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Soft nanosystems based on hydroxypiperidinium surfactants as adjuvants and micellar catalysts

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IR spectra were recorded on a Bruker Vector-22 Fourier-transform spectrophotometer in KBr pellets. ^{1}H NMR spectra were acquired on a on a Bruker AV-600 spectrometer (600 MHz). ESI mass spectra were recorded on an AmaZonX mass spectrometer

Piperidinium surfactants were synthesized by the reaction of the corresponding piperidine derivative (10 mM) and alkyl bromide (11 mM) in acetonitrile followed by recrystallization from acetone or ethyl acetate by analogy with [A. B. Mirgorodskaya, R. A. Kushnazarova, S. S. Lukashenko, L. Ya. Zakharova, *Russ. Chem. Bull*., 2019, **68**, 328 (*Izv. Akad. Nauk, Ser. Khim.*, 2019, 328)].

1-Dodecyl-4-hydroxy-1-(2-hydroxyethyl)piperidinium bromide (1a).

Yield 2.2 g (43.8%); white powder; mp 48-50°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.88 (t, 3H); 1.26-1.36 (m, 18H); 1.71 (m, 2H); 1.99 (m, 1H); 2.13 (m, 2H); 2.32 (m, 1H); 3.49 (m, 2H); 3.53 (m, 1H); 3.66 (m, 4H); 3.86 (m, 1H); 4.07 (m, 2H); 4.18 (m, 1H); 5.19 (s, OH). IR spectrum (KBr), ν/cm^{-1}: 3299, 2919, 2850.1471 1372, 2336.1252, 1165, 1135.1090, 1055.1010, 971, 926, 891.768, 719, 599. ESI mass spectrum, m/z: 314.4 $[M\text{-}Br]^+$. $C_{19}H_{40}NO_2Br$; Found,%: C 57.93; H 9.13; N 3.82; Br 19.51; Calculated,% C 57.86; H 10.22; N 3.55; Br 20.26.

4-Hydroxy-1-(2-hydroxyethyl)-1-tetradecylpiperidinium bromide (1b).

Yield 1.66 g (38%); white powder; mp 58-60°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.88 (t, 3H); 1.26-1.37 (m, 22H); 1.72 (m, 2H); 2.01 (m, 1H); 2.13 (m, 2H); 2.32 (m, 1H); 3.47 (m, 2H); 3.50 (m, 1H); 3.65 (m, 4H); 3.88 (m, 1H); 4.08 (m, 2H); 4.19 (d, 1H); 4.80 (s, OH). IR spectrum (KBr), ν/cm^{-1}: 3300, 2919, 2851.1471 1371, 1337.1254, 1170, 1125.1074, 1056.1040, 934, 926, 897, 764, 720, 610. Mass spectrum ESI, m/z: 342.50 $[M\text{-}Br]^+$. $C_{21}H_{44}NO_2Br$; Found,%: C 59.55; H 11.12; N 3.25; Br 18.78; Calculated,% C 59.70; H 10.50; N 3.32; Br 18.91.

1-Hexadecyl-4-hydroxy-1-(2-hydroxyethyl)piperidinium bromide (1c).

Yield 2.0 g (40%); white powder; mp 96-98°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.88 (t, 3H); 1.26-1.37 (m, 26H); 1.72 (m, 2H); 2.00 (m, 1H); 2.12 (m, 2H); 2.32 (m, 1H); 3.48 (m, 2H); 3.50 (m, 1H); 3.66 (m, 4H); 3.87 (m, 1H); 4.06 (m, 2H); 4.19 (d, 1H); 4.70 (s, OH). IR spectrum (KBr), ν/cm^{-1}: 3299, 2919, 2850.1471 1372, 1336.1252, 1165, 1135.1090, 1055.1010, 971, 926, 891.768, 719, 599. Mass spectrum ESI, m/z: 370.50 $[M-Br]^+$. $C_{23}H_{48}NO_2Br$; Found,%: C 60.95; H 11.23; N 3.18; Br 17.45; Calculated,% C 61.32; H 10.74; N 3.11; Br 17.73.

