Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Electronic Supplementary Infromation

Interactions of Emerging Contaminants with Model Colloidal Microplastics, C_{60} Fullerene, and Natural Organic Matter – Effect of Surface Functional Group and Adsorbate Properties

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List of Tables and Figures

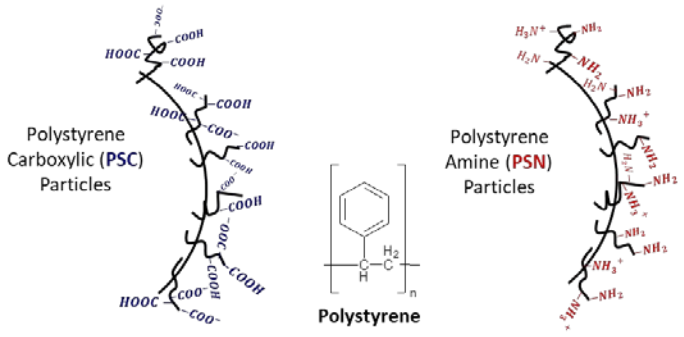

Figure S1 Depiction of the microparticles of different surface groups

Table S1 c_{max} and ΔG_{ads} values obtained from Langmuir fits of the adsorption data presented in Figure 2

AMP:m-PSC	Thermodynamic Parameters		CBZ:m-PSC	Thermodynamic Parameters	
pH	$c_{max} \times 10^{-6}$ (M)	ΔG_{ads} (kJ/mol)	pH	$c_{max} \times 10^{-6}$ (M)	ΔG_{ads} (kJ/mol)
4	15.0 ± 0.9	−40.5 ± 0.6	4	2.7 ± 0.2	−39.7 ± 0.7
7	26.8 ± 2.9	−40.3 ± 0.8	7	1.7 ± 0.2	−42.1 ± 1.1
10	31.3 ± 1.7	−41.1 ± 0.4	10	*Adsorption not detected*	
AMP:m-PSN	**Thermodynamic Parameters**		**CBZ:m-PSN**	**Thermodynamic Parameters**	
pH	$c_{max} \times 10^{-6}$ (M)	ΔG_{ads} (kJ/mol)	pH	$c_{max} \times 10^{-6}$ (M)	ΔG_{ads} (kJ/mol)
4	7.7 ± 0.6	−40.7 ± 0.8	4	4.8 ± 0.2	−36.9 ± 0.3
7	11.6 ± 0.6	−41.5 ± 0.4	7	4.8 ± 0.5	−40.4 ± 1.0
10	15.0 ± 0.9	−42.4 ± 0.7	10	5.0 ± 0.9	−35.2 ± 0.9

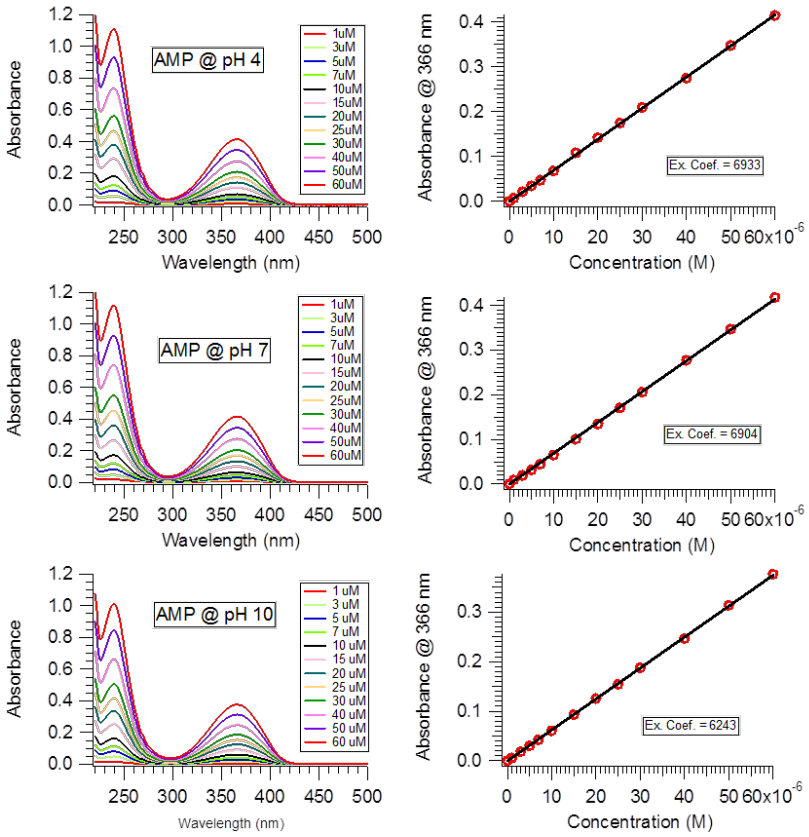

Figure S2 UV-Vis absorption spectra of AMP at different concentrations and the corresponding calibration curves as a function of pH

