

Supporting Information

Effect of humic acid on the sulfamethazine adsorption by functionalized multi-walled carbon nanotubes in aqueous solution: mechanisms study

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There are 9 figures and 3 tables.

There are 14 pages totlly.

Figure and tables

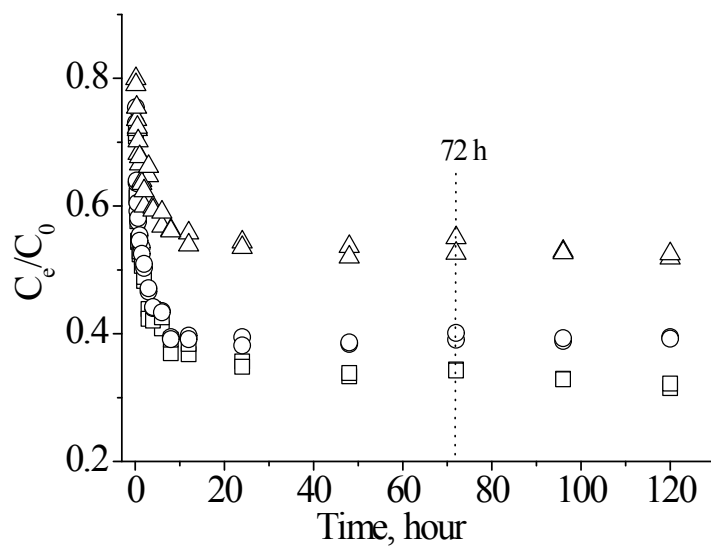


Fig. S1. Adsorption kinetics of HA onto P-MWCNT (\square), C-MWCNT (\circ), and H-MWCNT (Δ).

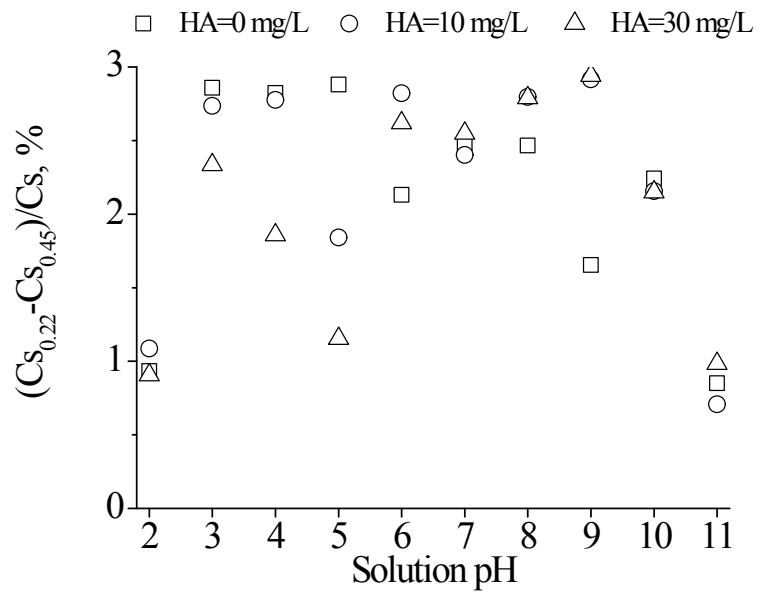


Fig. S2 The effect of membrane pore size on measurement of solubility of SMZ. $C_{s0.22}$ and $C_{s0.45}$ are the solubility of SMZ filtered by 0.22 μm and 0.45 μm , respectively.

