

The Potential of Colloidal Systems Based on Carbamate-Containing Hexadecylpiperidinium Surfactants in Biomedical Applications

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1-(2-(butylcarbamoyloxy)ethyl)-1-hexadecylpiperidinium bromide (1-CB(Bu)-P-16).

Yield 90.4 %. White solid. M.p. 65-68 °C. ¹H NMR spectrum (400 MHz, CDCl₃), δ, ppm (J, Hz): 0.87 t (N⁺-(CH₂)₁₅-CH₃, 3H, ³J_{HH} 6.8); 0.91 t (-NH-(CH₂)₃-CH₃, 3H, ³J_{HH} 7.3); 1.25-1.36 m (N⁺-(CH₂)₂-(CH₂)₁₃-CH₃, NH-(CH₂)₂-CH₂-CH₃, 28H); 1.50 m (NH-CH₂-CH₂-CH₂-CH₃, 2H); 1.68 m (N⁺-(CH₂)₂-CH₂-(CH₂)₂-N⁺, 2H); 1.81-2.00 m (N⁺-CH₂-CH₂-Alk, N⁺-CH₂-CH₂-CH₂-CH₂-CH₂-N⁺, 6H); 3.15 t (NH-CH₂-(CH₂)₂-CH₃, 2H, ³J_{HH} 7.2); 3.50 m (N⁺-CH₂-Alk, 2H); 3.66 m (N⁺-CH₂-CH₂-O-CO-, 2H); 3.83-3.87 m (N⁺-CH₂-(CH₂)₃-CH₂-N⁺, 4H); 4.52 m (N⁺-CH₂-CH₂-O-CO-, 2H). IR (KBr) ν: 3434, 3210, 3028, 2956, 2922, 2852, 1711, 1628, 1528, 1469, 1444, 1377, 1315, 1278, 1247, 1136, 1121, 1062, 1031, 1008, 975, 941, 929, 899, 861, 818, 779, 722, 643, 598 cm⁻¹. Elemental analysis calcd for C₂₈H₅₇BrN₂O₂ (%): C 63.02; H 10.77; Br 14.97; N 5.25. Found (%): C 62.95; H 10.73; Br 15.01; N 5.20. ESI mass spectrum, m/z: [M]⁺ 453.5 (calc m/z for C₂₈H₅₇BrN₂O₂ 533.7).