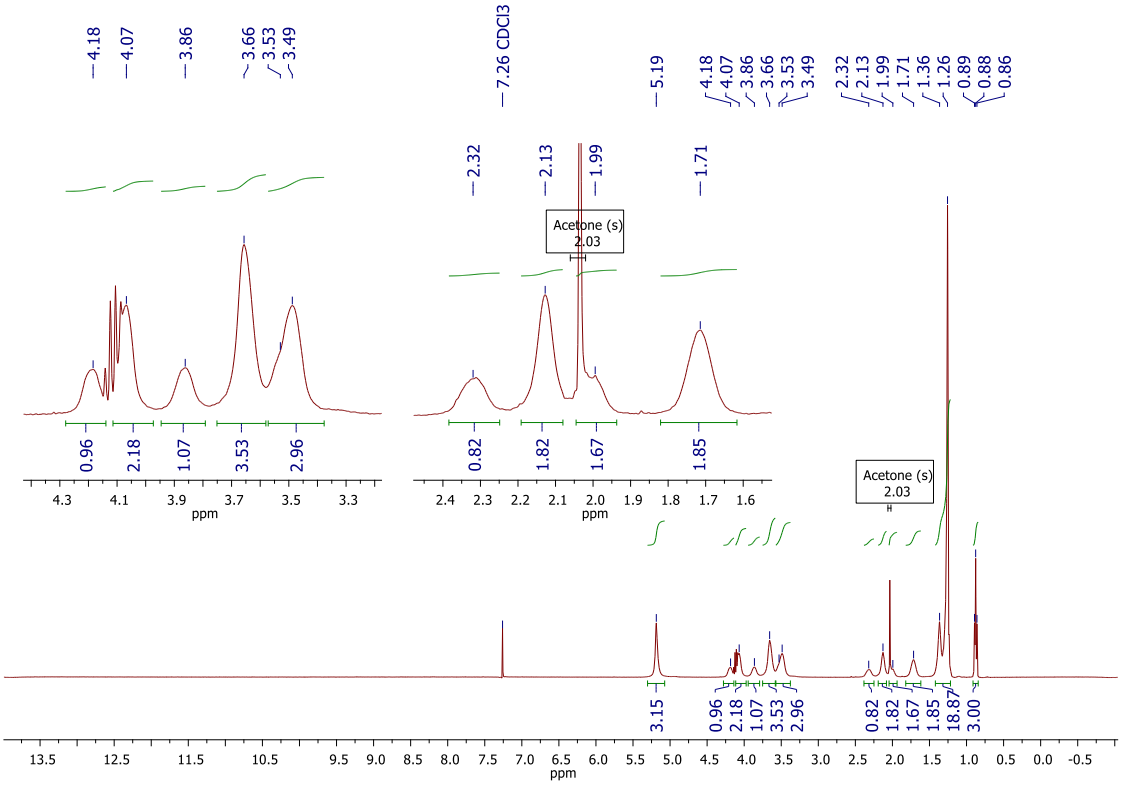

Figure S1. ^{1}H NMR spectrum of **1a**

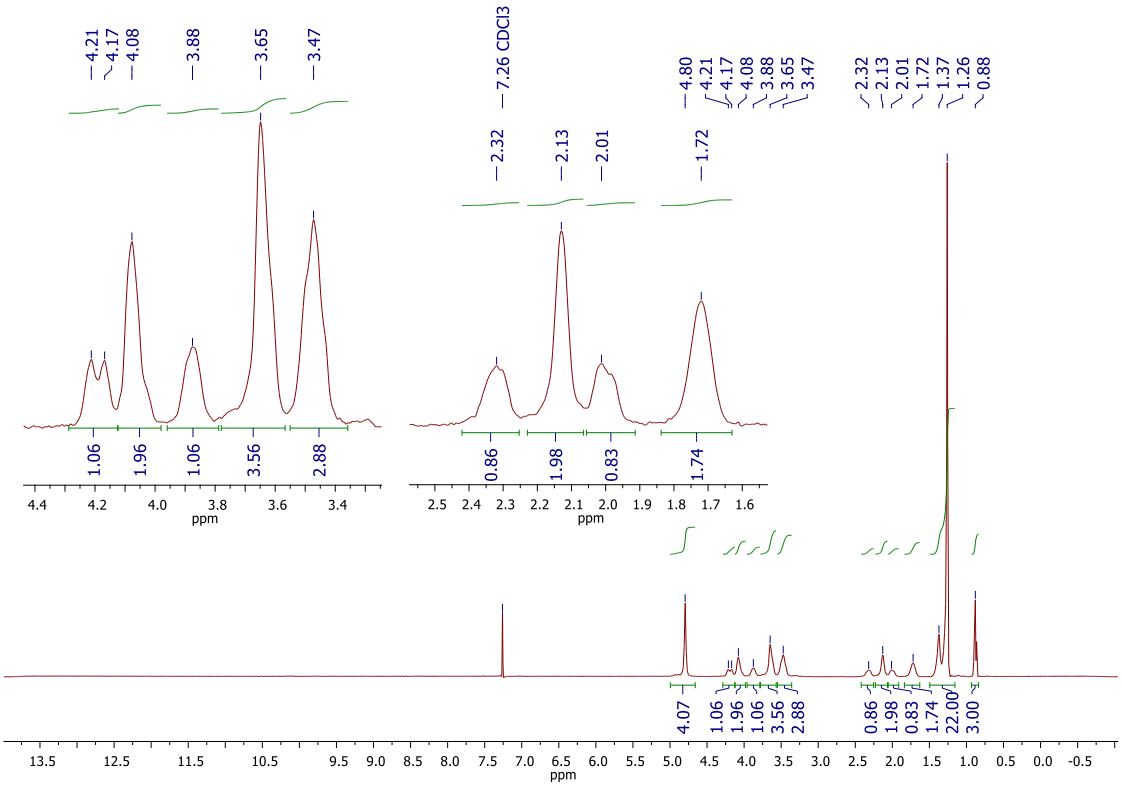

Figure S2. ^{1}H NMR spectrum of **1b**

