Supplementary data

Effect of microplastics on the binding properties of Pb(II) onto dissolved organic matter: insights from fluorescence spectra and FTIR combined with two-dimensional correlation spectroscopy

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This Supplementary data includes a total of 10 pages (including this page) with 2 sections for experimental, references, and 6 figures and 1 tables.

1. Data analysis

1.1. Fluorescence quenching analysis

Fluorescence quenching is an analytical technique based on the actual molecular contact between the fluorophore and the quenching agent with high sensitivity. The Modified Stern-Volmer equation[1-3] is used to fit the fluorescence quenching data of HA with the addition of Pb^{2+}:

$$\frac{F_0}{F_0 - F} = \frac{1}{f \cdot K_M \cdot C_M} + \frac{1}{f}$$

Where, F_0 represents the initial fluorescence intensity, that is, the fluorescence intensity of HA without heavy metal ions or PSMPs added. F represents the measured fluorescence intensity, and the fluorescence intensity of HA after adding heavy metal ions or PSMPs. f represents the proportion of metal-bound fluorophores to the initial fluorescence. K_M and C_M are the conditional stability constant and the total heavy metal concentration, respectively. The f and K_M values are calculated by plotting a linear relationship between $F_0/(f_0\text{-}f)$ and $1/C_M$.

1.2. two-dimensional correlation spectroscopy (2D-COS) analysis

2D-COS analysis for the SF and FTIR spectral data was performed using the 2D Shige software to further explore the sites and sequential orders for the interaction of EPS with PSMPs.[4, 5]

(2D-Shigeversion 1.3, https://sites.google.com/site/Shigemorita/home/2dshige)

The graphs were further plotted by use of Origin 9.0 software.

2. Reference

1 X Li, B Wu, Q Zhang, et al. Complexation of humic acid with Fe ions upon persulfate/ferrous oxidation: Further insight from spectral analysis [J]. *J Hazard Mater*, **2020**, 399: 123071.

2 N Habibul, W Chen. Structural response of humic acid upon binding with lead: A spectroscopic insight [J]. *Sci Total Environ*, **2018**, 643: 479-85.

3 Y Ding, M Liu, S Peng, et al. Binding characteristics of heavy metals to humic acid

before and after fractionation by ferrihydrite [J]. *Chemosphere*, **2019**, 226: 140-8.

4 Y Park, S Jin, I Noda, et al. Emerging developments in two-dimensional correlation spectroscopy (2D-COS) [J]. *Journal of Molecular Structure*, **2020**, 1217.

5 H Luo, Q Cheng, Q Fan, et al. FT-IR and synchronous fluorescence two-dimensional correlation spectroscopic analysis on the binding properties of mercury onto humic acids as influenced by pH modification and sulfide addition [J]. *Sci Total Environ*, **2022**, 819: 152047.

