Electronic Supplementary Material (ESI) for Environmental Science: Water Research & Technology.

Cephalexin interaction with biosolids-derived dissolved organic matter: binding mechanism and implications for adsorption by biochar and clay

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Table S1. Physicochemical characteristics of biochar and montmorillonite used in adsorption study.

Material	N_2 specific surface area (m^2 g^{-1})	Cation exchange capacity (meq 100 g^{-1})	%C	%N	Particle size (µm)
Date palm petiole biochar	71.07	1.48	71.03	0.25	<180
SWy-1[a]	31.82	76.4			1.15[1]

[a] SWy-1 surface area and cation exchange capacity from The Clay Minerals Society (clays.org/sourceclays_data/)

Table S2. Basic chemical and optical characteristics of DOM used in experiments. Properties were determined in deionized water. Standard deviations of replicated measurements (n=3) are presented in parentheses.

% C	$SUVA_{254}$ (L mg^{-1} C m^{-1})	Fluorescence index (FI)	Humification index (HIX)	Biological fluorescence index (BIX)	pH
38.4 (0.002)	1.01 (0.06)	1.7 (0.03)	0.36 (0.01)	1.15 (0.04)	5.78 (0.03)

Table S3. Ryan-Weber fitting parameters for cephalexin-DOM binding at experimental pH values.

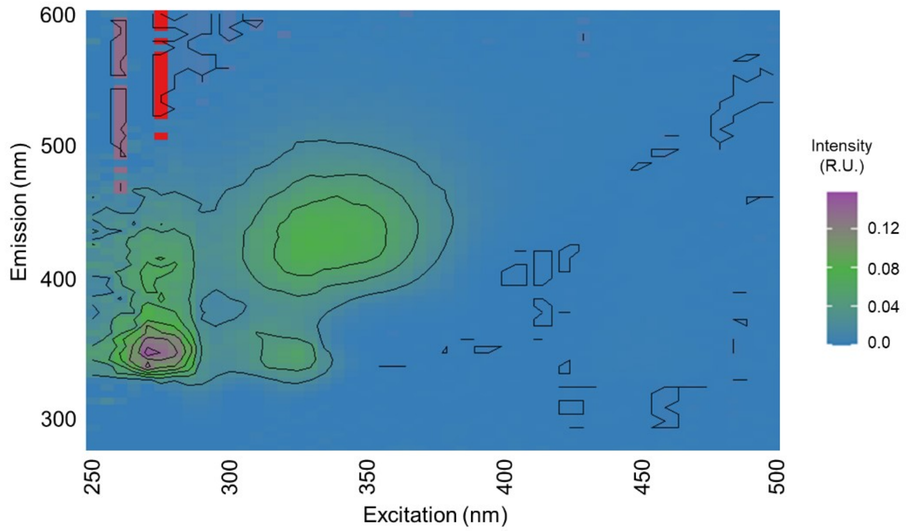
pH	Log K_c	L_t (M)	Root-mean-square error
4.0	8.48	$8.57 \bullet 10^{-4}$	$4.36 \bullet 10^{-2}$
5.0	7.16	$2.48 \bullet 10^{-3}$	$4.94 \bullet 10^{-2}$
7.0	5.33	$3.99 \bullet 10^{-3}$	$2.26 \bullet 10^{-2}$

Table S4. Ryan-Weber fitting parameters for cephalexin-DOM binding at experimental background ionic strength values and cation charges.

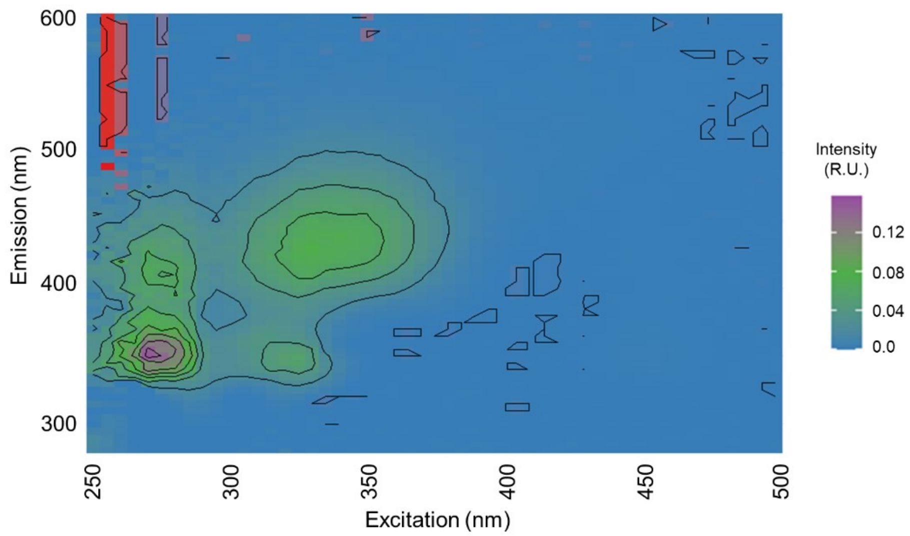
Background ionic strength condition	Background cation	Log K_c	L_t (M)	Root-mean-square error
DDIW	N/A	6.00	$2.41 \bullet 10^{-3}$	$4.29 \bullet 10^{-2}$
I = 0.10 M	Na^+	6.41	$2.16 \bullet 10^{-3}$	$1.99 \bullet 10^{-2}$
I = 0.10 M	Ca^{+2}	5.93	$1.78 \bullet 10^{-3}$	$4.31 \bullet 10^{-2}$

