Electronic Supplementary Material (ESI) for Environmental Science: Atmospheres.

Supporting Information Section

Effect of Aromatic Ring Substituents on the Ability of Catechol to Produce Brown Carbon in Iron(III)-Catalyzed Reactions

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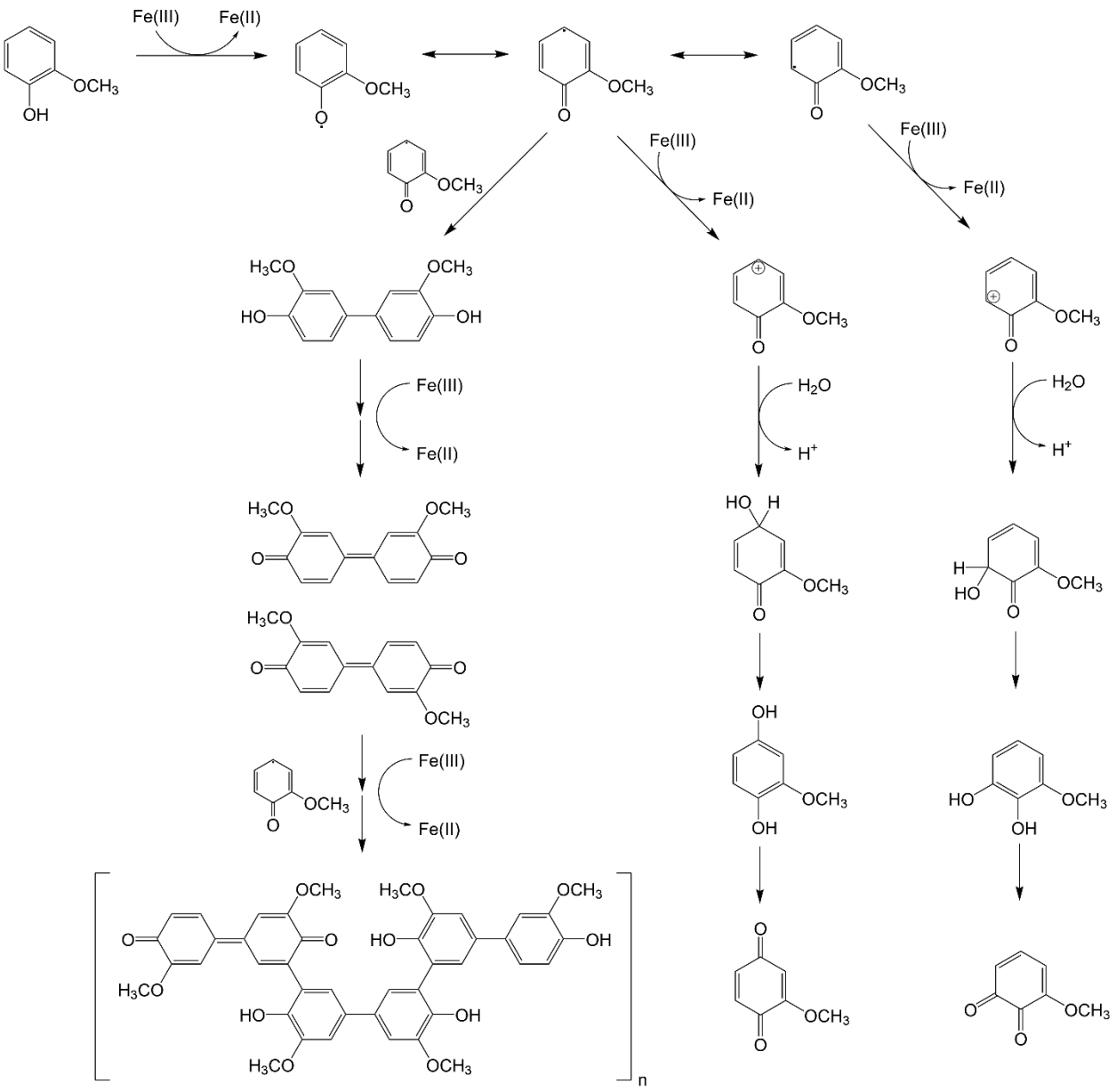

Scheme S1: Mechanism for the oxidation of guaiacol in the presence of excess iron under dark conditions leading to the formation dimers [*Hwang et al.*, 2008] and eventually polyguaiacol [*Crawford et al.*, 1981].

Crawford, R. L., L. E. Robinson, and R. D. Foster (1981), Polyguaiacol: a Useful Model Polymer for Lignin Biodegradation Research, *Applied and Environmental Microbiology*, *41*(5), 1112-1116.