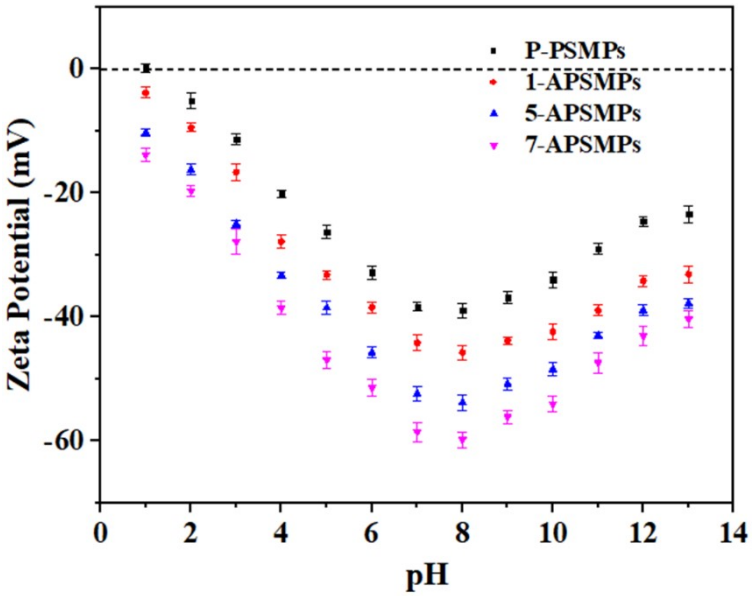
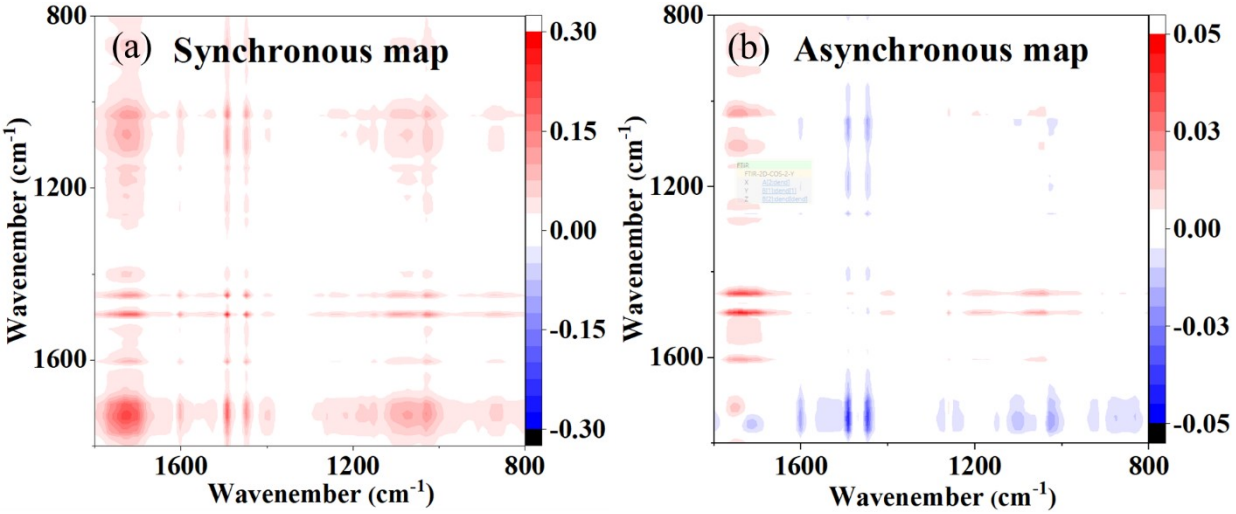


Figure S1 The zeta potentials of pristine and aged PSMPs.



64 Figure S2 2D-FTIR-COS of PSMPs

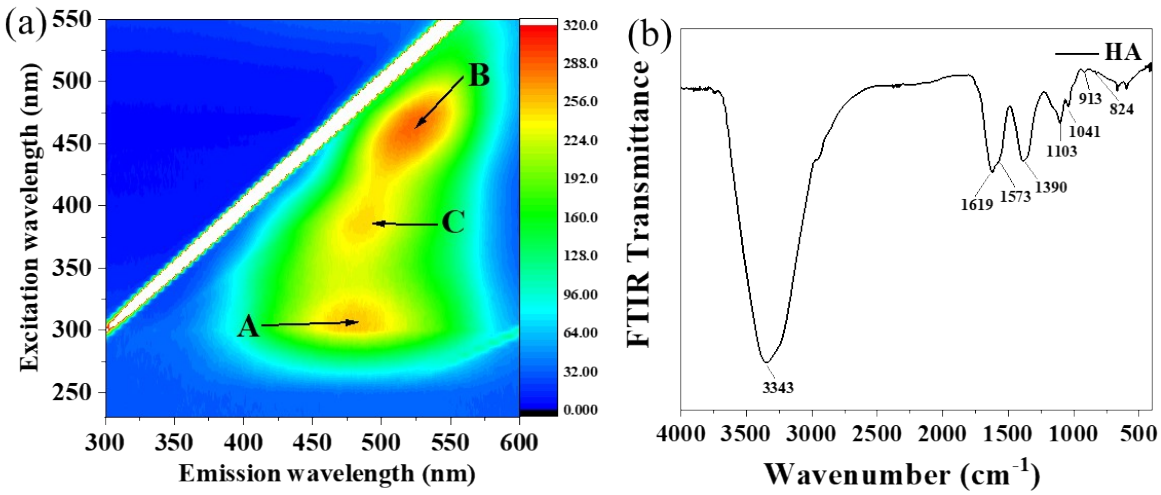


Figure S3 3D-EEM fluorescence spectroscopy (a) and FTIR (b) of HA.

