1 **Supplementary Materials**

2 Molecular-scale investigation on the photochemical

3 transformation of dissolved organic matter after immobilization

4 by iron minerals with FT-ICR MS

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23 Text S1 FT-ICR MS data processing

24   Molecular formulas containing the elements C, H, O, N, and S were performed

25 according to basic chemical standards using in-house software. The molecular

26 parameters (m/z, H/C, O/C, etc.), derived from peak formula assignments were

27 expressed as intensity-weighted average (wa) values. Therefore, these values directly

28 reflected the relative contribution of each m/z peak to the entire DOM mass spectrum.

29 The modified aromaticity index (AI), the double bond equivalent (DBE) and Kendrick

30 quality defect (KMD) were calculated for each assigned molecular formula.

31   Van Krevelen diagrams was used to distinguish compound classes in samples on

32 the basis of O/C and H/C plots. According to van Krevelen diagrams, compounds were

33 classified into seven categories by elemental ratios: (1) lipids (H:C = 1.5-2.0; O:C = 0-

34 0.3); (2) proteins (H:C = 1.5-2.2; O:C = 0.3-0.67); (3) carbohydrates (H:C = 1.5-2.0;

35 O:C = 0.67-1.2); (4) unsaturated hydrocarbons (H:C = 0.7-1.0; O:C = 0-0.1); (5) lignins

36 (H:C = 0.7-1.5; O:C = 0.1-0.67); (6) condensed aromatic structures (H:C = 0.2-0.7; O:C

37 = 0-0.67); and (7) tannin (H:C = 0.5-1.5; O:C = 0.67-1.2). To accurately describe the

38 impact of mineral types on DOM adsorption and photochemical transformation

39 processes. In the analysis of adsorption data, van Krevelen diagrams mainly display the

40 DOM molecules in the solution after adsorption. In case of photochemical degradation,

41 van Krevelen diagrams mainly demonstrate the DOM molecules DOM molecules

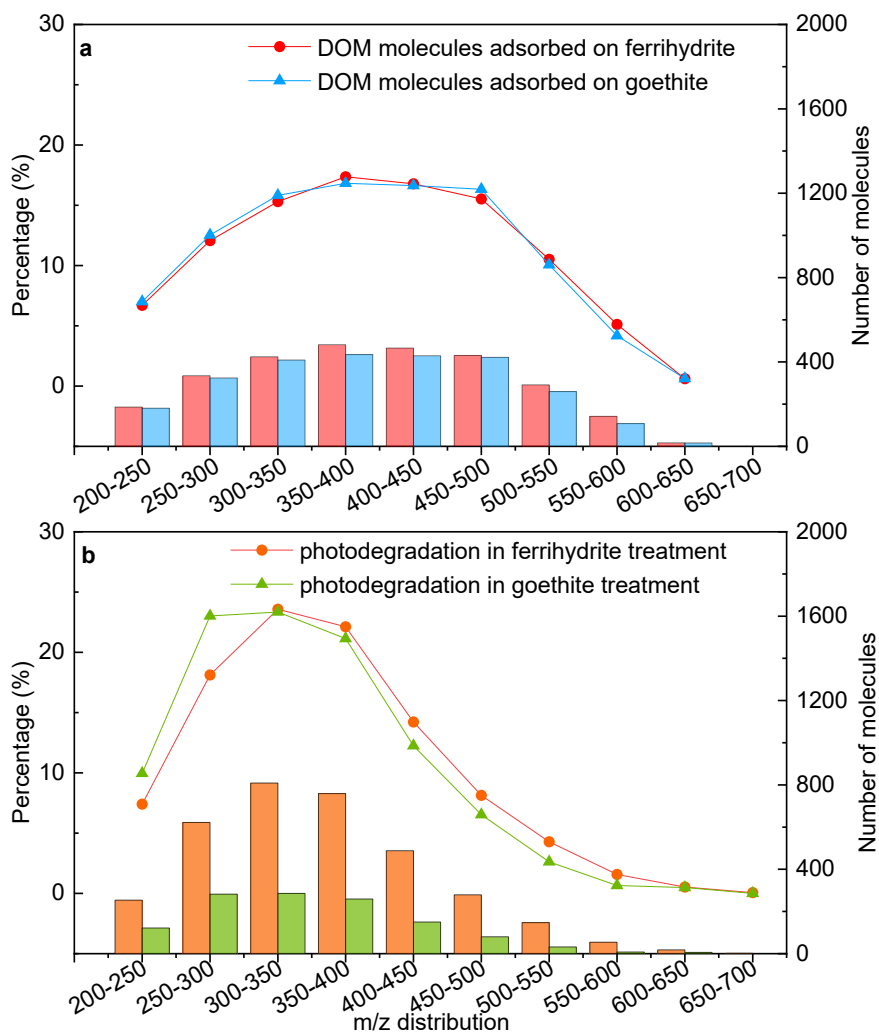42 eluted from iron oxyhydroxides.