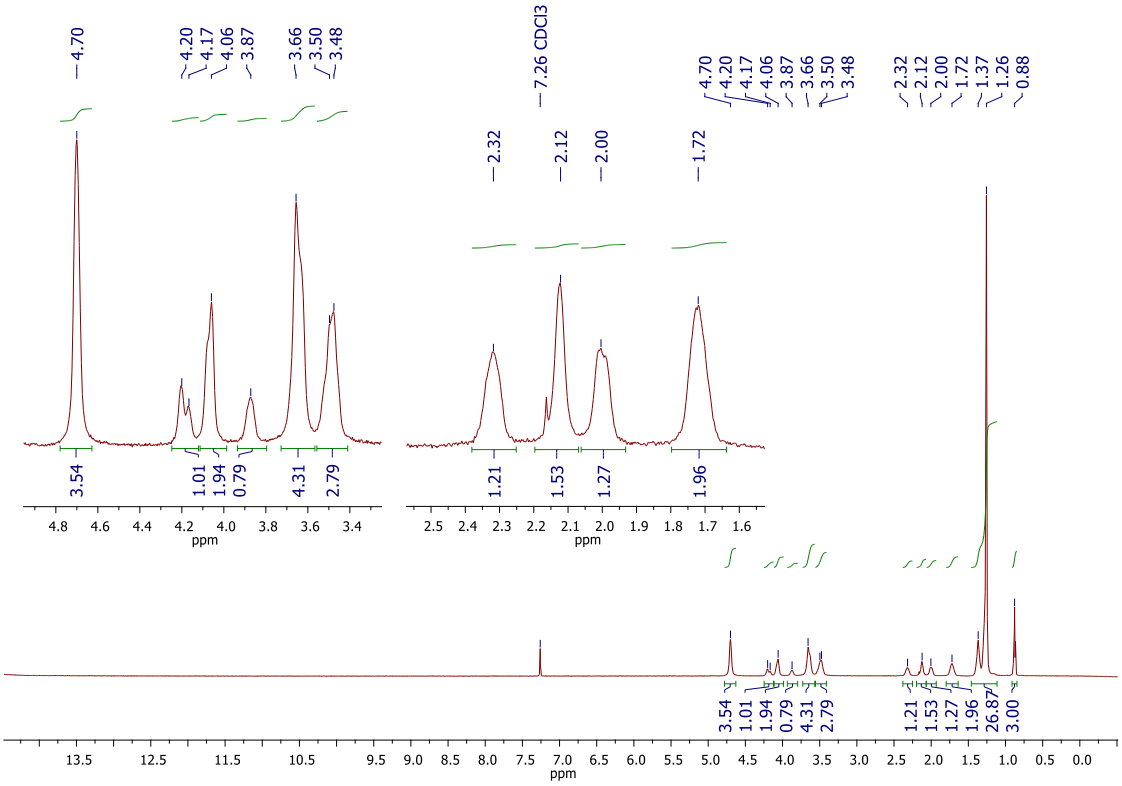

Figure S3. ^{1}H NMR spectrum of **1c**

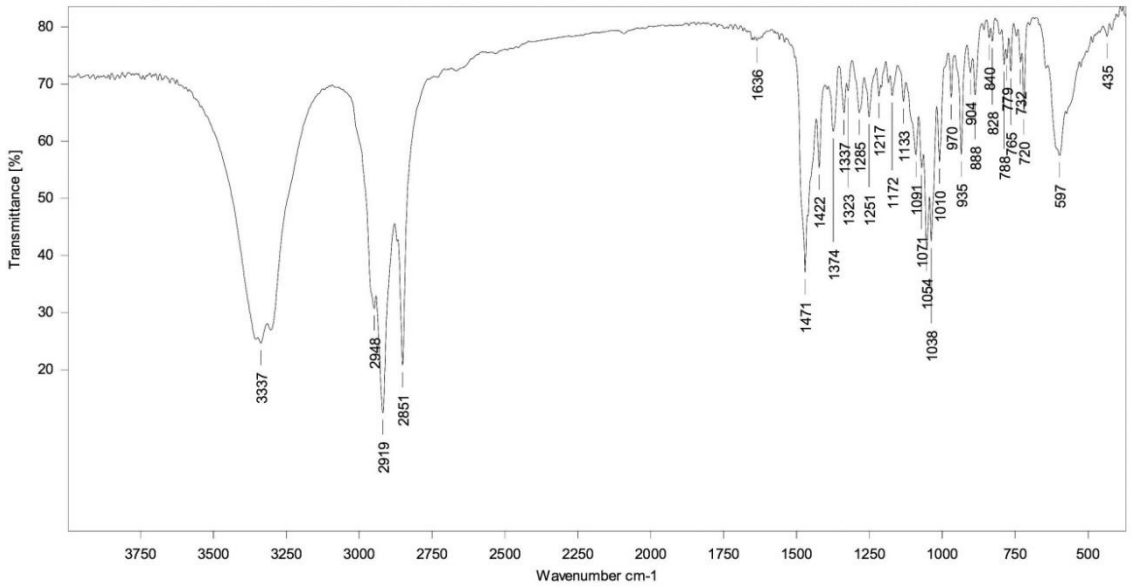