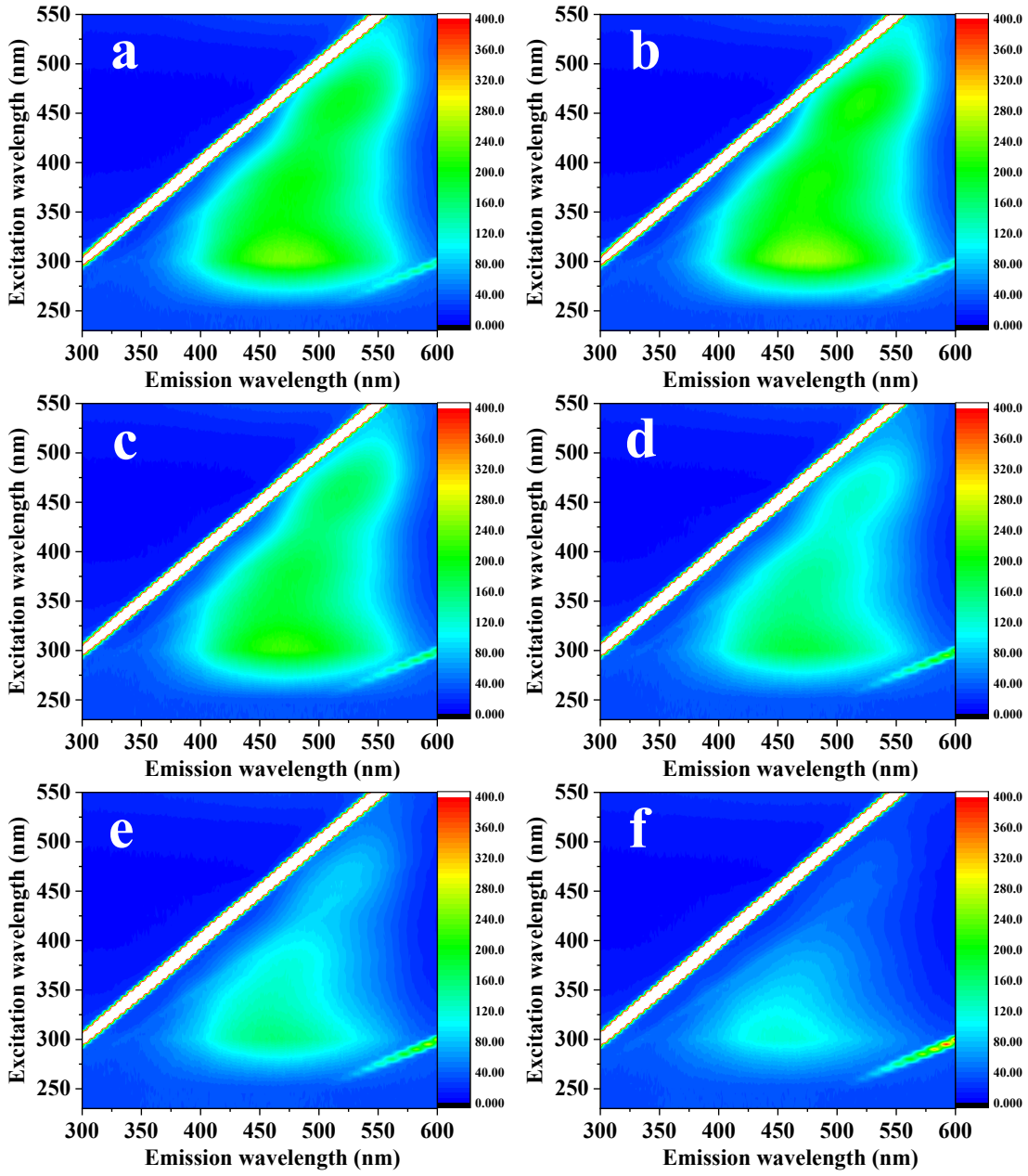


Figure S4 3D-EEM of HA after Pb^{2+} adsorption

(the concentraion of Pb^{2+} are: 0.50, 1.0, 2.0, 5.0, 10 and 20 $mg \cdot L^{-1}$).