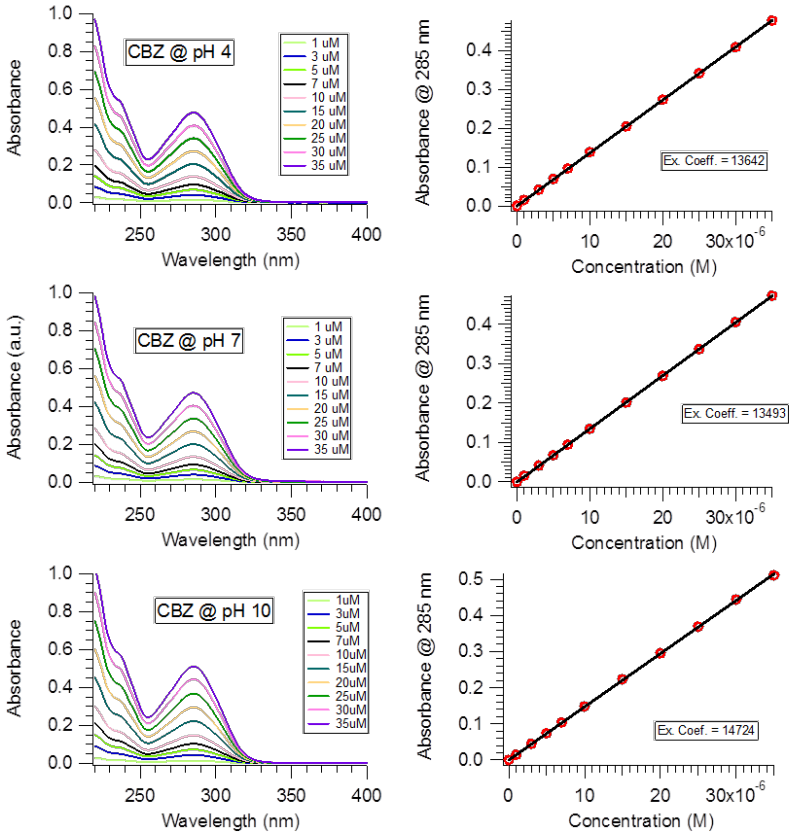

Figure S3 UV-Vis absorption of spectra of CBZ at different concentrations and the corresponding calibration curves as a function of pH

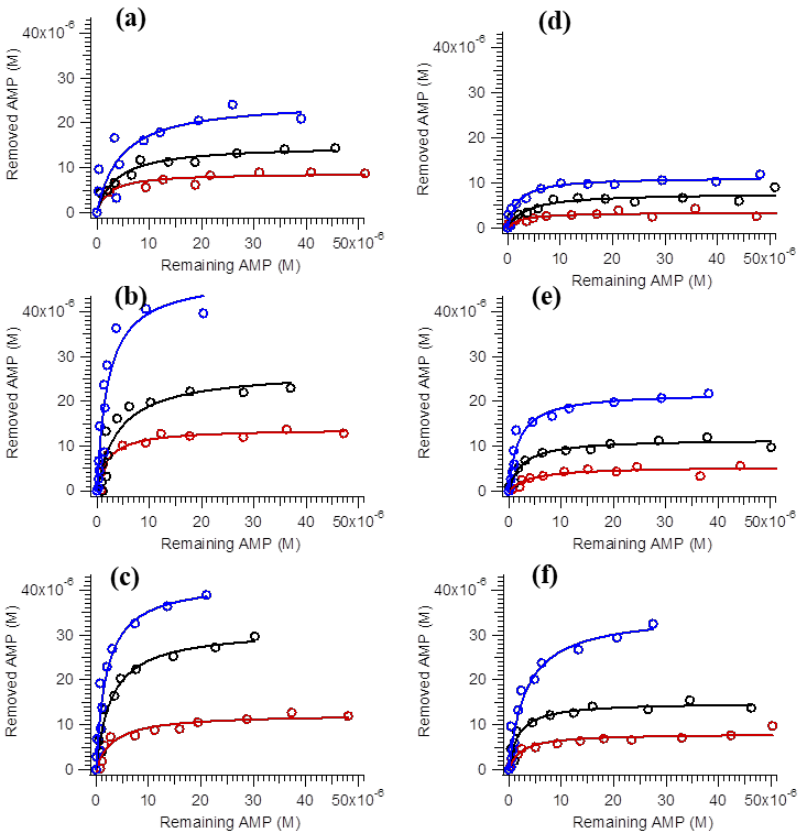

Figure S4 Adsorption isotherms of AMP onto *m*-PSC in (a) pH 4 (b) pH 7 and (c) pH 10 solution and onto m-PSN in (d) pH 4 (e) pH 7 and (f) pH 10 solution for three number densities: 0.5 (red), 1.0 (black), 2.0 (blue) × 10^8 particles mL^{-1}

