Electronic Supplementary Information

Nanocarriers from dicationic bis-imidazolium amphiphiles and their interaction with anionic drugs

Lucía Casal-Dujat, ^ab Peter C. Griffiths, *c Carlos Rodriguez-Abreu, d Conxita Solans, Sarah Rogers, f and Lluïsa Pérez-García *c Carlos Rodriguez-Abreu, d Conxita Solans, c Sarah Rogers, f and Lluïsa Pérez-García *c Carlos Rodriguez-Abreu, d Conxita Solans, c Carlos Rodriguez-Abreu, d Carlos Rodrig

Characterization of 1

¹H NMR: Varian Gemini 300 (300 MHz). ¹³C NMR: Varian Gemini 400 (100 MHz). NMR spectra were determined in CDCl₃ and the chemical shifts are expressed in parts per million (ppm) relative to the central peak of the solvent. Thin Layer Chromatography (TLC) was performed on Merck coated 60 F₂₅₄ silica gel plates; the spots were located with UV light and developed with an iodine/silica or (1% w/v) potassium permanganate solution. Mass Spectra (MS): Electrospray (ESI) in Agilent (2006) LC/MSD-TOF mass spectrometer. High Resolution Mass Spectra (HR-MS): Electrospray (ESI) with high resolution in Agilent (2006) LC/MSD-TOF mass spectrometer. Melting points are incorrected and were measured by Gallenkamp Melting point instrument using crystal capillaries purchased from Afora.

1: ${}^{1}H$ NMR (300 MHz, CDCl₃): 0.87 (t, J=6 Hz, 6H, CH₃); 1.25-1.32 (m, 20H, (CH₂)₅); 1.90 (m, 4H, N-CH₂-C**H**₂); 4.27 (t, J=7.5 Hz, 4H, N-CH₂); 5.64 (s, 4H, CH₂); 7.17 (dd, J=6 Hz, J=9 Hz, 1H, Ar-H(5)); 7.29 (s, 2H, Im-H(4)); 7.62 (d, 2H, J=9 Hz, Ar-H(4,6)); 8.13 (s, 1H, Ar-H(2)); 8.20 (t, 2H, Im-H(5)); 10.45 (s, 2H, Im-H(2))... ${}^{13}C$ NMR (100 MHz, CDCl₃): 14.2 (CH₃); 22.7-31.8 ((CH₂)₆); 50.4 (N-CH₂); 52.5 (CH₂); 121.9 (Im-C(4)); 123.7 (Im-C(5)); 130.1 (Ar-C(4,5,6)); 130.6 (Ar-C(2)); 134.9 (Ar-C(1,3))/(ImC(2)); 136.8 (Ar-C(1,3))/(ImC(2)). MS (ESI) m/z: (232.2, [(M-2Br)/2]²⁺, 100%); (351.3, [M-(CH₂)₇-CH₃), -2Br]⁺, 21%); (464.4, [M-2Br]⁺, 4%); (543.3, [M-Br]⁺, 5%). HRMS (ESI) m/z: (C₃₀H₄₈N₄Br₂ – Br)⁺ calculated 543.3056, found 543.3078; (C₃₀H₄₈N₄Br₂ – 2Br)²⁺ calculated 232.1934, found 232.1941. R_f: 0.36 (CH₂Cl₂:MeOH, 9:2

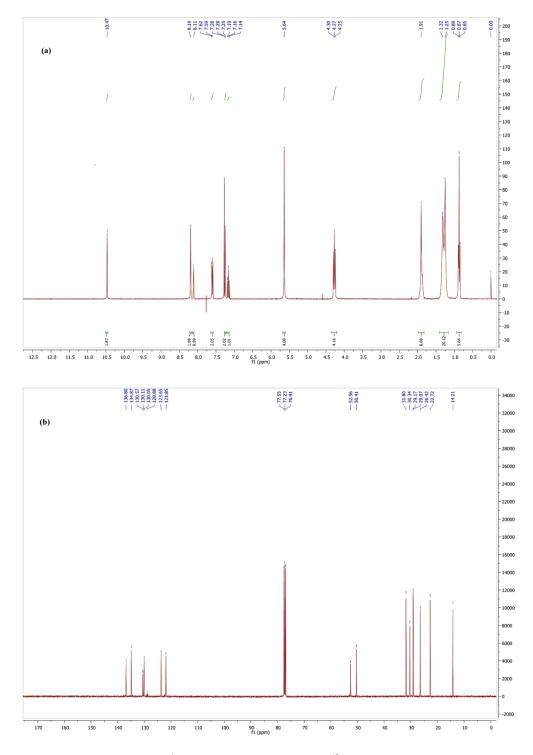


Fig S1. NMR spectra for 1: (a) 1 H NMR (300 MHz, CDCl₃) and 13 C NMR (100 MHz, CDCl₃).

Fluorescence emission spectra of pyrene containing surfactant solution

Fig. 2 shows an example of the experimental results for **2** by plotting the intensity as a function the wavelength for increasing concentration of surfactant (0.2 – 1.2 mM) in aqueous solution with a fixed concentration of pyrene (10^{-6} M). The fluorescence intensity was normalized by I_1/I_3 (I_1 and I_3 correspond to the wavelengths of 373 nm and 384 nm, respectively).

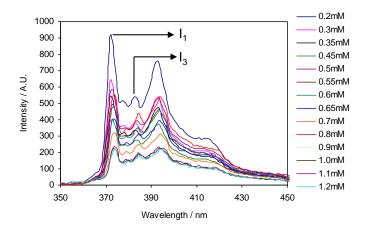


Fig. S2 Fluorescence spectra of aqueous solutions of 2.

SANS curve for 1

The flat SANS curves showed in Fig. 3S suggest that surfactant molecules of $\bf 1$ in 10 mM and 15 mM aqueous solutions at 25°C do not have the capability to self-assemble into aggregates.

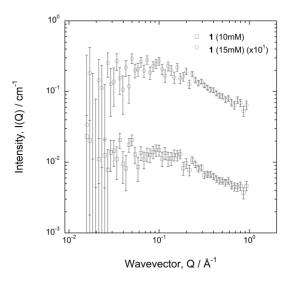


Fig. S3 SANS curves obtained for 10~mM and 15~mM aqueous solutions containing 1.