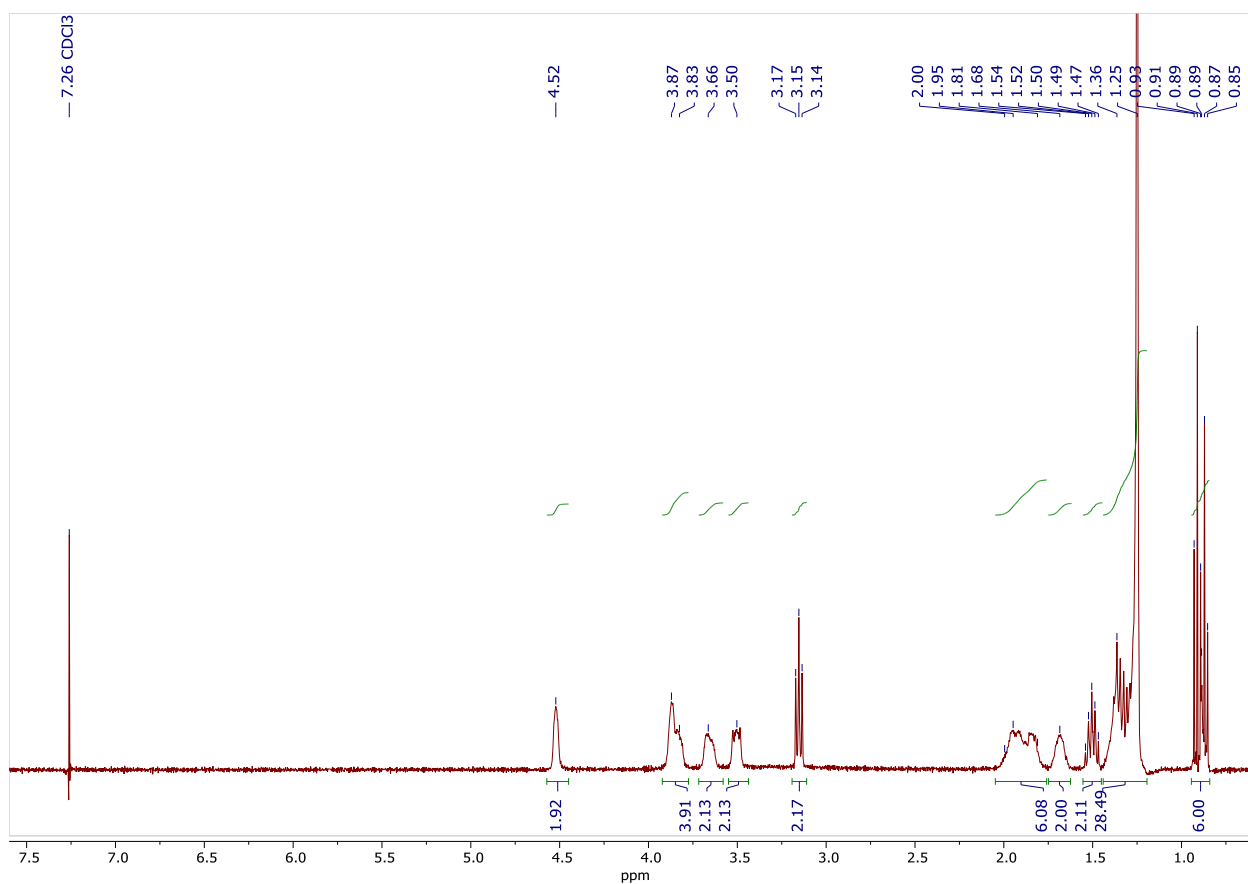


Figure S1. NMR ¹H spectrum of 1-CB(Bu)-P-16.