Figure S4. IR spectrum (KBr) **of 1a**

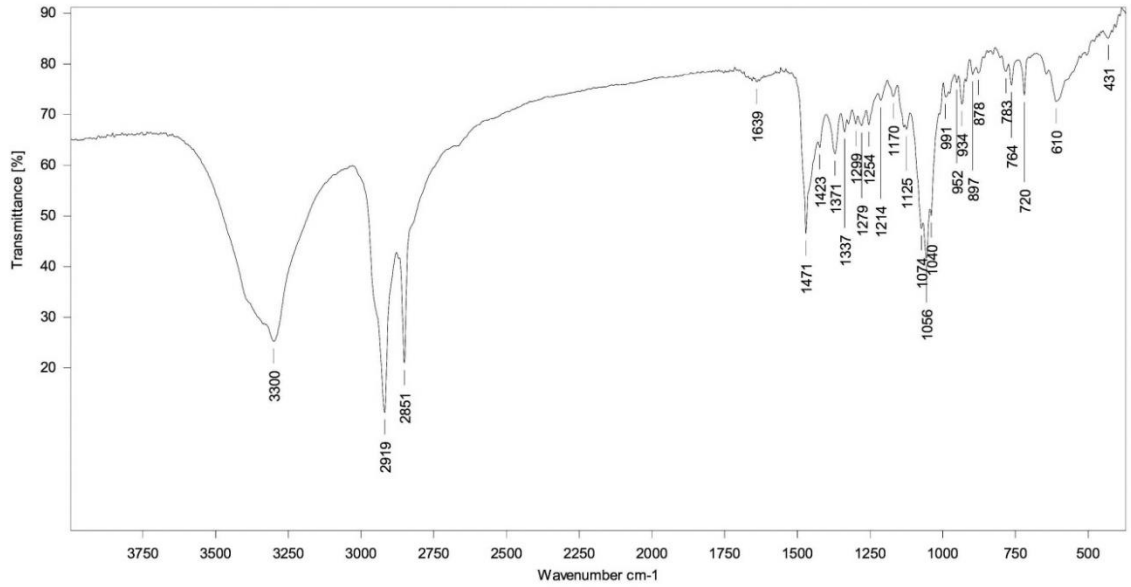

Figure S5. IR spectrum (KBr) of **1b**

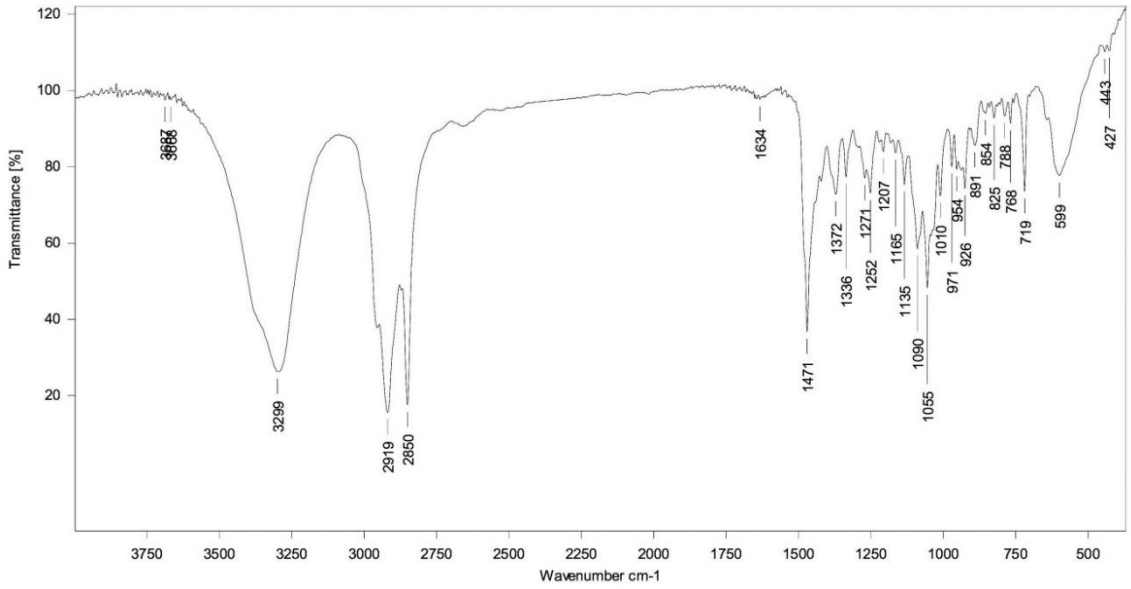