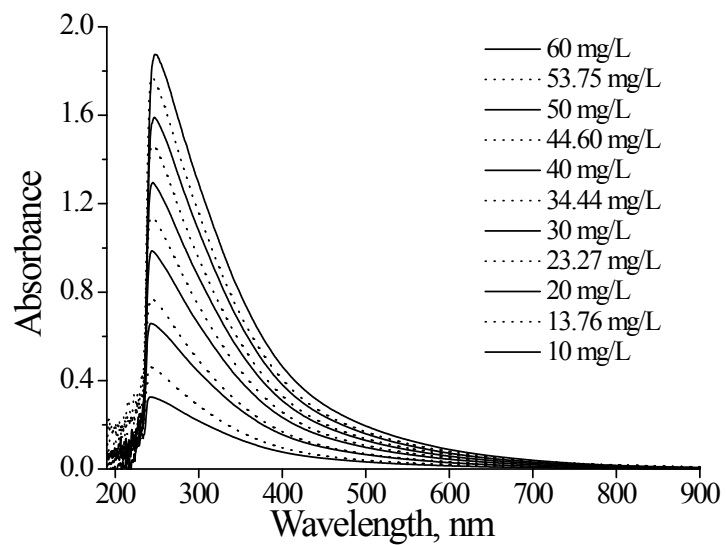


Fig. S3. Ultraviolet-visible absorbance spectra of HA with concentrations from 10 to 60 mg L⁻¹ at 190–900 nm. The solid line represents the HA concentration before adsorption and the dotted line shows the HA concentration at adsorption equilibrium.

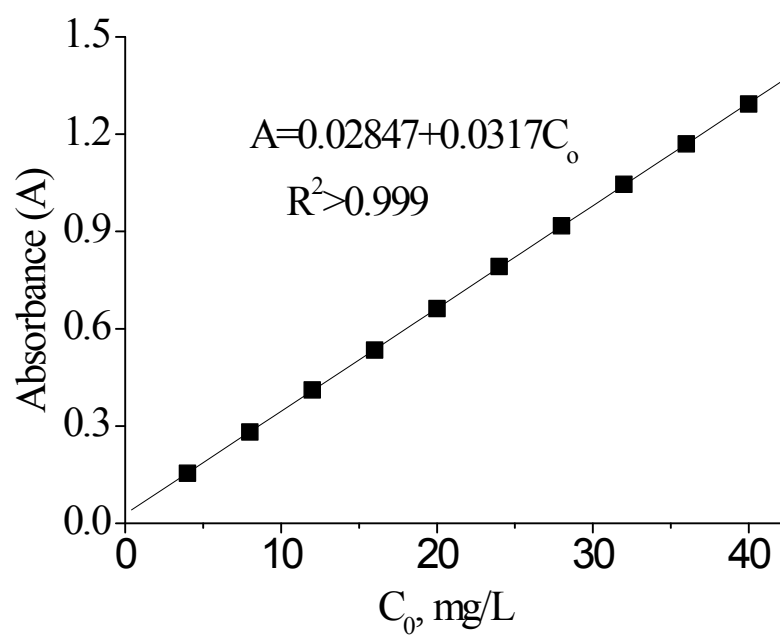


Fig. S4. HA concentration-absorbance calibration curve.

