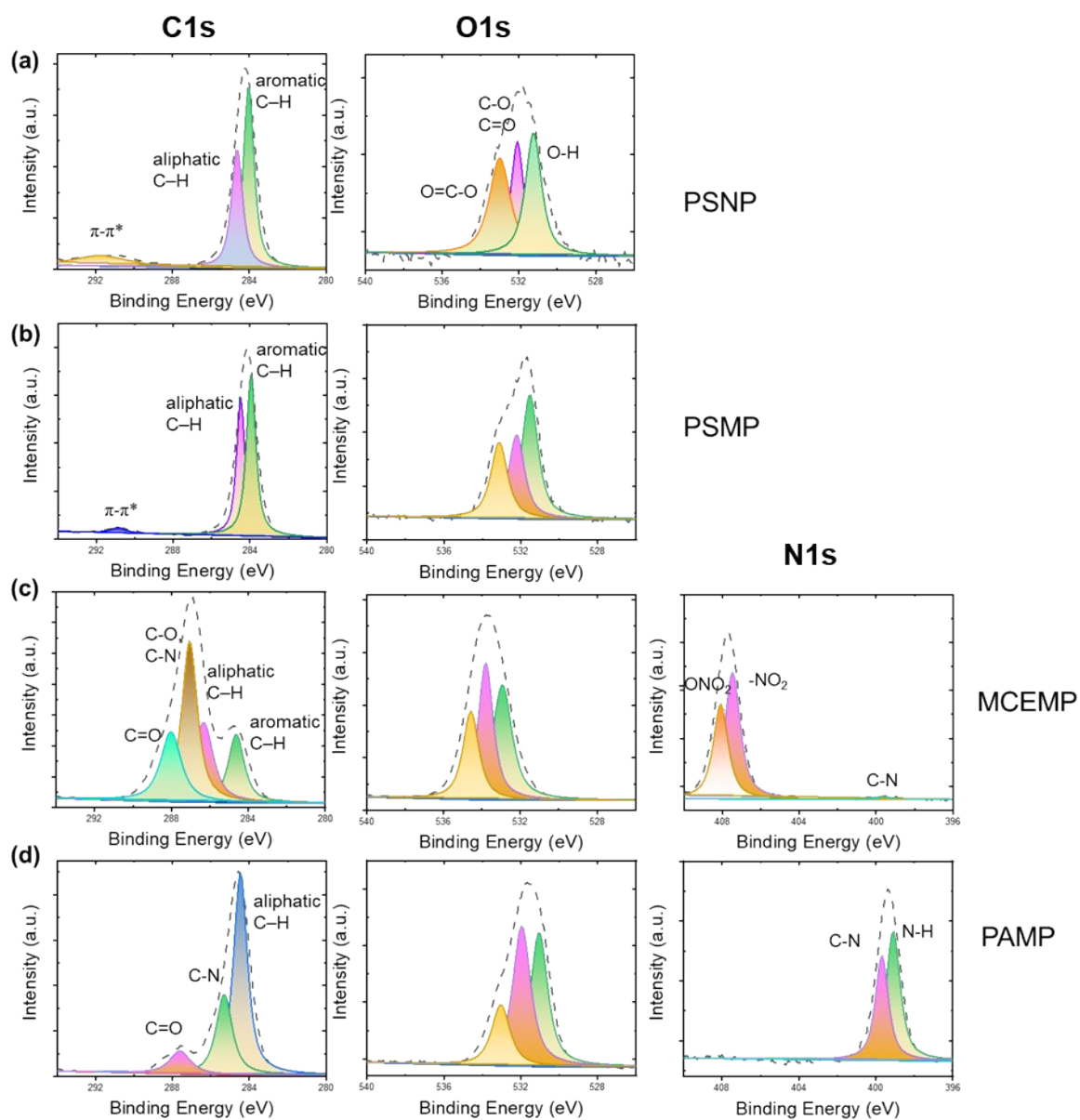


Fig. S1. XPS spectra of C1s, O1s, N1s of (a) PSNP, (b) PSMP, (c) MCEMP, and (d) PAMP.