Figure S6. IR spectrum (KBr) of **1c**

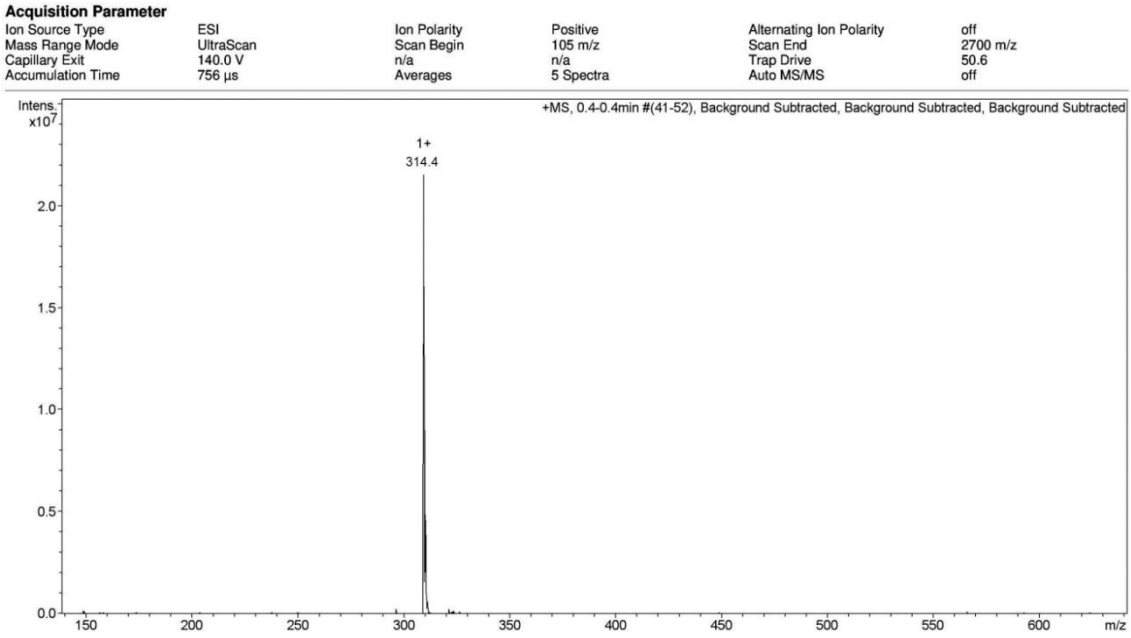

Figure S7. ESI mass spectrum of **1a**

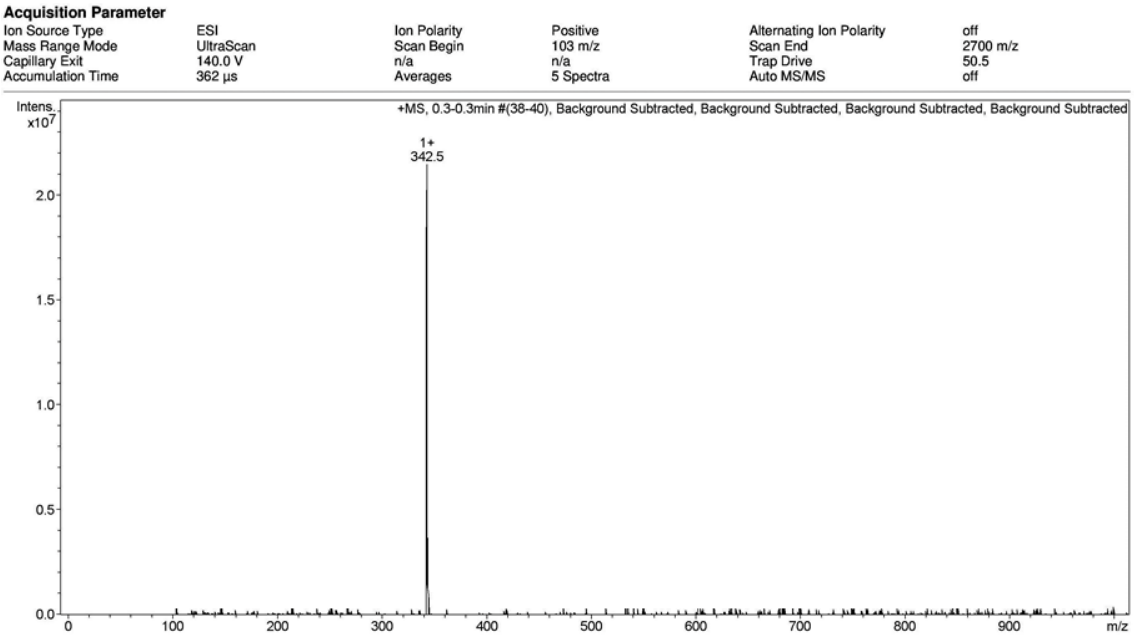