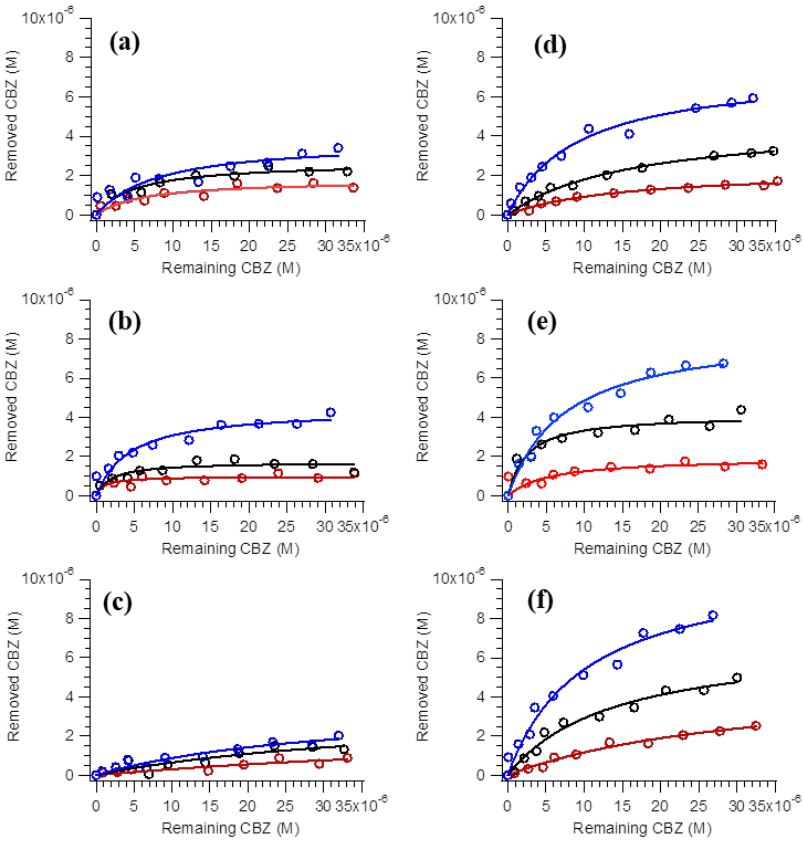

Figure S5 Adsorption isotherms of CBZ onto *m*-PSC in (a) pH 4 (b) pH 7 and (c) pH 10 solution and onto m-PSN in (d) pH 4 (e) pH 7 and (f) pH 10 solution for three number densities: 0.5 (red), 1.0 (black), 2.0 (blue) × 10^8 particles mL^{-1}

