PAMAM dendrimer for mitigating humic foulant

Priyanka Bhattacharya,^{*a,b*} Nathan Conroy,^{*c*} Apparao M. Rao,^{*a*} Brian A. Powell,^{*c*} David A. Ladner,^{*c*} and Pu Chun Ke^{**a*}

^a Department of Physics and Astronomy, Clemson University, Clemson, SC 29634, USA. E-mail: pcke11@clemson.edu

^bApplied Materials Science, Pacific Northwest National Laboratory, PO Box 999, Richland, WA 99352, USA.

^c Department of Environmental Engineering and Earth Sciences, Clemson University Clemson, SC 29634, USA.

Electronic Supplementary Information

Experimental Details

I. Materials. Generation 5 amine-terminated PAMAM dendrimers (G5-NH₂, MW 28,826 g/mol) were purchased from Dendritech Inc. in aqueous solution and used as received. HA was purchased from Sigma Aldrich in powder form and dissolved in deionized (DI) water to form a stock solution of 500 mg/L.

II. Methods.

The HA solution was filtered using 0.2 µm syringe filters (Whatman) prior to all experiments. All experiments were performed at room temperature.

- Dynamic light scattering and zeta potential: The hydrodynamic size of the control HA and G5-PAMAM solutions were measured using dynamic light scattering in 1 mm path length plastic cuvettes (S90, Malvern Instruments). The hydrodynamic sizes of the supernatants of the G5-HA complexes were also measured under identical conditions. Zeta potential measurements were conducted in disposable zeta potential plastic cuvettes using a Zetasizer (Nano ZS, Malvern Instruments).
- 2. Fluorescence measurements: HA solution was prepared by diluting from the stock in DI water and increasing concentrations of G5-PAMAM were added to the HA solution in a 1 mm path length quartz cuvette. After 30 sec of gentle shaking, the mixtures were allowed to incubate for 5 min and their fluorescent emission spectra between 400-600 nm were recorded for an excitation of 320 nm and Ex/Em slit widths of 10/20 nm on a Cary Eclipse fluorescence spectrophotometer (Varian, Inc.). The emission spectra were corrected for their respective blanks (HA and dendrimers only). Measurements were recorded on three samples for statistical error analysis.
- **3. UV-vis absorbance measurements:** For the determination of optimal dendrimer concentration, first HA solutions of 75-125 mg/L were prepared by diluting the stock solution with DI water. The pH of the prepared HA solutions was 5.5. Then, G5-PAMAM of gradient concentrations were added to the HA

solutions in 2 mL Eppendorf tubes. The mixtures were incubated for 24 h on a lab rotor (Labquake, Barnstead). The samples were then centrifuged in a Minispin (Eppendorf) at the rate of 5,000 rpm (4,515g RCF) for 15 min and the absorbance of the supernatants was read on a UV-vis spectrophotometer (Biomate 3) in quartz cuvettes.

4. ATR-FTIR: ATR-FTIR analyses were performed on a Thermo Nicolet 6700 FTIR with a single bounce diamond Smart iTR cell. The precipitate shown in the Fig. 2 inset was recovered by centrifugation, dried at 40°C, and then placed directly onto the ATR crystal for ATR-FTIR analysis. Standard data collection parameters were 32 scans at 4 cm⁻¹ resolution. A flux of nitrogen was passed through the instrument to remove CO₂(g).

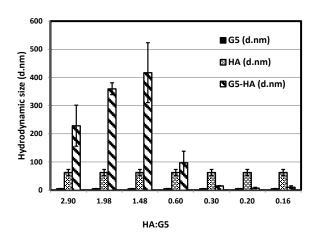


Fig. S1 Hydrodynamic sizes of HA, G5-PAMAM and G5-HA complexes in the respective supernatants at different HA:G5-PAMAM ratios.

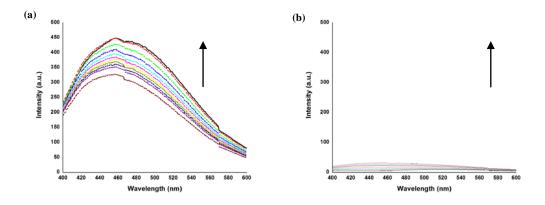


Fig. S2 Fluorescence emission spectra of (a) HA and (b) G5-PAMAM at different concentrations. Arrow indicates direction of increasing concentrations.