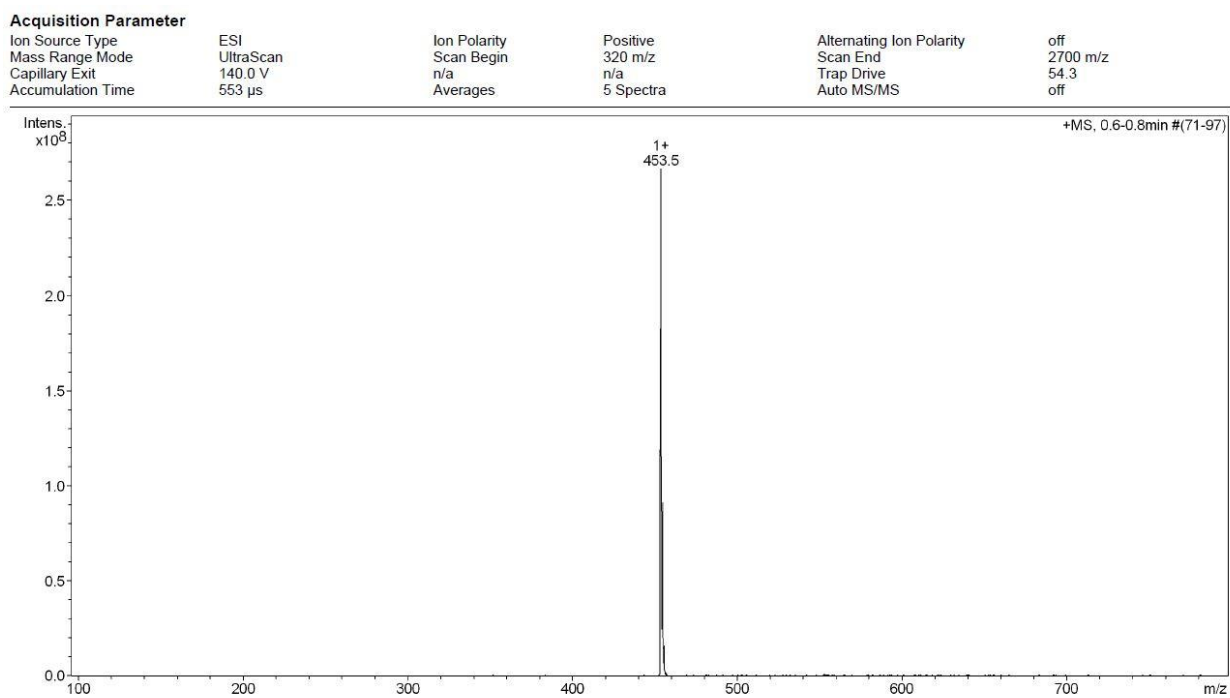


Figure S2. ESI mass spectrum of 1-CB(Bu)-P-16.

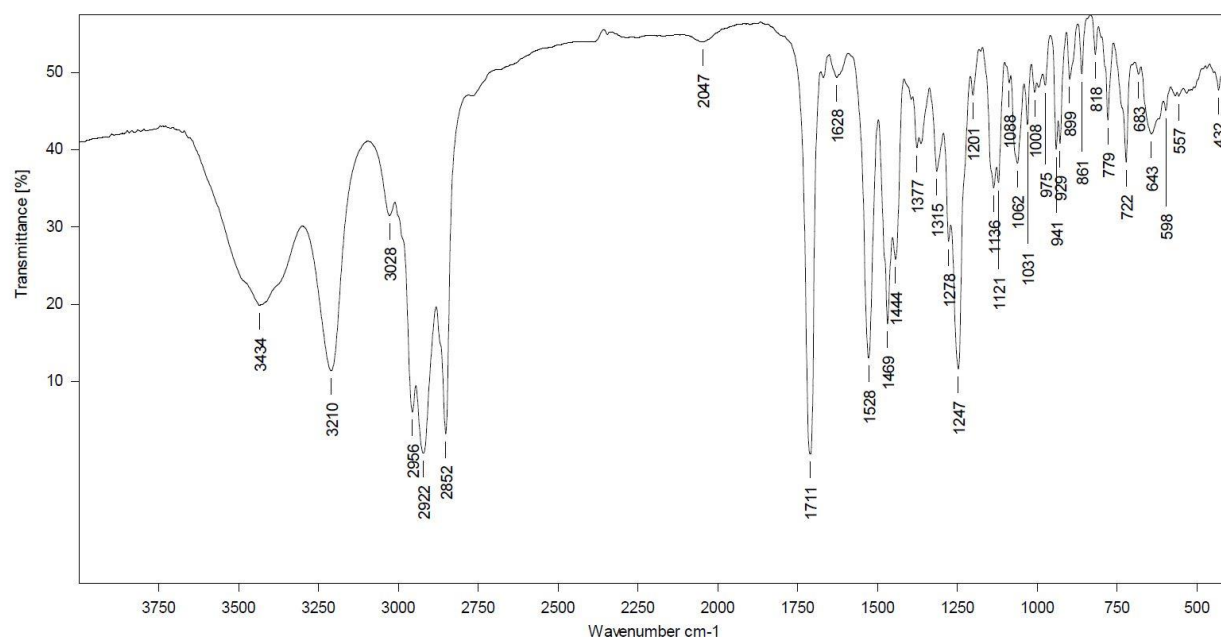


Figure S3. IR spectrum of 1-CB(Bu)-P-16.

3-(butylcarbamoyloxy)-1-hexadecyl-1-methylpiperidinium bromide (3-CB(Bu)-P-16).