Figure S1. EEMs of 50 ppm cephalexin collected at a) pH = 4.0, b) pH = 5.0 and c) pH = 7.0.

a)



b)



c)

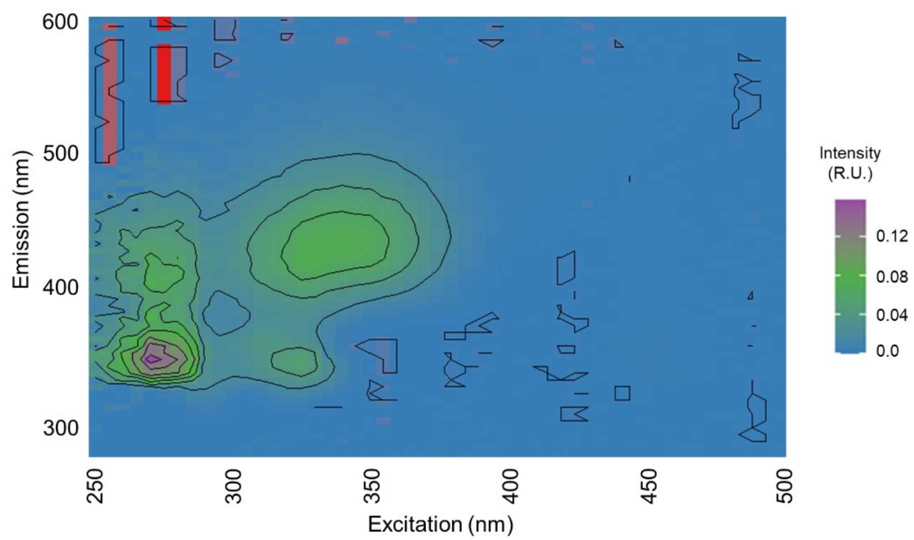
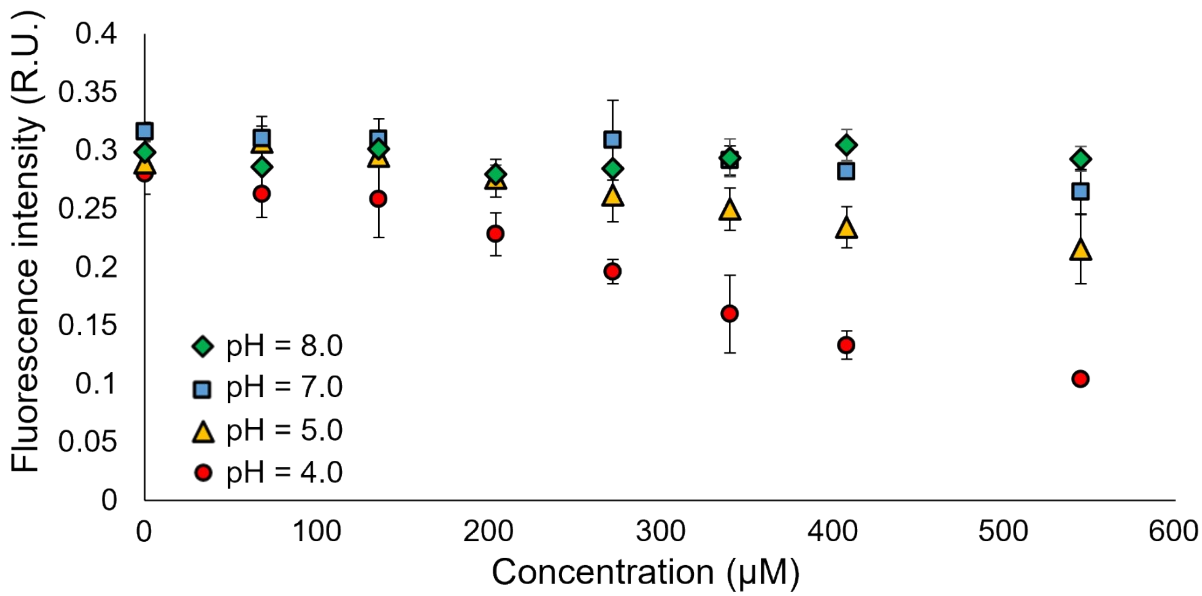


Figure S2. Fluorescence intensities versus cephalexin concentration for [DOM] = 2.5 mg C L^{-1} in synthetic wastewater at pH = 4.0 (red), 5.0 (yellow), 7.0 (blue) and 8.0 (green). Error bars



represent standard deviations of experimental replicates (n=3).