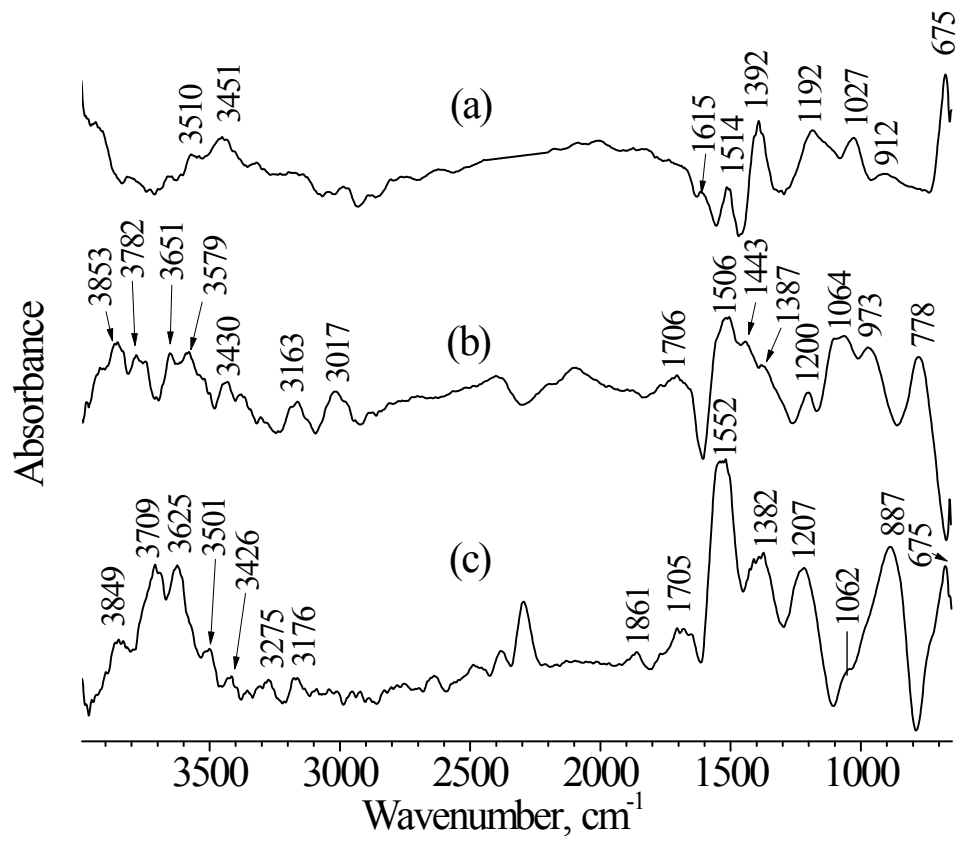


Fig. S5. μ -FTIR spectra of P-MWCNT (a), C-MWCNT (b), and H-MWCNT (c).

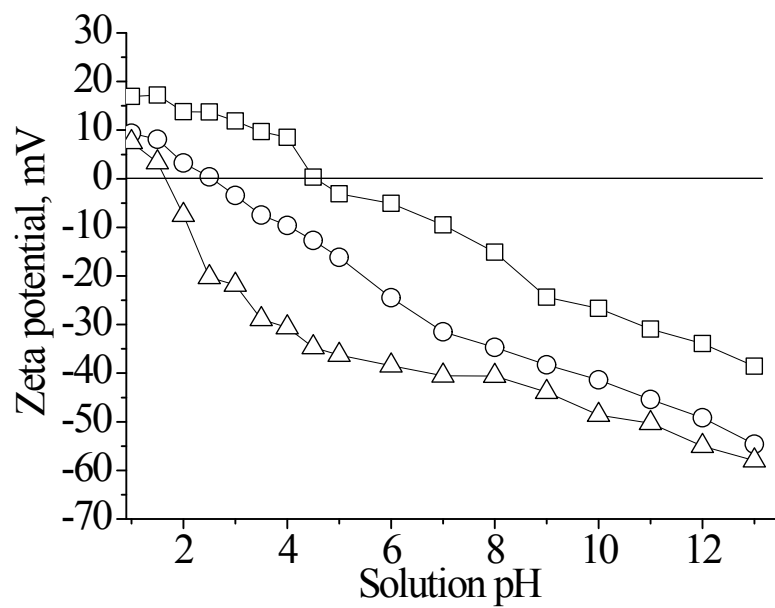


Fig. S6. Zeta potential of P-MWCNT (\square), C-MWCNT (\circ), and H-MWCNT (Δ) as a function of pH.