Yield 82.3 %. White solid. M.p. 77-80 °C. ^1H NMR spectrum (600 MHz, CDCl_3), δ , ppm (J, Hz): 0.87 t ($\text{N}^+(\text{CH}_2)_{15}\text{-CH}_3$, 3H, $^3J_{\text{HH}}$ 7.1); 0.91 t ($-\text{NH}(\text{CH}_2)_3\text{-CH}_3$, 3H, $^3J_{\text{HH}}$ 7.3); 1.24-1.36 m ($\text{N}^+(\text{CH}_2)_2\text{-(CH}_2\text{)}_{13}\text{-CH}_3$, $\text{NH}(\text{CH}_2)_2\text{-CH}_2\text{-CH}_3$, 28H); 1.45-1.50 m ($\text{NH-CH}_2\text{-CH}_2\text{-CH}_2\text{-CH}_3$, 2H); 1.66-2.25 m ($\text{N}^+\text{-CH}_2\text{-CH}_2\text{-(CH}_2\text{)}_{13}\text{-CH}_3$, $\text{N}^+\text{-CH}_2\text{-CH-(CH}_2\text{)}_2\text{-CH}_2\text{-N}^+$, 6H); 3.13-3.16 m ($\text{CO-NH-CH}_2\text{-(CH}_2\text{)}_2\text{-CH}_3$, 2H); 3.18, 3.40 two m ($\text{N}^+\text{-CH}_3$, 3H); 3.29-3.34, 3.42-3.74, 3.90-3.99 three m ($\text{N}^+\text{-CH}_2\text{-Alk}$, $\text{N}^+\text{-CH}_2\text{-CH-(CH}_2\text{)}_2\text{-CH}_2\text{-N}^+$, 6H); 4.34, 4.45 two m ($\text{N}^+\text{-CH}_2\text{-CH-O}$, 1H). IR (KBr) ν : 3326, 2919, 2852, 1718, 1625, 1575, 1467, 1376, 1250, 1125, 1081, 1024, 915, 722, 626 cm^{-1} . Elemental analysis calcd for $\text{C}_{27}\text{H}_{55}\text{BrN}_2\text{O}_2$ (%): C 62.41; H 10.67; Br 15.38; N 5.39. Found (%): C 62.36; H 10.70; Br 15.32; N 5.37. ESI mass spectrum, m/z : $[\text{M}]^+$ 340.27 (calc m/z for $\text{C}_{27}\text{H}_{55}\text{BrN}_2\text{O}_2$ 519.65).