Figure S8. ESI mass spectrum of **1b**

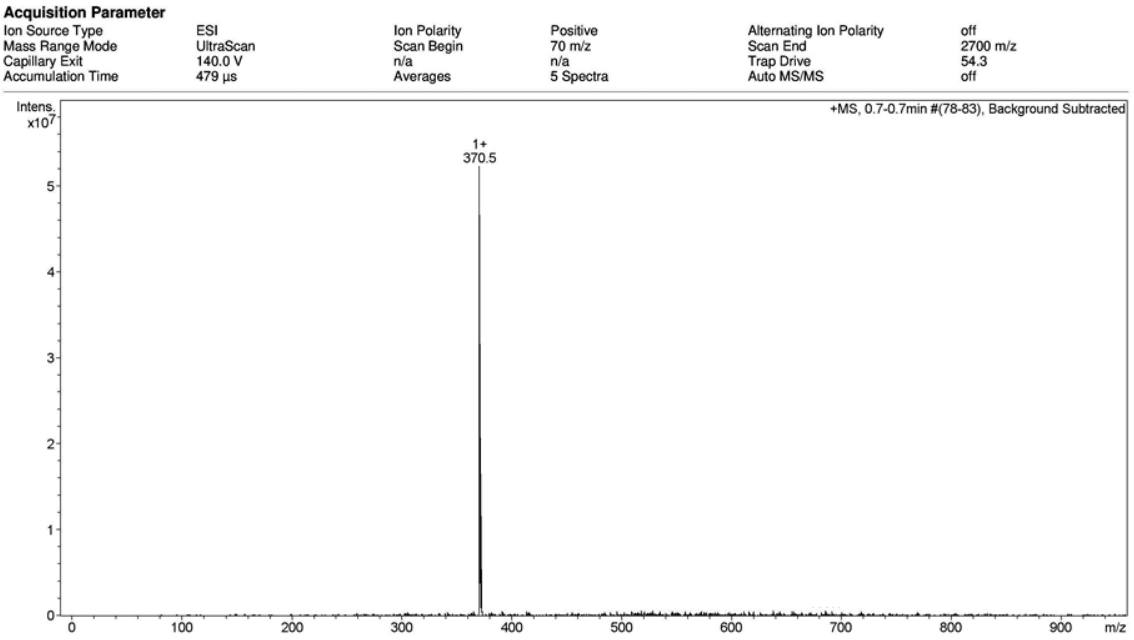

Figure S9. ESI mass spectrum of **1c**

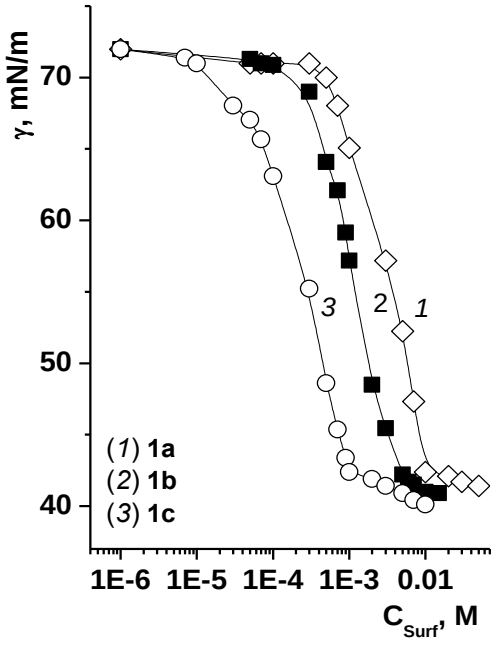

Figure S10. Surface tension isotherms of **1a-c** (CMC values are 1.1 mM and 0.9 mM for compounds **2** and **3**, respectively)