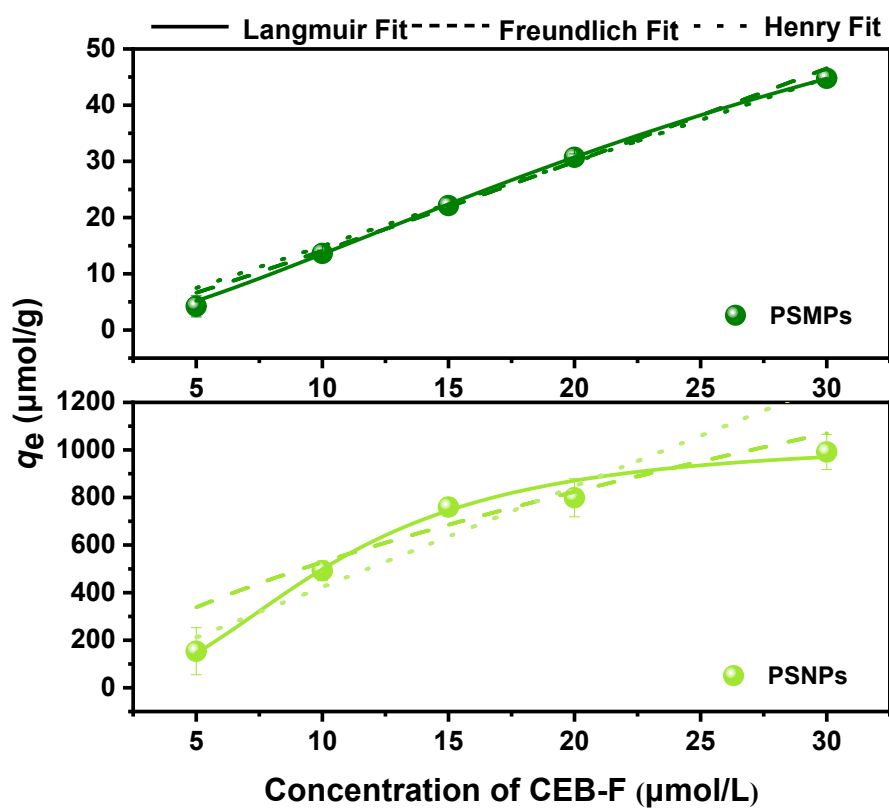


Fig. S2. Adsorption isotherms for the adsorption of CEB-F on PSMPs and PSNPs fitted by the Langmuir, Freundlich, and Henry model.

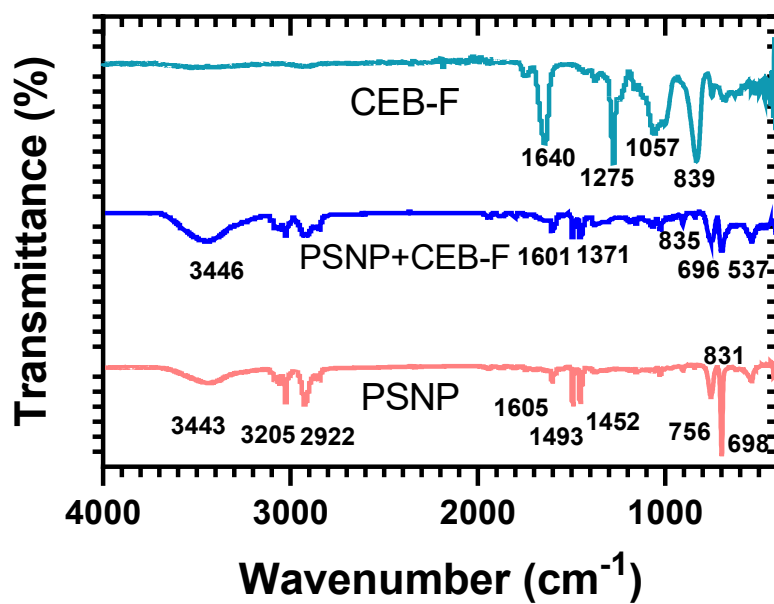


Fig. S3. FTIR spectra of pure CEB-F, PSNPs, and PSNP adsorption of CEB-F.