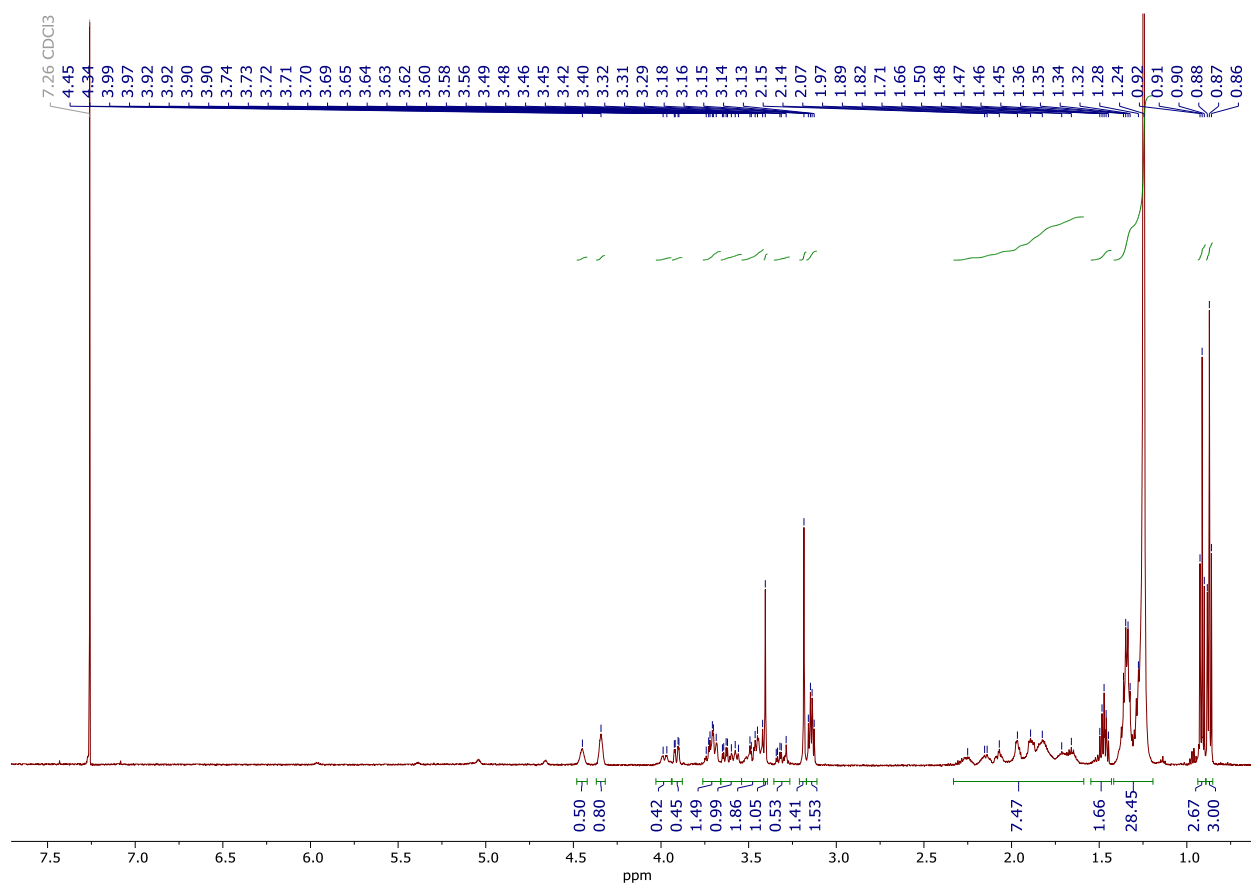


Figure S4. NMR ^1H spectrum of 3-CB(Bu)-P-16.

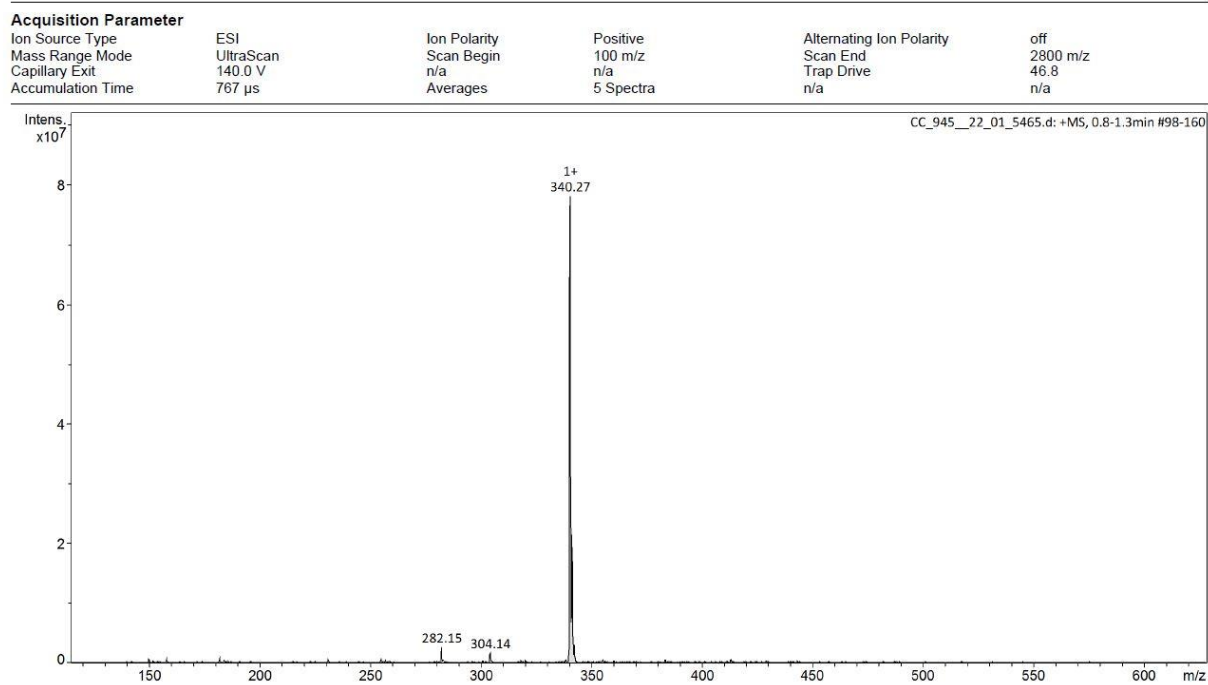


Figure S5. ESI mass spectrum of 3-CB(Bu)-P-16.