Figure S3. Cephalexin charge and chemical speciation variation with pH. Experimental pH values are denoted by the dashed vertical lines. Dissociation constants were determined experimentally by Mrestani et al.[2]

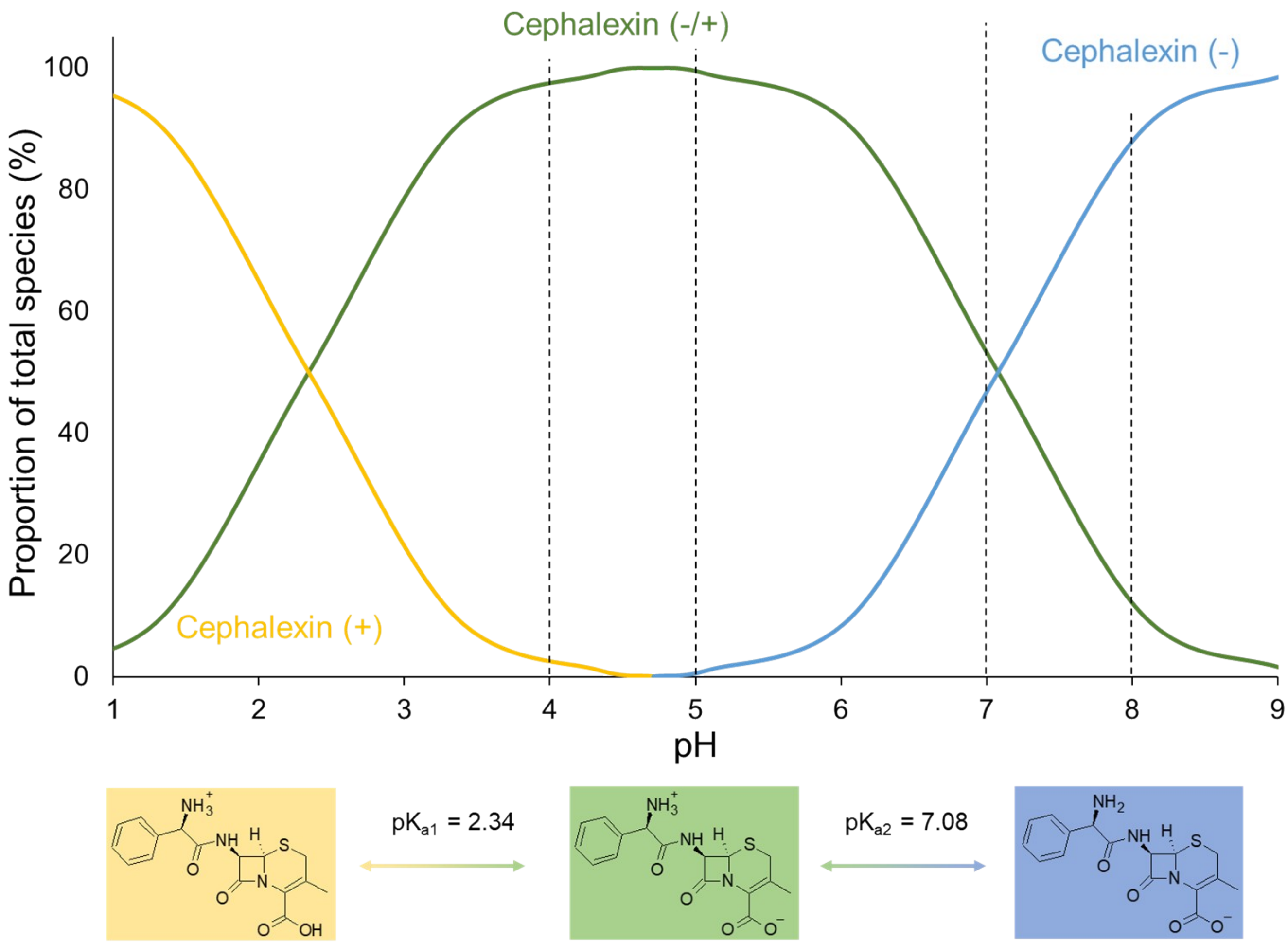


Figure S4. Relationship between log K_c and pH for cephalexin-DOM binding in a synthetic wastewater matrix