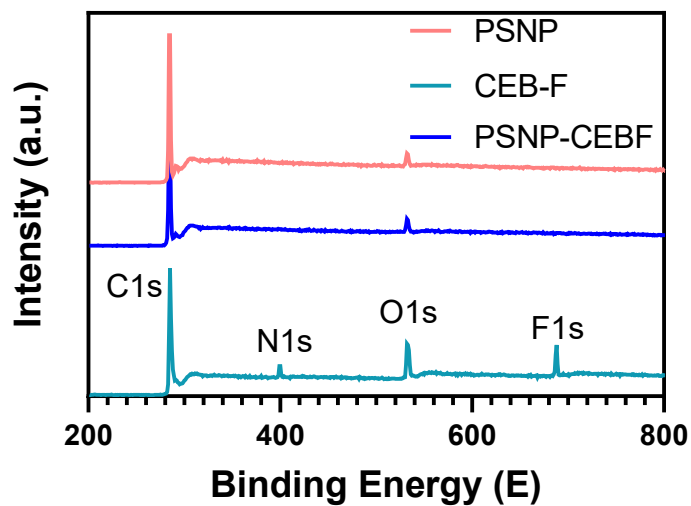


Fig. S4. XPS survey spectra of CEB-F, PSNPs, and PSNP after adsorption of CEB-F.

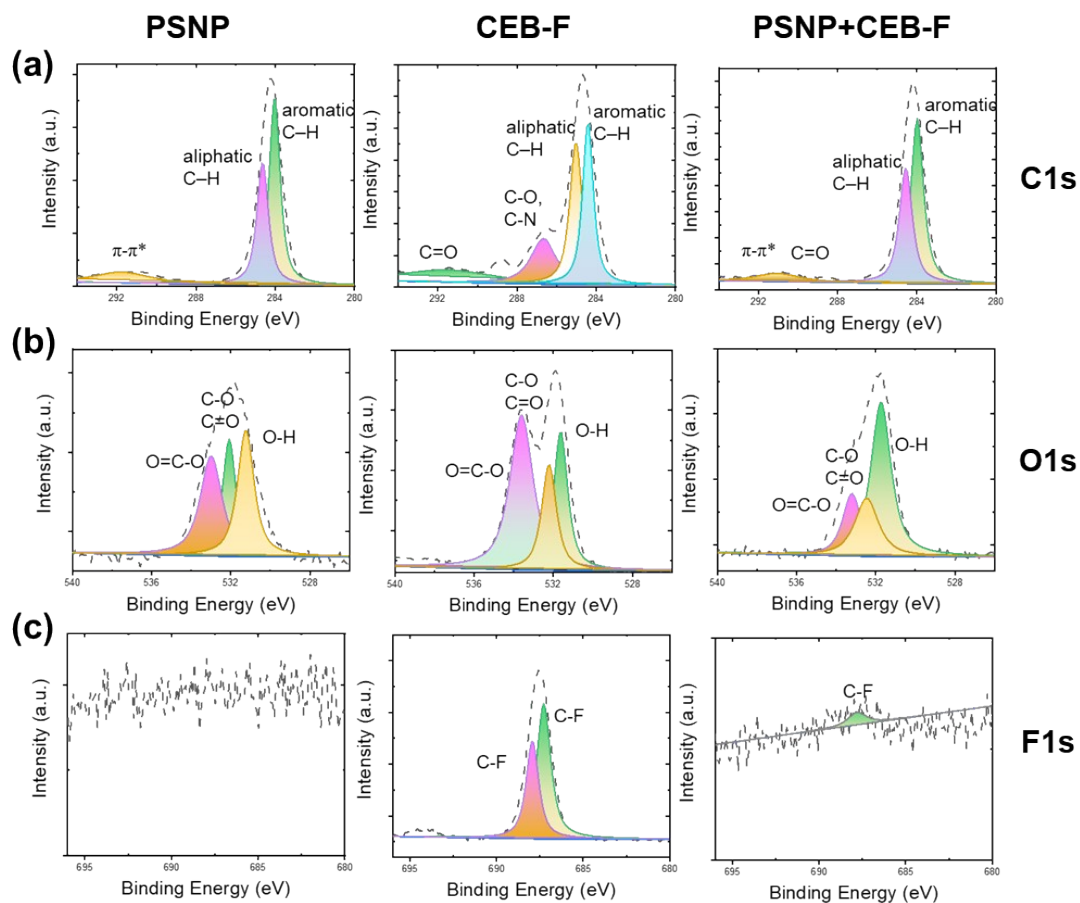


Fig. S5. XPS spectra of C1s (a), O1s (b), F1s (c) of PSNP, pure CEB-F, and PSNP-CEB-F.