Hwang, S., C. H. Lee, and I. S. Ahn (2008), Product identification of guaiacol oxidation catalyzed by manganese peroxidase, *Journal of Industrial and Engineering Chemistry*, *14*(4), 487-492.

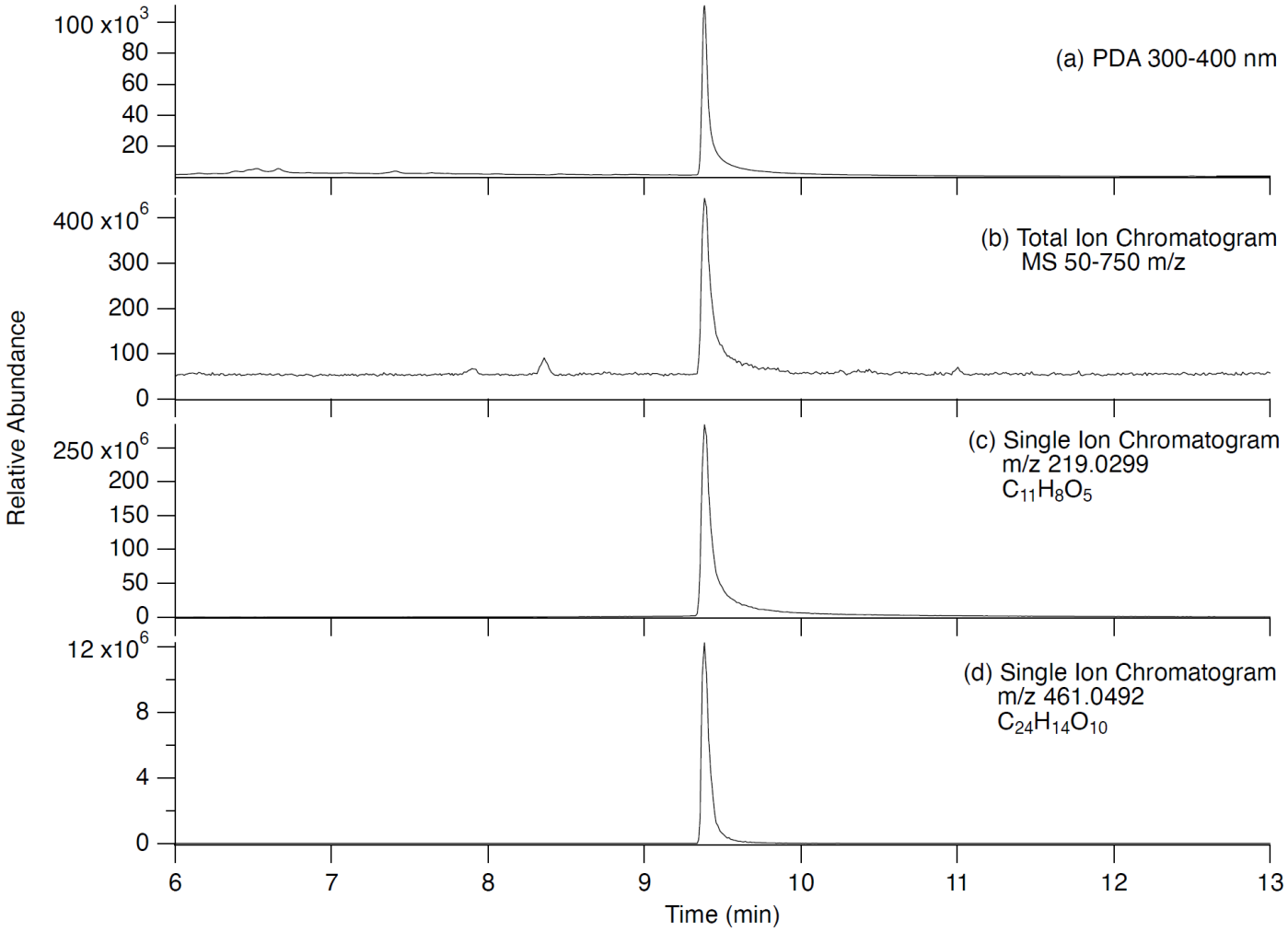

Figure S1: UPLC-PDA-HRMS data for the 3-HC + Fe(III) reaction products: (a) photodiode array (PDA) chromatogram; (b) total ion current (TIC) chromatogram; and (c & d) single ion monitoring (SIM) chromatograms. The TIC and SIM chromatograms were corrected for the 0.06 min delay time between PDA and Orbitrap detectors. The formulas listed correspond to neutral compounds observed as deprotonated ions at the specified *m/z* values.

