

Supporting Information

A Smart Supramolecular Hydrogel of N^a-(4-n-Alkyloxybenzoyl)-L-histidine Exhibiting pH-Modulated Properties” by T. Patra, A. Pal and J. Dey*

Chemical Identification of Amphiphiles

C₈-OBH: Yield 65%, M.P 145-147°C (d). $[\alpha]_D^{25}$ (0.5%, CH₃OH) = 6.80°, FT-IR (KBr, cm⁻¹): 3398,3304,3155, 2925, 2853, 1718, 1637, 1538, 1508,1400,1313,1250. ¹H-NMR: δ_H (400 MHz, CD₃OD): 7.7 (2H, d, J8.8, Ph-*H*), 6.9 (2H, d, J8.8, Ph-*H*), 7.95 (1H, d, J8.8, *NH*), 8.49 (1H, s, CCHN), 7.2 (1H, s, NCHN), 4.72 (1H, dd, J₁5.2, J₂5.2, CH(NH)COOH), 4.0 (2H, t, J6.5, O-CH₂), 3.33 (2H, dd, J7.6 CHCH₂), 1.8 (2H, m, CH₂-CH₂-O), 1.47(2H, m, CH₂-CH₂-CH₂-O), 1.32 (8H, m, alkyl chain), 0.9 (3H, t, J6.4, CH₃).

C₆-OBH: Yield 76%, M.P 144°C (d). $[\alpha]_D^{25}$ (0.5%, CH₃OH) = 8.58°, FT-IR (KBr, cm⁻¹): 3395,3302,3155, 2925, 2853, 1716, 1637, 1538, 1504,1400,1313,1250. ¹H-NMR: δ_H (400 MHz, D₂O/NaOD): 7.4 (2H, d, J8.8, Ph-*H*), 6.7 (2H, d, J8.8, Ph-*H*), 7.38 (1H, s, CCHN), 6.63 (1H, s, NCHN), 4.33 (1H, dd, J₁5.2, J₂5.2, CH(NH)COOH), 3.79 (2H, t, J6.5, O-CH₂), 2.92 (2H, dd, J7.6 CHCH₂), 1.48 (2H, m, CH₂-CH₂-O), 1.13(2H, m, CH₂-CH₂-CH₂-O), 1.42 (4H, m, alkyl chain), 0.93 (3H, t, J6.4, CH₃).

C₁₀-OBH: Yield 62%, M.P 155°C (d). $[\alpha]_D^{25}$ (0.5%, CH₃OH) = 6.78°, FT-IR (KBr, cm⁻¹): 3398,3302,3154, 2925, 2853, 1715, 1634, 1535, 1508,1400,1313,1250. ¹H-NMR: δ_H (400 MHz, D₂O/NaOD): 7.75 (2H, d, J8.8, Ph-*H*), 6.76 (2H, d, J8.8, Ph-*H*), 7.41 (1H, s, CCHN), 6.76 (1H, s, NCHN), 4.63 (1H, dd, J₁5.2, J₂5.2, CH(NH)COOH), 3.49 (2H, t, J6.5, O-CH₂), 3.08 (2H, dd, J7.6 CHCH₂), 1.58 (2H, m, CH₂-CH₂-O), 1.29 (14H, m, alkyl chain), 0.91 (3H, t, J6.4, CH₃).

C₁₂-OBH: Yield 58%, M.P 161°C (d). $[\alpha]_D^{25}$ (0.5%, CH₃OH) = 5.56°, FT-IR (KBr, cm⁻¹): 3398,3302,3154, 2925, 2853, 1716, 1637, 1540, 1508,1400,1313,1250. ¹H-NMR: δ_H (400 MHz, D₂O/NaOD): 7.74 (2H, d, J8.8, Ph-*H*), 6.73 (2H, d, J8.8, Ph-*H*), 7.4 (1H, S, CCHN), 6.73 (1H, S, NCHN), 4.62 (1H, dd, J₁5.2, J₂5.2, CH(NH)COOH), 3.5 (2H, t, J6.5, O-CH₂), 3.06 (2H, dd, J7.6 CHCH₂), 1.54 (2H, m, CH₂-CH₂-O), 1.27 (18H, m, alkyl chain), 0.90 (3H, t, J6.4, CH₃).

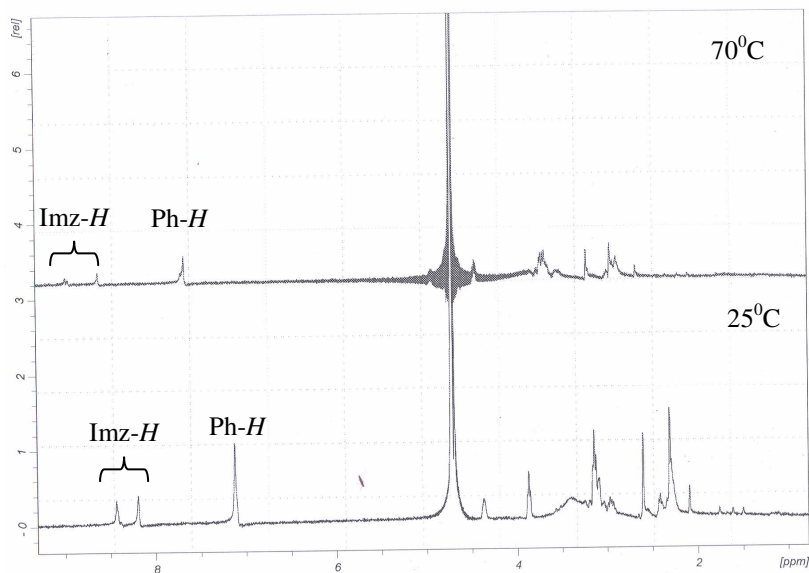


Figure S1. Representative ¹H NMR spectra of 10 mM C₈-OBH hydrogel in pH 8 phosphate buffer at 25 °C and 70 °C.