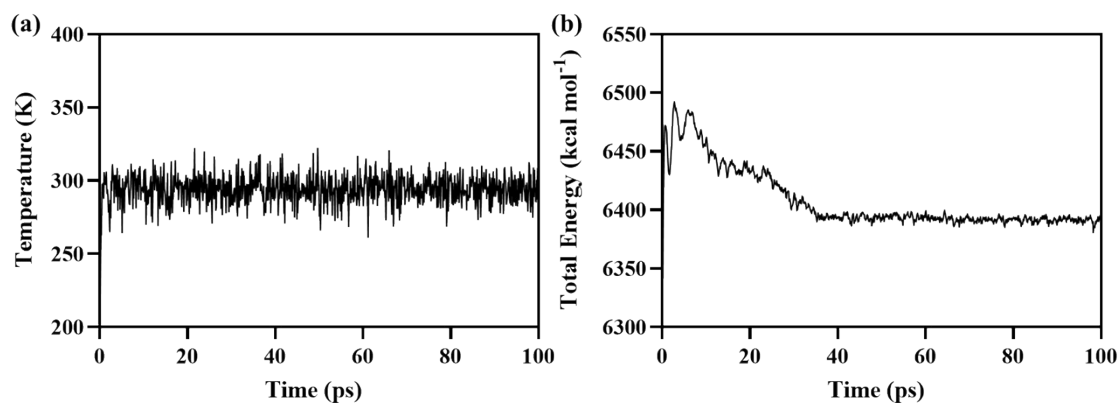


Fig. S6. The temperature (a) and (b) the energy versus time curves of the CEB-F and PSNPs during the final NPT MD simulation process.

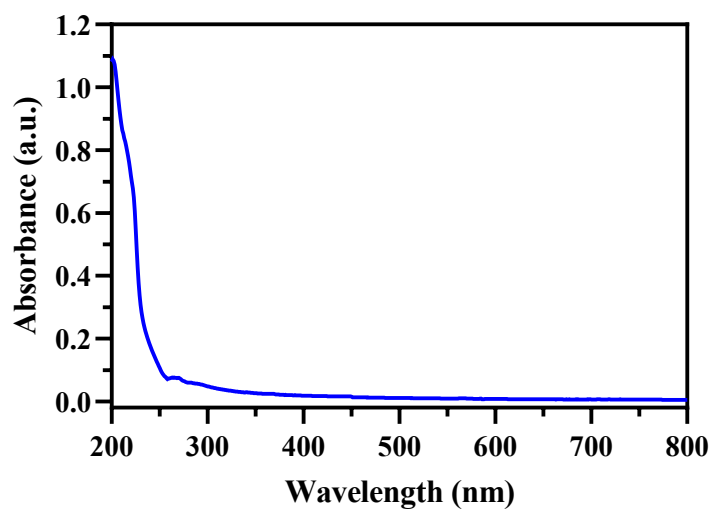


Fig. S7. UV-vis spectra of 5 mg L⁻¹ of PSNPs in water.