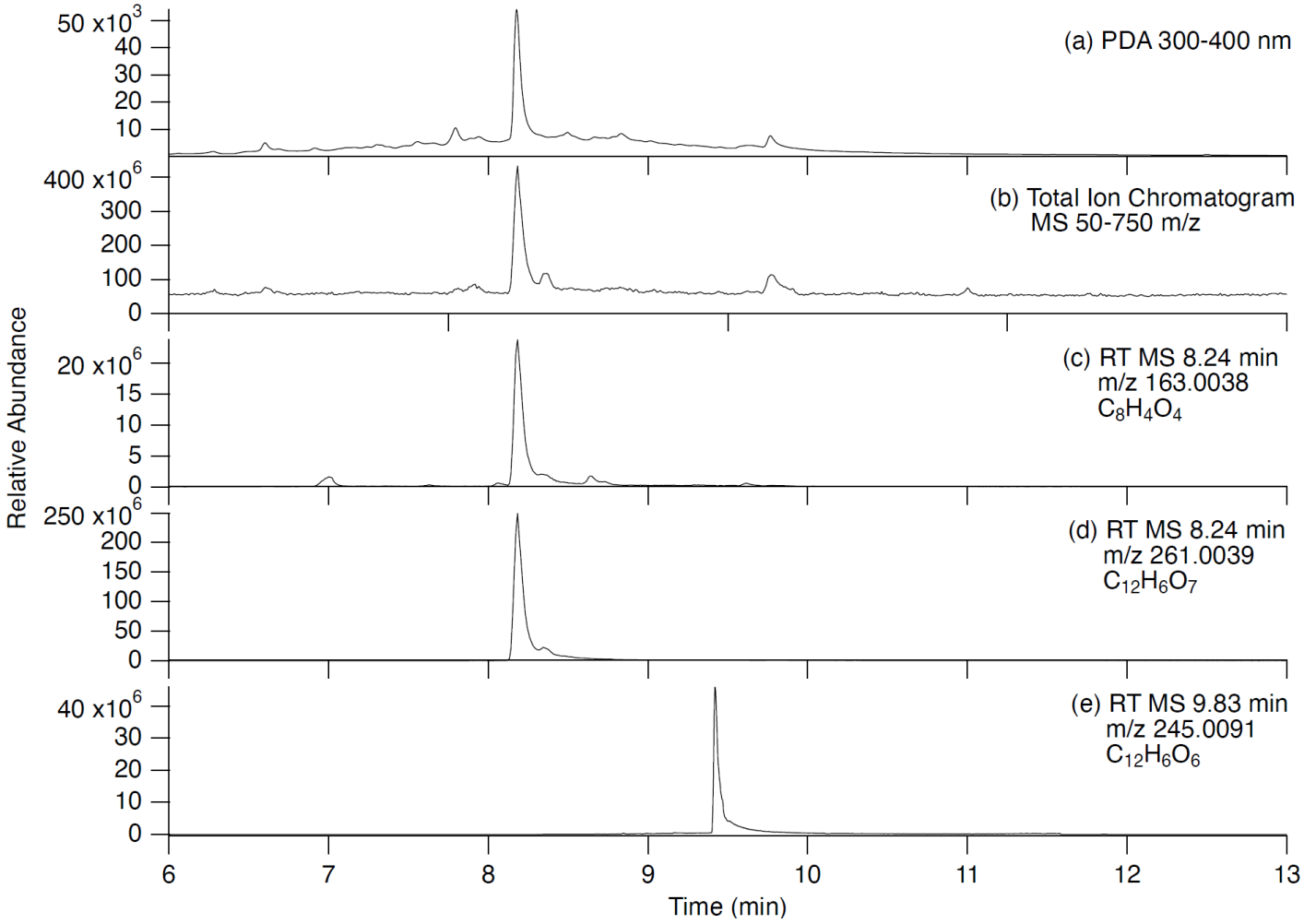

Figure S2: UPLC-PDA-HRMS data for the 4-HC + Fe(III) reaction products: (a) photodiode array (PDA) chromatogram; (b) total ion current (TIC) chromatogram; and (c & d) single ion monitoring (SIM) chromatograms. The TIC and SIM chromatograms were corrected for the 0.06 min delay time between PDA and Orbitrap detectors. The formulas listed correspond to neutral compounds observed as deprotonated ions at the specified *m/z* values.