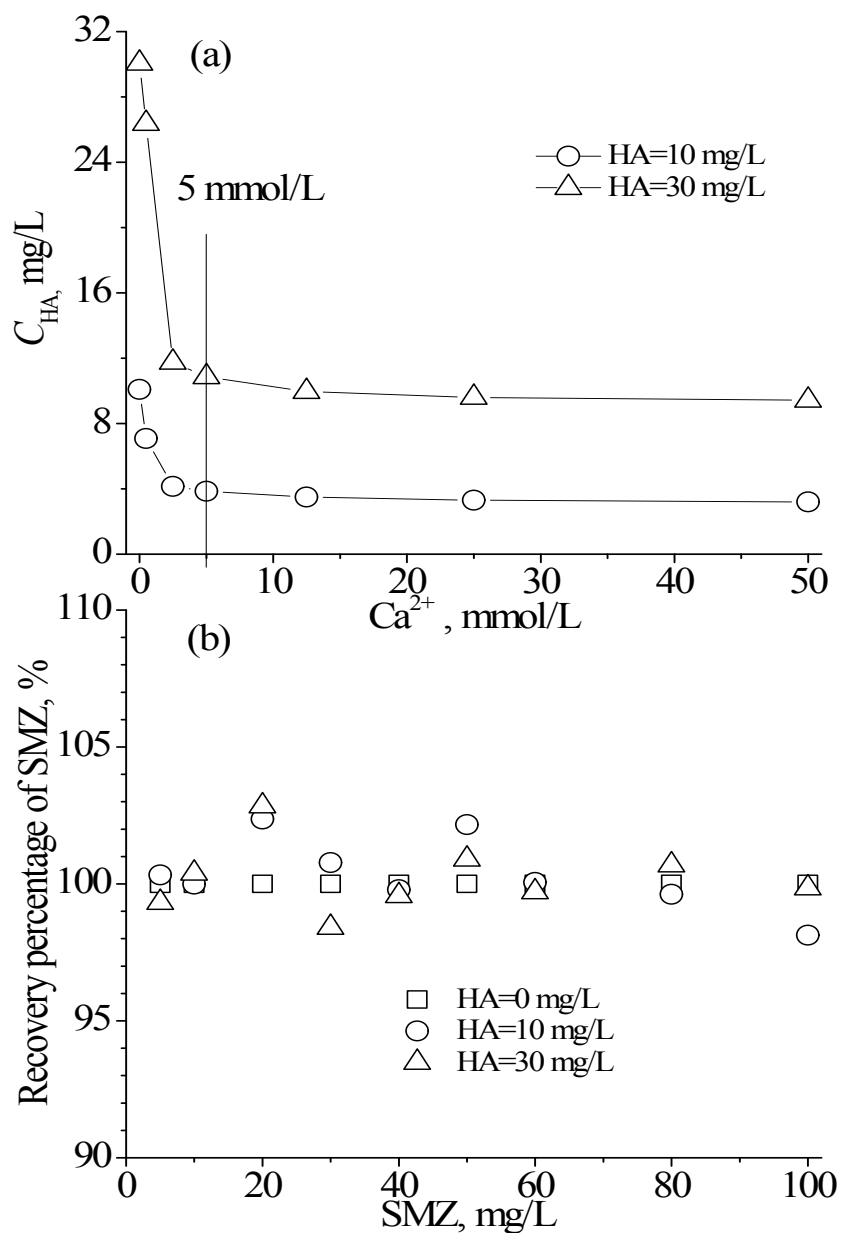


Fig. S7. Effect of HA on SMZ adsorption. (a) Concentration of HA as affected by Ca^{2+} (0–100 mM). The initial concentrations of HA were 10 and 30 mg/L. C_{HA} is the concentration of HA at which HA precipitation was caused by Ca^{2+} and separated using a 0.45 μm hydrophilic membrane filter. (b) Recovery percentage of SMZ. The HA was precipitated by Ca^{2+} and was separated immediately using a 0.45 μm hydrophilic membrane filter.

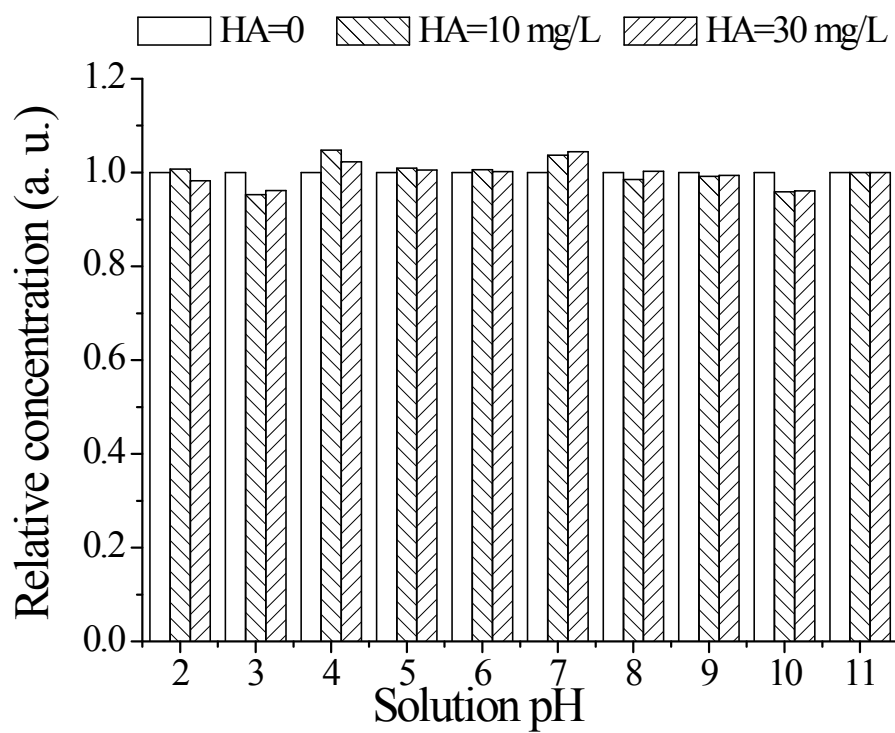


Fig. S8. Relative solubility based on a background solution (value = 1) of SMZ in the presence of HA.