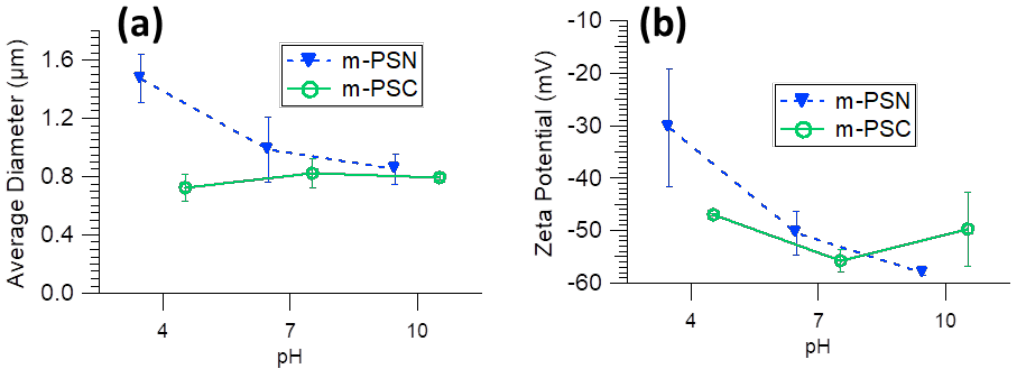

Figure S6 Initial particle size (a) and zeta-potential (b) as a function of pH

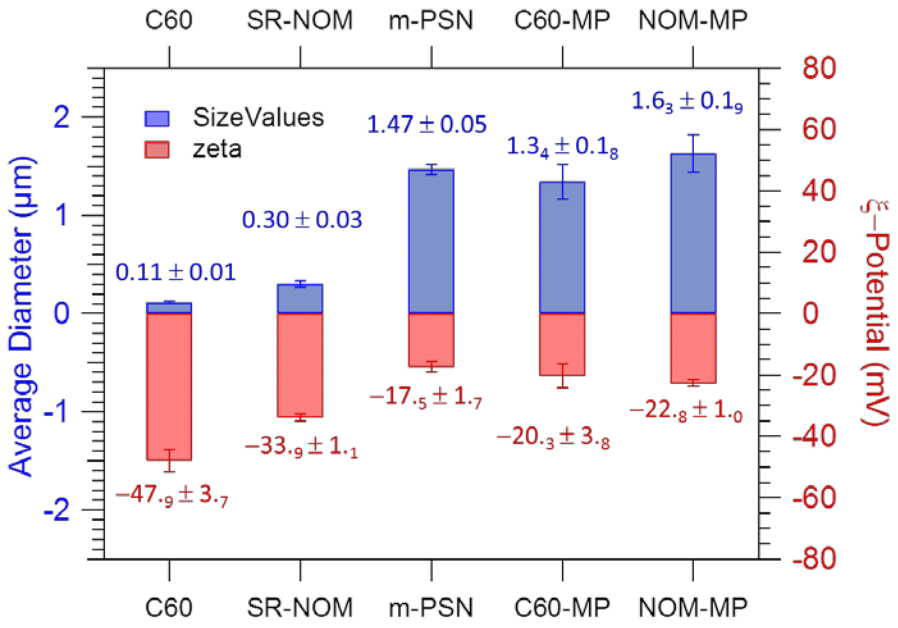

Figure S7 The average size (hydrodynamic diameter, left axis) and ξ-potential (right axis) of colloids used in this study. These measurements are based on dynamic light scattering. The size and ξ-potential were collected at the particle (m-PSN, C_{60}-MP, and NOM-MP) number density of $1 \times 10^{8}\ mL^{-1}$. As for the C_{60} and SR-NOM, the concentrations are 115 ppm and 139 u[C60] for SR-NOM and C_{60}, respectively.

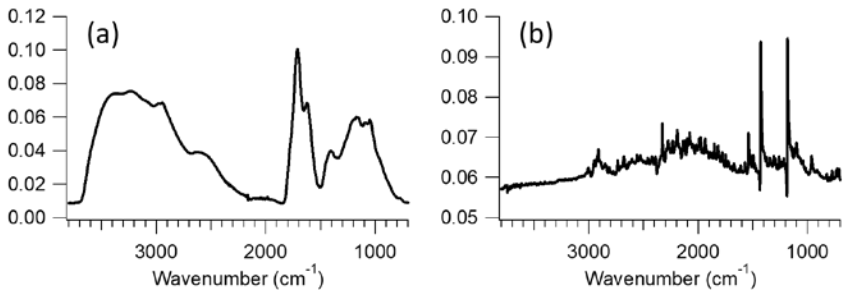

Figure S8 ATR-FTIR spectra of (a) SR-NOM solids and (b) C_{60} powder.

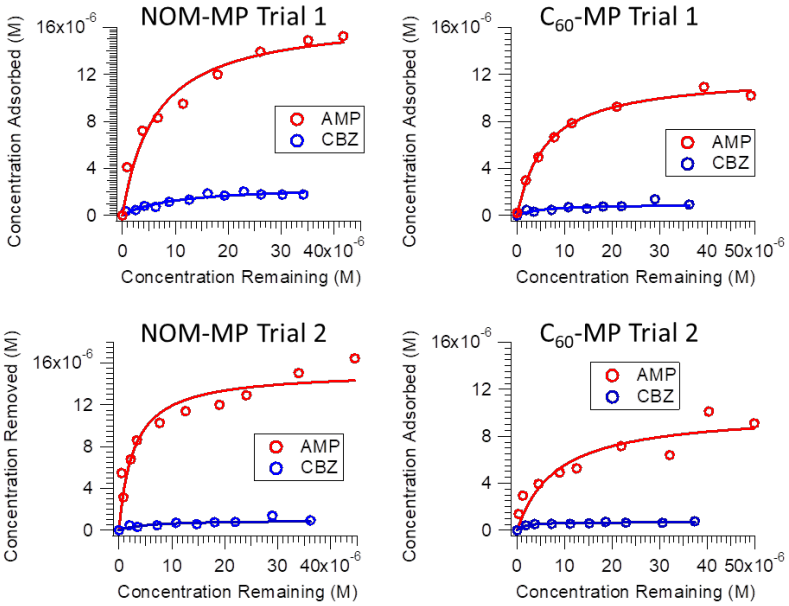

Figure S9 Replicates of CBZ and AMP adsorption isotherms of onto NOM-MP and C_{60}-MP in 0.1 M PBS (pH 7.4). The markers correspond to experimental data. The solid curves represent fitting of experimental data with Langmuir isotherm model.