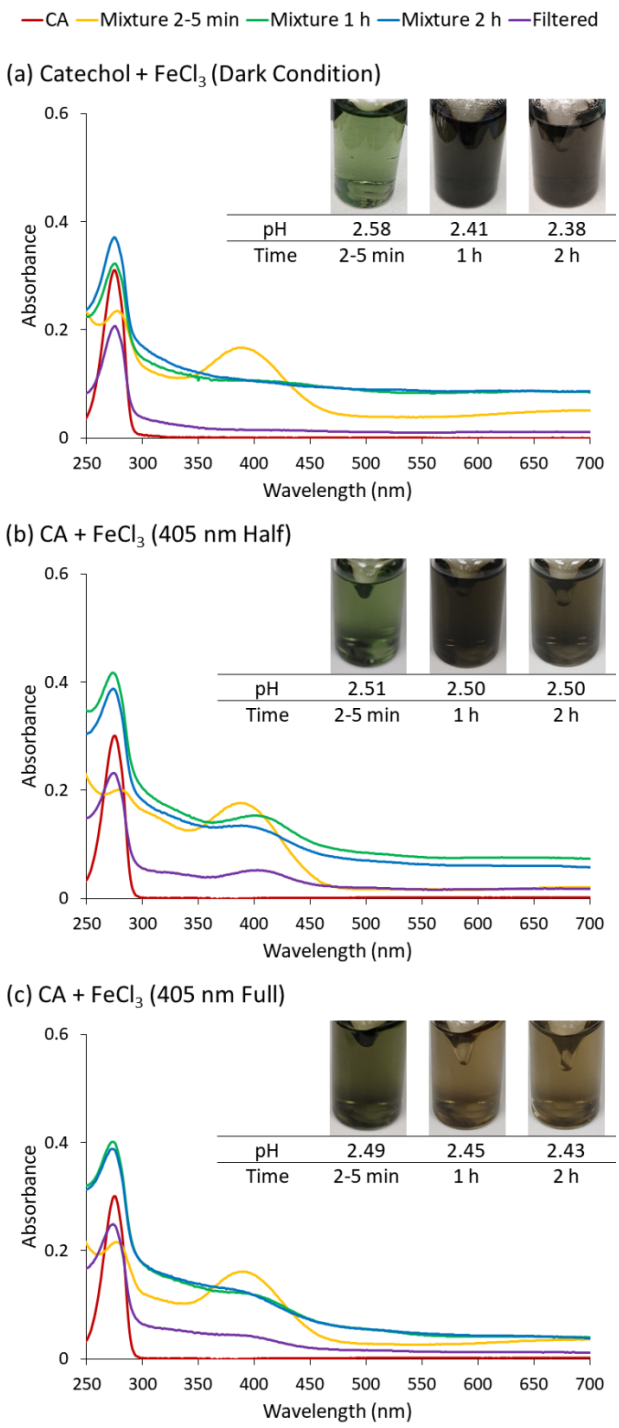

Figure S3: The effect of 405 nm irradiation on particle formation of CA and Fe(III) at different levels of UV LED intensity (0%, 50%, 100%) . Different colors of traces correspond to spectra of CA before mixing (red), 2-5 min after mixing (orange), 1 h after mixing (green), 2 h after mixing (blue), and filtered solution (purple).

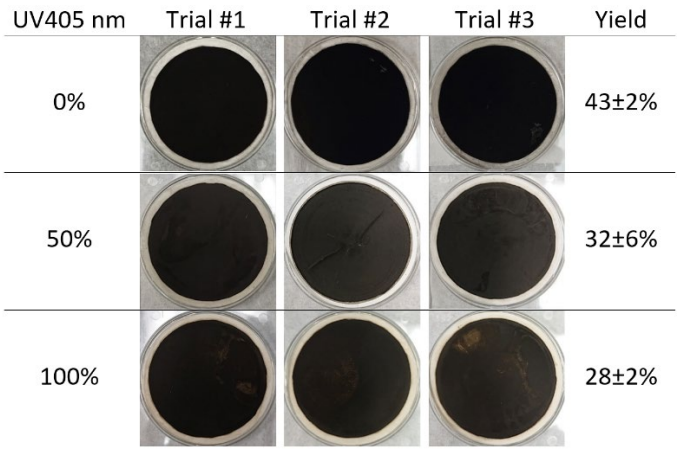

Figure S4: Photographs of filters containing particles after 2 h or reaction, filtration, and drying for pyrocatechol (CA) under different intensities of 405 nm UV irradiation. The last column contains the average (n=3) effective mass yield in percent.