Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A. This journal is © The Royal Society of Chemistry 2020

## 1 Supporting Information

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3	Co-existence of humic acid enhances reductive removal of diatrizoate via
4	depassivating zero-valent iron under aerobic conditions
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27 Fig. S1. SEM (a) and XRD (b) characterization of the mZVI after received.









33 Fig. S3. FT-IR spectra of bulk HA and iron residuals exposure to oxygenate solutions

34 in the presence of 100 mg/L HA over 24 h.

Table S1	. Major infrared	l absorption	bands of HA.
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Wavenumber (cm <sup>-1</sup> )	Vibration
3700-3300	-OH stretching
1365	-OH deformation
1370	C-H deformation of CH <sub>2</sub> and CH <sub>3</sub> groups
1460	aliphatic C-H
2926	asymmetric C-H stretching of aliphatic –CH <sub>2</sub>
2856	symmetric C-H stretching of aliphatic –CH <sub>2</sub>
1255	C-O stretching of phenolic
1720	C-O vibration of carboxyl
1590	stretching of aromatic C=C
1090	C-O stretching in polysaccharides



40 Fig. S4. (a) Heat released per injection of Fe<sup>3+</sup> binding to HA; (b) non-linear regression
41 of heat vs. Fe<sup>3+</sup> dosage.



45 Fig. S5. (a) Aqueous DTA after the interaction of DTA with 2.0 g/L ferrihydrite (Fhy), 46 lepidocrocite (Lpd), maghematite (Mag), and Fe<sub>3</sub>O<sub>4</sub> for 10 h in the absence and 47 presence of 40.0 mg-C/L HA; (b) the DTA concentration in the ZVI/air system with 48 adding different scavengers (methanol for both •OH and Fe(IV), isopropanol for •OH), 49 experimental conditions:  $[ZVI]_0 = 2.0 \text{ g/L}, [DTA]_0 = 20.0 \text{ mg/L}, [HA]_0 = 40.0 \text{ mg-C/L},$  $50 [methanol]_0 = [isopropanol]_0 = 0.5 \text{ M}.$ 





Fig. S6. CVs of ZVI in the absence and presence of 40.0 mg-C/L HA and ZVI with the
starting potentials from -1.5 to -1.7 V in Na<sub>2</sub>SO<sub>4</sub> electrolyte solution.





56 Fig. S7. Mass spectrometry of LC-ESI-MS for the transformed products from DTA by





59 Fig. S8. Mass spectrometry of LC-ESI-MS for the transformed products from DTA by

60 ZVI and 40.0 mg-C/L HA systems under aerobic conditions.



64 Fig. S9. pH variations after addition of 2.0 g/L mZVI in the absence and presence of

40.0 mg-C/L HA with initial pH adjusted to 3.0.



69 **Fig. S10.** Variations of Fe(II) and Fe(III) (a) and ratio of dissolved organic carbon 70 (DOC) (C) to the initial organic carbon ( $C_0$ ) of HA (b) after the mixing of 600  $\mu$ M Fe(II) 71 or Fe(III) with 40.0 mg-C/L HA. As for avoiding the precipitation of Fe(II)/Fe(III), the 72 initial pH of solutions used in Fe(II) and Fe(III) experiments were respectively adjusted 73 to 5.0 and 2.8.



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76 Fig. S11. EPR spectra selectively showing the Fe(III) signal region for HA + Fe(III).

77 The concentrations of HA and Fe(III) were 40.0 mg-C/L and 2.0 mM, respectively.



80 Fig. S12. Photographs and the turbidity presented by the absorbance value at 660 nm of HA-Fe suspensions with different  $\mathrm{Fe}^{3+}$  concentration and

 $82\ 40.0$  mg-C/L HA in steady-state conditions.

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Fig. S13. SEM images of ZVI collected at 24 h following exposure to pH 3.0
oxygenated solution in the presence of 40.0 mg-C/L HA, with suspected Fe-NOM
aggregates surrounding the ZVI particles.



89 Fig. S14. XPS Fe 2p spectra of ZVI solids collected in the control and HA (40.0 mg-

90 C/L) systems after reacting for 2 h.



93 Scheme S1. Reductive removal pathway of DTA in the ZVI aerobic systems. Noting
94 that DTA-1 and DTA-2 were the transformed products of the systems without addition
95 of HA, while DABA can be detected in the presence of HA.