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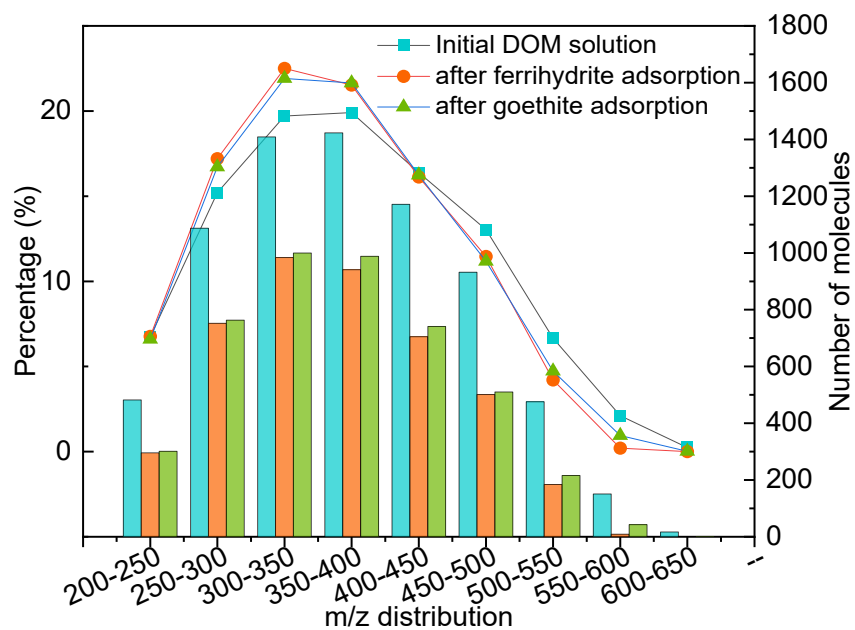
Fig. S1. Mass distribution (the bar graph on the right) and percentage content (The line chart on the left) of DOM species in initial solution and residual after adsorption by ferrihydrite and goethite.

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51 **Fig. S2.** The molecular weight distribution (bar chart on the right) and percentage

52 content (line chart on the left) of DOM (a) adsorbed by ferrihydrite and goethite and

53 DOM (b) photodegradation after adsorption.

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55 Table S1 Intensity-weighted average molecular parameters and the number of formulas

56 of DOM derived from assigned molecular formulas.

parameters	Initial DOM solution	after ferrihydrite adsorption	after goethite adsorption
molecules number	7148	4372	4563
m/zwa (Da)	349.41	338.54	339.95
Cwa	17.52	16.99	17.03
Hwa	23.69	23.26	24.82
Owa	6.42	6.23	6.13
O/Cwa	0.38	0.37	0.37
H/Cwa	1.41	1.42	1.50
DBEwa	6.40	6.06	5.27

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59 Table S2 $AI_{mod, wa}$ index of DOM absorbed by iron minerals before and after sunlight.

	$AI_{mod,wa}$
DOM adsorbed by goethite	0.35
DOM adsorbed by ferrihydrite	0.31
DOM adsorbed by goethite after sunlight	0.024
DOM adsorbed by ferrihydrite after sunlight	-0.0016

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