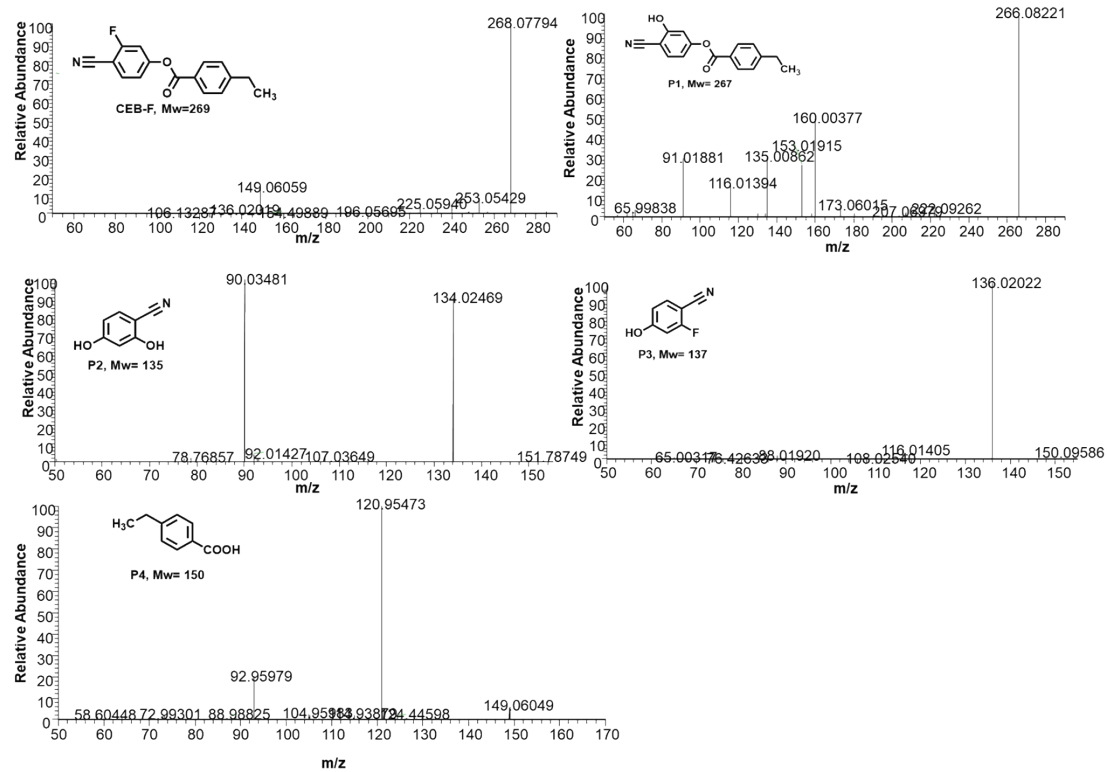


Fig. S8. UPLC-Q-Exactive Orbitrap-MS identification for the CEB-F and associated four primary phototransformation products (P1-P4).