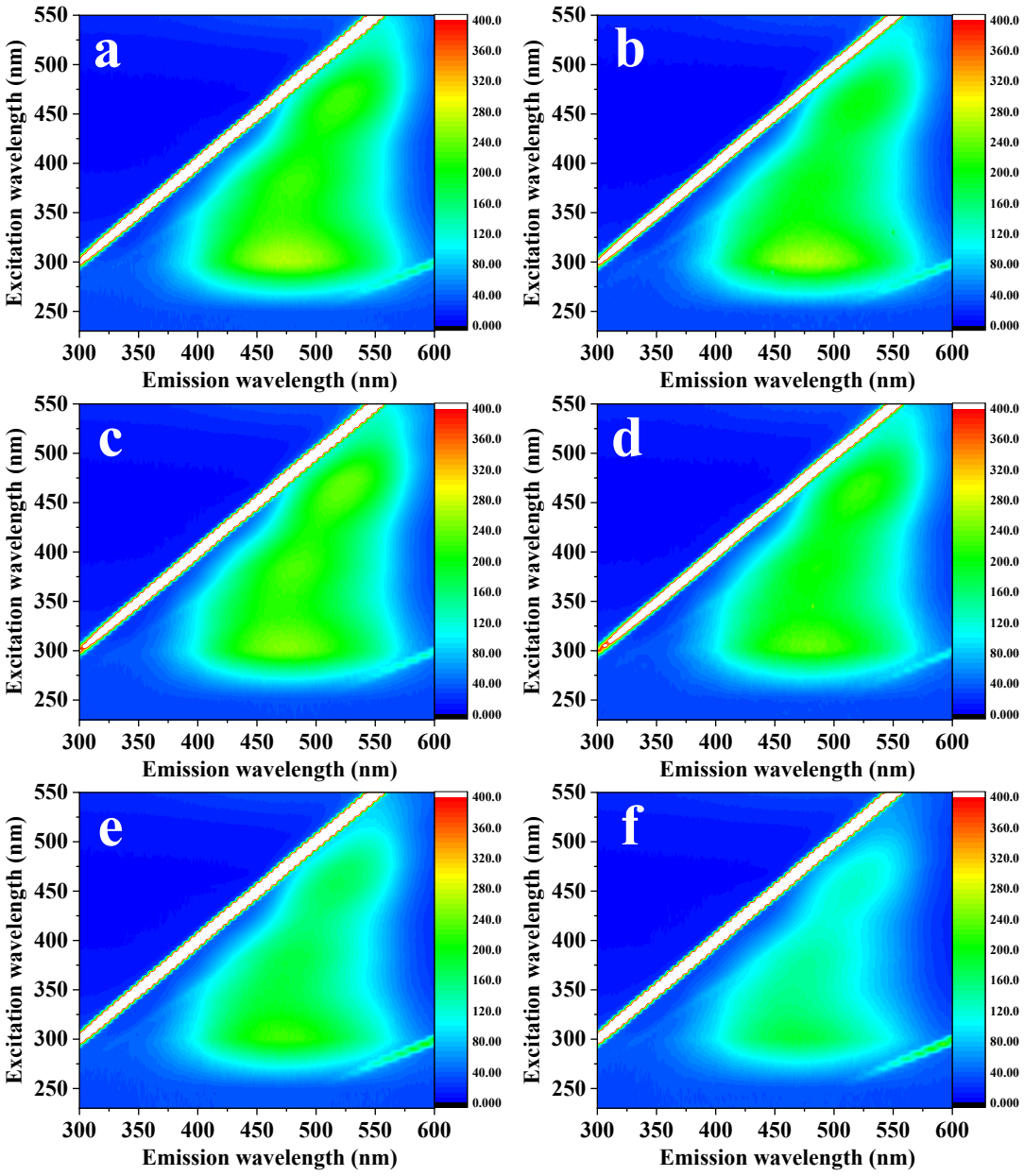


Figure S5 3D-EEM of HA after PSMPs adsorption

(the concentraion of PSMPs are: 0.10, 1.0, 5.0, 10, 50 and 100 mg·C·L^{-1}).