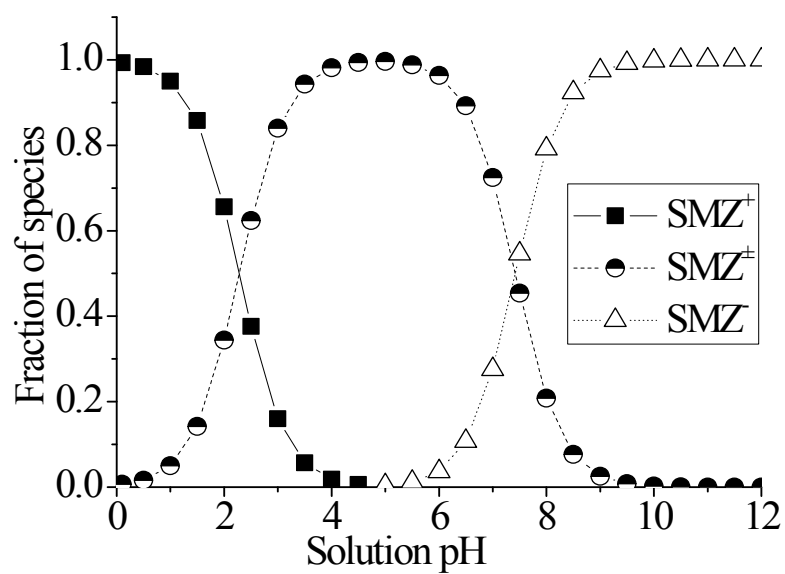


Fig. S9. The species distribution for SMZ at different solution pH.

Table S1 Basic MWCNTs structural properties ^a.

Name	Outer diameter ^b (nm)	Inner diameter ^b (nm)	Carbon content ^c (%)	Oxygen content ^c (%)	Surface area ^d (m ² ·g ⁻¹)	Mesopore volume ^d (cm ³ ·g ⁻¹)	Micropore volume ^d (cm ³ ·g ⁻¹)
P-MWCNTs	10-20	5-10	99	0.85	167	0.619	0.016
C-MWCNTs	10-20	5-10	97	2.16	178	0.629	0.015
H-MWCNTs	10-20	5-10	92	7.07	185	0.756	0.024

^a The data are herein presented in Table. S1 were firstly published in Chen et al., 2009 ¹.

^b The diameters were determined by transmission electron microscope (TEM);

^c The carbon and oxygen contents were determined by X-ray photoelectron spectroscopy (XPS);

^d The surface area and pore volume were determined by nitrogen gas adsorption and desorption at 77k with ASAP2000 (Micromeritics Instrument Corporation).

Table S2 Elemental compositions and ¹³C NMR estimates of carbon distributions for HA.

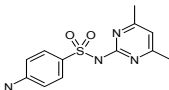
sample	Elemental composition (%) ^a				Ash(%) ^a	(O+N)/C ^b	Integration of NMR results (%)		
	C	H	O	N			Aliphatic C	Aromatic C	Aliphaticity ^c
AHA	57.07	3.25	36.85	1.47	1.36	0.50	22.3	53.7	0.42

^a Mass-based percentages. The C, H and N were determined by CHN Elemental Analyzer (EA 1112, Thermo Finnigan, Italia), the ash were determined using combustion the processed ash at 750 °C for 4 hour, and the oxygen content were calculated by mass difference [Oxygen content = 100 % -(C content +H content +N content)].

^b Molar-based ratios.

^c Aliphaticity was calculated as aliphatic C (0-109 ppm)/aromatic C (109-163 ppm) ratio². The major structural carbons were measured using a 300M Hz NMR spectrometer (Bruker AV300, Switzerland).

Table S3 Structural and physicochemical properties of sulfamethazine.

Compound	CAS number ^a	Chemical structure ^a	Molecular weight (g·mol ⁻¹)	Water solubility (g·L ⁻¹) ^b	pKa ^c
sulfamethazine	57-68-1		278.33	Fig. 5(a)	2.28 7.42

^a from chemBlink Database of Chemicals from Around the World

<http://www.chemblink.com/products/57-68-1.htm>

^b The water solubility of SMZ were determined at temperature 298 K.

^c Reference from ³⁻⁵.

Literature cited

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