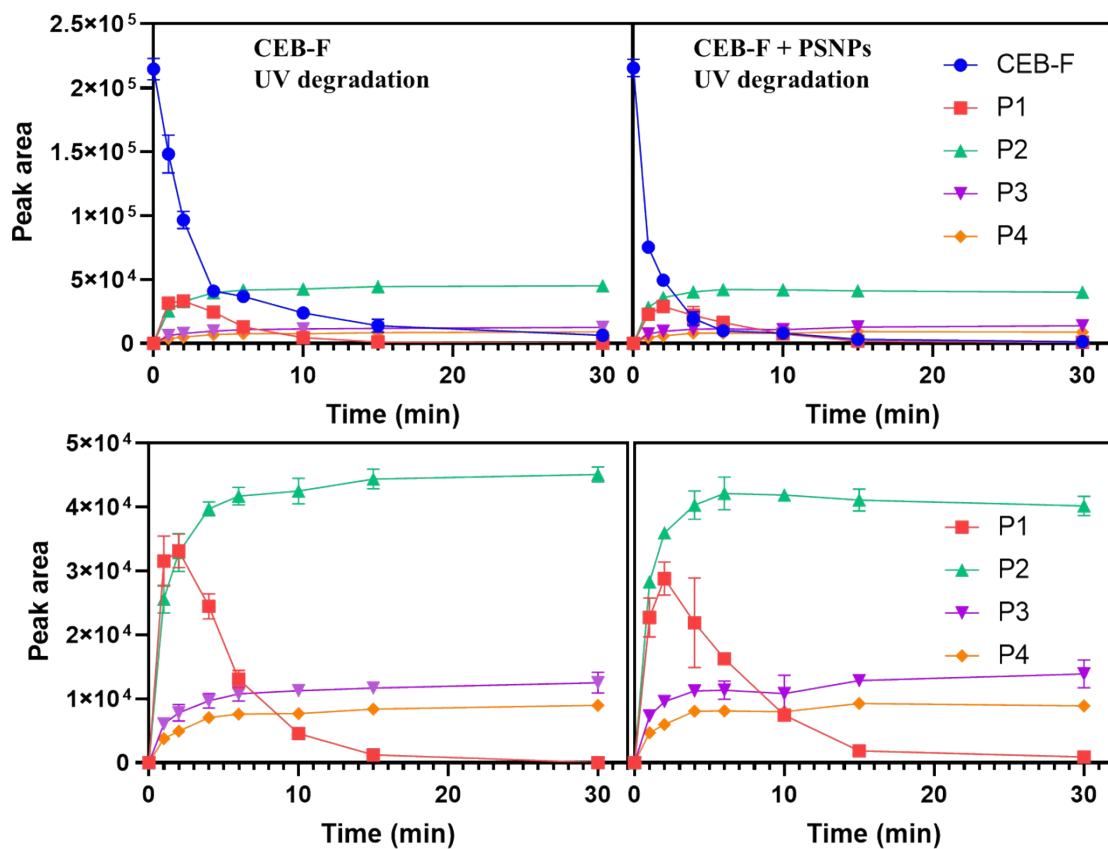


Fig. S9. Peak areas for CEB-F and associated four primary phototransformation products (P1-P4) when undergoes HPLC spectrum over the reaction time course.

Table S1. Fitness of dynamics models for CEB-F sorption on different plastics.

plastics	Pseudo-first-order			Pseudo-second-order			Intraparticle diffusion model			
	q_e ($\mu\text{mol/g}$)	k_1 (min^{-1})	R^2	q_e ($\mu\text{mol/g}$)	k_2 ($\mu\text{mol/g/min}$)	R^2	k_1	C_1	k_2	C_2
MCEMP	10.8453	0.0193	0.9792	13.0914	0.0017	0.9444	1.0251	1.3188	-0.1522	12.636
PAMP	6.9769	0.0062	0.9919	9.6208	0.0005	0.9915	0.3961	0.7374	0.1764	2.6603
PSMP	14.1503	0.6609	0.9977	14.3319	0.0914	0.9806	3.2035	5.1871	0.0174	13.8
PSNP	589.4106	0.0570	0.9969	672.9721	0.0009	0.0796	81.087	18.932	-0.8264	589.24

Table S2. Fitness of isotherm parameters for CEB-F sorption on different plastics.

Plastics	Langmuir		Freundlich			Henry		
	q_{max} ($\mu\text{mol/g}$)	k_L ($\text{L}/\mu\text{mol}$)	R^2	k_F ($\mu\text{mol/g}$) \cdot ($\mu\text{mol/L}$) ^{- $1/n$}	$1/n$	R^2	k_D (L/g)	R^2
PSMP	95.1760	0.0049	0.9996	1.1496	1.0882	0.9928	1.4949	0.9978
PSNP	1037.3882	0.0029	0.9851	120.3109	0.6425	0.8708	42.3969	0.9655

Table S3. Primary properties of various water samples.

Parameter	Unit	Pearl River water	Tap water	WWTP effluent water	South China Sea water
pH	-	7.37	7.28	7.03	8.15
TOC	mg L^{-1}	4.123	1.037	5.239	1.235
Na^+	mg L^{-1}	17.88	12.07	39.54	11289
K^+	mg L^{-1}	5.01	3.52	11.37	403
Cu^{2+}	$\mu\text{g L}^{-1}$	0.83	/	0.62	47.22
Mg^{2+}	mg L^{-1}	4.07	2.11	8.24	1507
Al^{3+}	$\mu\text{g L}^{-1}$	5.77	18.9	10.58	4.31
Cl^-	mg L^{-1}	15.62	12.37	51.24	19387
HCO_3^-	mg L^{-1}	5.13	2.87	3.52	6.57
SO_4^{2-}	mg L^{-1}	29.54	17.39	42.57	3305

Table S4. Calculated total energy of complex and each molecule and binding energy of CEB-F/PSNPs.

	Total energy (kcal mol ⁻¹)	Binding energy (kcal mol ⁻¹)
PS	6101.0632	-
CEB-F	39.2836	-
CEB-F-PS	6091.9393	-48.4075