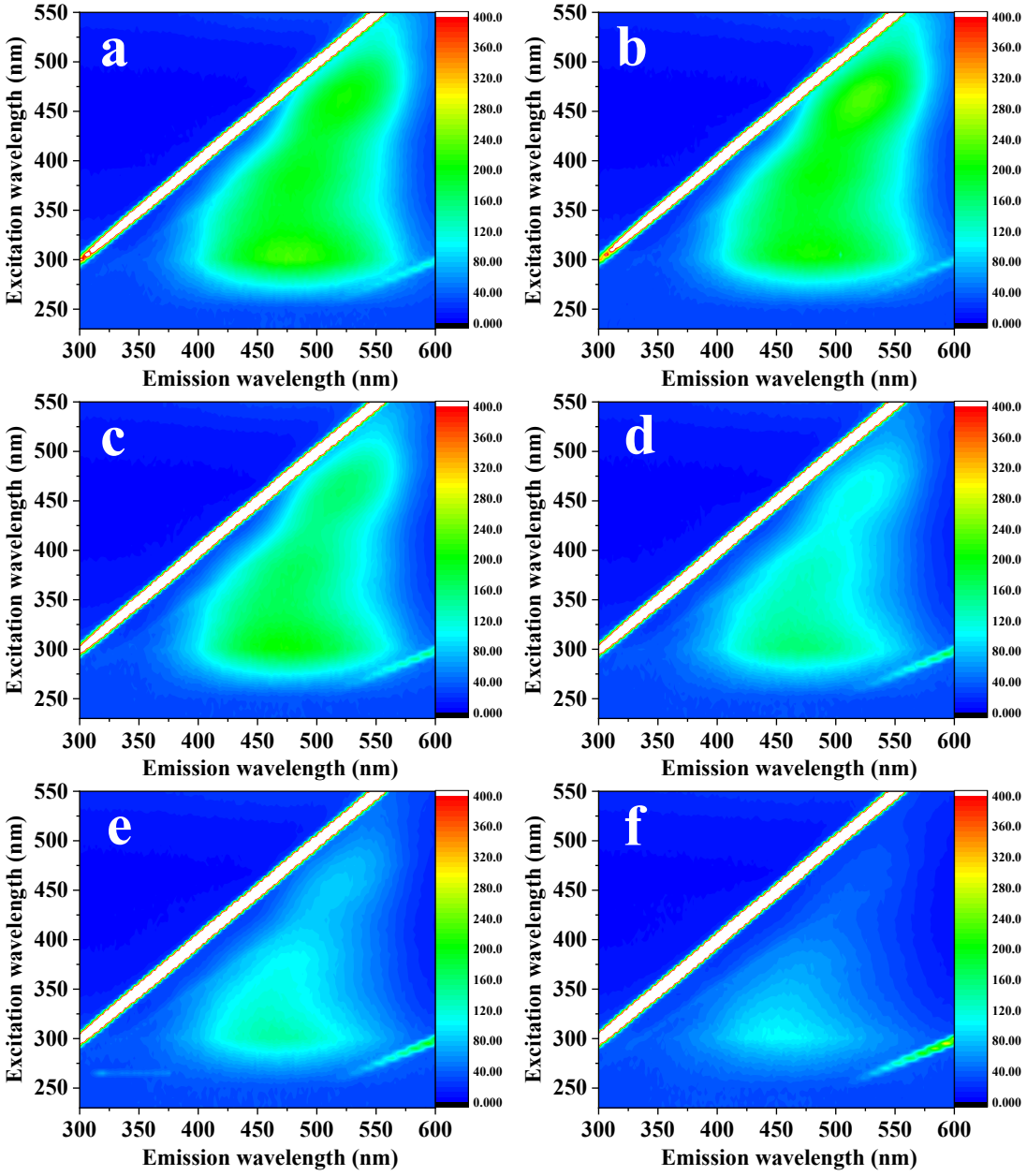


Figure S6 3D-EEM of HA after Pb^{2+} adsorption in HA-PSMPs-Pb^{2+} system (HA: PSMPs = 1:1) (the concentraion of Pb^{2+} are: 0.50, 1.0, 2.0, 5.0, 10 and 20 $mg \cdot L^{-1}$).

79 Table S1 The BET surface of the pristine PSMPs and aged PSMPs.

Materials	BET surface area ($m^2 \cdot g^{-1}$)	Average pore diameter (nm)	Micropore volume ($cm^3 \cdot g^{-1}$)
P-PSMPs	3.68	1.51	0.00131
1-APSMPs	13.6	1.52	0.00392
5-APSMPs	46.1	1.54	0.0134
7-APSMPs	54.8	1.63	0.0156

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