

## Supporting Information:

### Can Molecules with Anionic Head and Poly(ethylene glycol) methyl ether Tail Self-assemble in Water? A Surface tension, Fluorescence Probe, Light Scattering, and Transmission Electron Microscopic Investigation

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**Materials.** Poly(ethylene glycol)methyl ether methacrylate (MW 300 and 1100), and 3-mercaptopropionic acid were obtained from Aldrich and were used without further purification. The fluorescence probes, 1-anilinonaphthalene (AN), 1,6-diphenyl-1,3,5-hexatriene (DPH), and pyrene (Py) were procured from Aldrich (Milwaukee, WI, USA) and were purified by repeated recrystallization from an ethanol-acetone mixture. Good quality organic solvents employed in this work were purified and dried whenever necessary. All aqueous solutions were prepared using Milli-Q water (~18 M $\Omega$ ), pH 6.6.

**Synthesis.** Compound A was synthesized by thiol-ene “click” chemistry following a method reported in the literature.<sup>1</sup> Briefly poly(ethylene glycol)methyl ether methacrylate was first freed from inhibitor by passing through a SiO<sub>2</sub> column and elution by methanol. Pure poly(ethylene glycol)methyl ether methacrylate was then reacted with 3-mercaptopropionic acid in methanol at room temperature for 6 hours. The compound A<sub>1</sub> and A<sub>2</sub> were obtained as white solid after evaporation of the solvent and were then purified by column (Al<sub>2</sub>O<sub>3</sub>) chromatography using 5:1 (v/v) ethyl acetate/pet ether mixture. The compounds were characterized by FT-IR, <sup>1</sup>H NMR, and <sup>13</sup>C NMR spectroscopy. The reaction

of NaHCO<sub>3</sub> with A<sub>1</sub> or A<sub>2</sub> in THF-water mixture overnight gave the sodium salt, SA<sub>1</sub> or SA<sub>2</sub>. The solid product thus obtained was purified by repeated precipitation from diethylether.

### Chemical Identification

**Amphiphile A<sub>1</sub>.** State. Solid, and hygroscopic, Yield 79%, FTIR (KBr cm<sup>-1</sup>). Peak at 3600 cm<sup>-1</sup> (broad) shows the presence of O-H stretching, 1742 cm<sup>-1</sup> shows presence of C=O stretching of ester group and 636 cm<sup>-1</sup> shows presence of C-S stretching. <sup>1</sup>H NMR (CDCl<sub>3</sub>, δ ppm): 1.45 (CH<sub>3</sub>, t, 9H), 2.18 (CH<sub>3</sub>-CH<sub>2</sub>-N, m, 4H), 2.42 (2H, s, OH), 2.81 (6H, m, N-CH<sub>2</sub>, S-CH<sub>2</sub>-CH<sub>2</sub>-N), 3.25 (5H, m, S(CH<sub>2</sub>-CHCH<sub>3</sub>)CH<sub>2</sub>CH<sub>2</sub>N), 3.88 (3H, s, CH<sub>3</sub>-O), 4.10 (4H, m, long chain glycolic CH<sub>2</sub>, CHCH<sub>2</sub>OH), 4.23 (2H, m, CH-CH<sub>2</sub>-OH), 4.77 (2H, t, C(O)OCH<sub>2</sub>). <sup>13</sup>C-NMR. (CDCl<sub>3</sub>, 400 MHz) δ (ppm) 174.5 (COOCH<sub>2</sub>), 169.1 (COOH), 68.7, 69.5, 70.5, 70.9, 73.6 (ether CH<sub>2</sub>), 54.9 (OCH<sub>3</sub>), 42.4 (SCH<sub>2</sub>CH), 36.2 (SCH<sub>2</sub>CH), 35.9 (SCH<sub>2</sub>CH<sub>2</sub>COOH), 28.1 (SCH<sub>2</sub>CH<sub>2</sub>COOH), 15.1 (CH<sub>3</sub>).

**Amphiphile A<sub>2</sub>.** State. Solid and hygroscopic, Yield 80%, FTIR (KBr cm<sup>-1</sup>). Peak at 3600 cm<sup>-1</sup> (broad) shows the presence of O-H stretching, 1741 cm<sup>-1</sup> shows presence of C=O stretching of ester group and 637 cm<sup>-1</sup> shows presence of C-S stretching. <sup>1</sup>H NMR (CDCl<sub>3</sub>, δ ppm): 1.40 (CH<sub>3</sub>, t, 9H), 2.127 (CH<sub>3</sub>-CH<sub>2</sub>-N, m, 4H), 1.92 (2H, s, OH), 2.31 (6H, m, N-CH<sub>2</sub>, S-CH<sub>2</sub>-CH<sub>2</sub>-N), 2.75 (5H, m, S(CH<sub>2</sub>-CHCH<sub>3</sub>)CH<sub>2</sub>CH<sub>2</sub>N), 3.38 (3H, s, CH<sub>3</sub>-O), 3.60 (m, long chain glycolic CH<sub>2</sub>, CHCH<sub>2</sub>OH), 3.73 (2H, m, CH-CH<sub>2</sub>-OH), 4.27 (2H, t, C(O)OCH<sub>2</sub>). <sup>13</sup>C-NMR. (CDCl<sub>3</sub>, 400 MHz) δ (ppm) 176.3 (COOCH<sub>2</sub>), 168.4 (COOH), 67.8, 68.6, 70.9, 71.5, 74.1 (ether CH<sub>2</sub>), 55.9 (OCH<sub>3</sub>), 43.4 (SCH<sub>2</sub>CH), 36.5 (SCH<sub>2</sub>CH), 36.4 (SCH<sub>2</sub>CH<sub>2</sub>COOH), 27.9 (SCH<sub>2</sub>CH<sub>2</sub>COOH), 14.8 (CH<sub>3</sub>).

References:

- 1 C. Rim, L.J. Lahey, G.P.H. Zhang and D.Y. Son *Tetrahedron Lett.* 2009, **50**, 745-747.