Table S2 Average c_{max}, Γ_i and ΔG_{ads} for the AMP and CBZ adsorption on C_{60}-MP and NOM-MP in 0.1M PBS (pH 7.4)

Pharmacetical: Substrate	$c_{max} \times 10^{-6}$ (M)	Γ_i $(molecules/nm^2)$	ΔG_{ads} (kJ/mol)
AMP:NOM-MP	16.1 ± 1.2	17.2 ± 4.8	-40.3 ± 1.4
CBZ:NOM-MP	3.7 ± 1.6	4.0 ± 2.0	-37.7 ± 0.6
AMP:C60-MP	10.4 ± 1.5	7.5 ± 2.0	-39.1 ± 0.4
CBZ:C60-MP	0.8 ± 0.2	0.6 ± 0.2	-41.3 ± 2.3

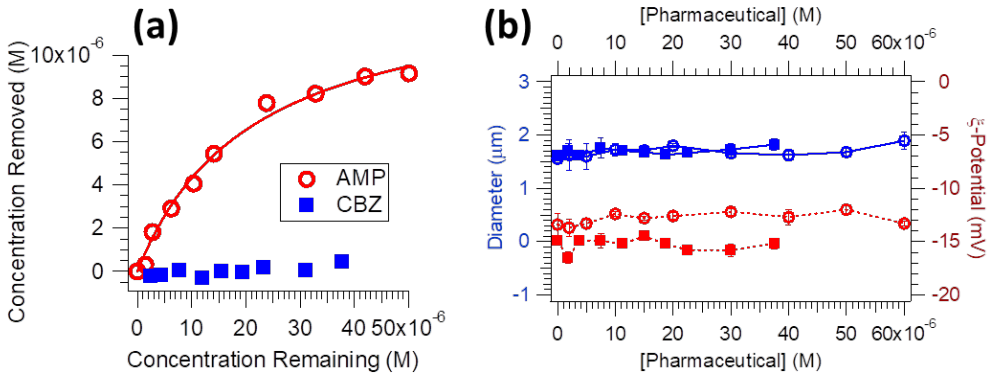

Figure S10 Control Experiment – (a) adsorption isotherms and (b) the corresponding size (blue) and zeta potential measurements (red) of AMP (circle) and CBZ (square) onto m-PSN in 0.1 M PBS (pH 7.4).

Table S3 Average c_{max} and ΔG_{ads} for the AMP and CBZ adsorption on the surrogate m-PSN particle in 0.1M PBS (pH 7.4)

Pharmaceutical: Substrate	$c_{max} \times 10^{-6}$ (M)	ΔG_{ads} (kJ/mol)
AMP:m-PSN	13.4 ± 0.9	-36.2 ± 0.4
CBZ:m-PSN	*Adsorption not detected*	

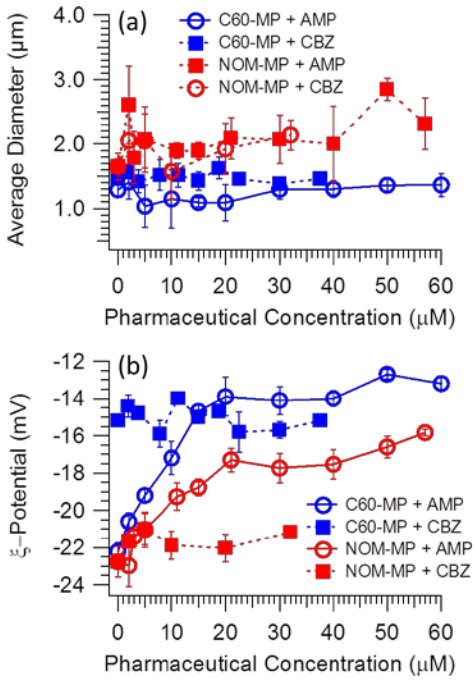

Figure S11. Size (a) and (b) zeta-potential measurement of colloidal C_{60}-MP (blue) and NOM-MP (red) as a function of AMP (circle) and CBZ (square) concentration. Each data point represents average of at least three measurements.