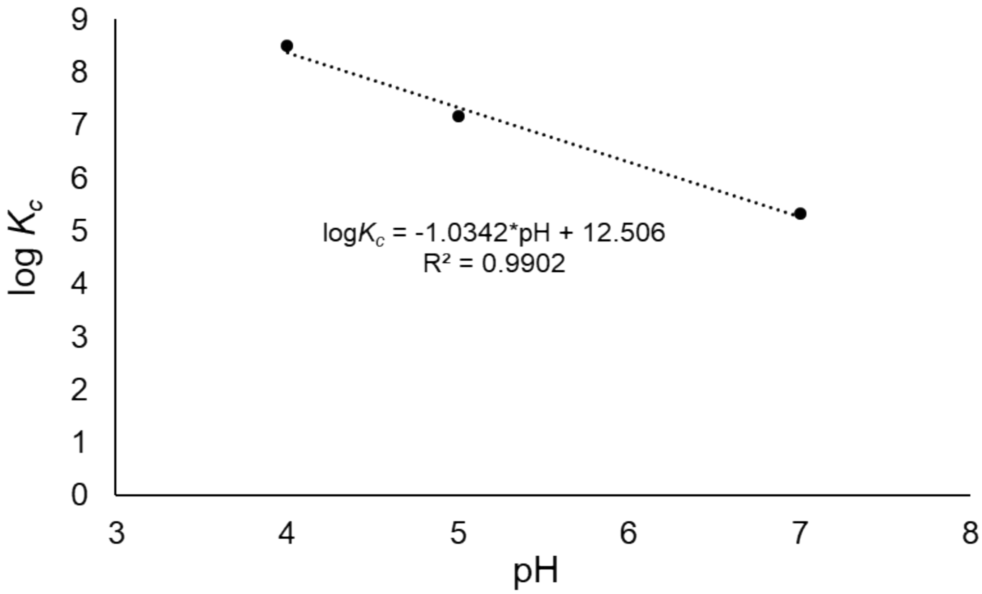
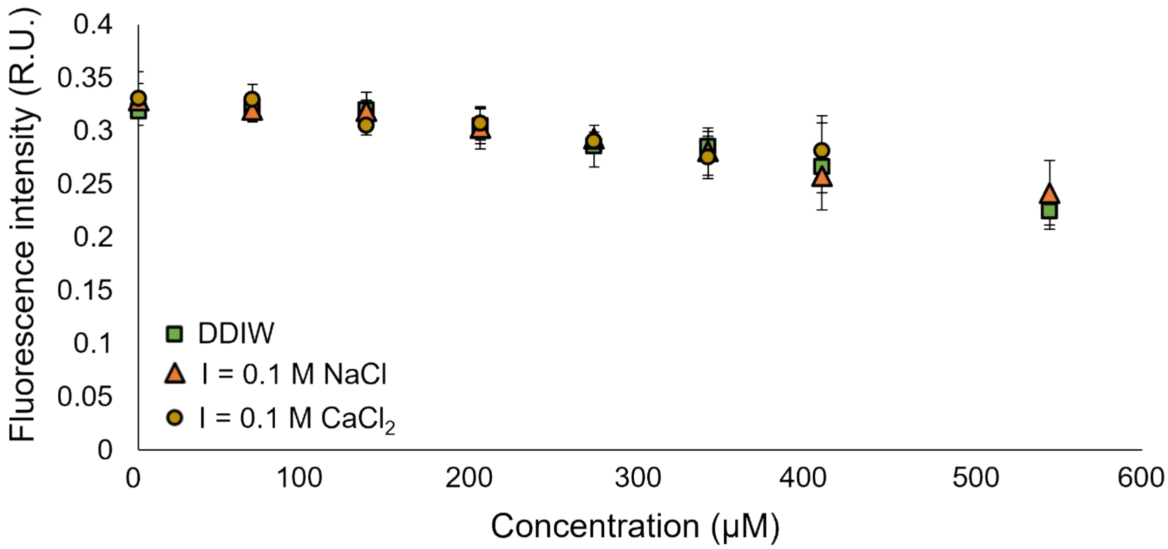


Figure S5. Fluorescence intensities versus cephalexin concentration for [DOM] = 2.5 mg C L^{-1} in ultrapure water (green), I = 0.1 M NaCl (orange) and I = 0.1 M $CaCl_2$ (brown). Error bars represent standard deviations of experimental replicates (n=3).



References

1. M.A. Anderson and P.M. Bertsch, Electrophoretic Mobility and Particle Size of Clays Using Laser Doppler Velocimetry-Photon Correlation Spectroscopy, Soil Sci. Soc. Am. J., 1993, 57, 1641-1643.
2. Y. Mrestani, R. Neubert, A. Munk and M. Wiese, Determination of dissociation constants of cephalosporins by capillary zone electrophoresis, J. Chromatogr. A, 1998, 803, 273-278.