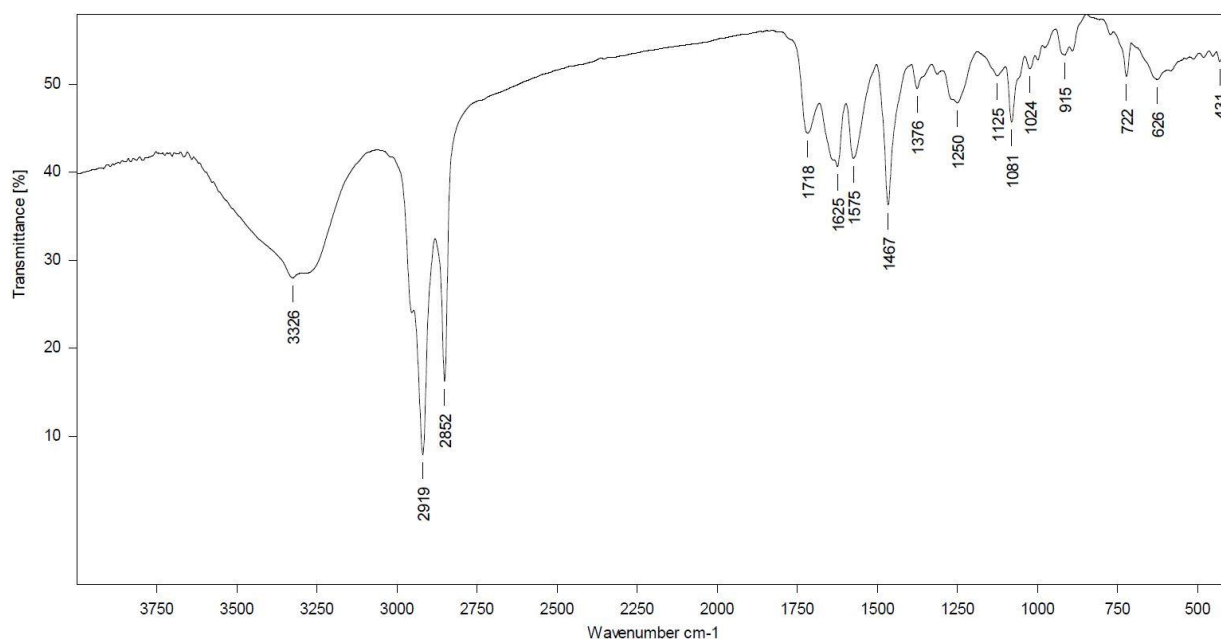


Figure S6. IR spectrum of 3-CB(Bu)-P-16.

4-(butylcarbamoyloxy)-1-(2-(butylcarbamoyloxy)ethyl)-1-hexadecylpiperidinium bromide (1,4-CB(Bu)-P-16). Yield 78.6 %. White solid. M.p. 175-178 °C. ^1H NMR spectrum (400 MHz, CDCl_3), δ , ppm: 0.85-0.93 m ($\text{N}^+(\text{CH}_2)_{15}\text{-CH}_3$, $-\text{NH}(\text{CH}_2)_3\text{-CH}_3$, 9H); 1.24-1.37 m ($\text{N}^+(\text{CH}_2)_2\text{-(CH}_2)_{13}\text{-CH}_3$, $\text{NH}(\text{CH}_2)_2\text{-CH}_2\text{-CH}_3$, 30H); 1.49 m ($\text{NH-CH}_2\text{-CH}_2\text{-CH}_2\text{-CH}_3$, 4H); 1.68 m ($\text{N}^+\text{-CH}_2\text{-CH}_2\text{-Alk}$, 2H); 2.07 m ($\text{N}^+\text{-CH}_2\text{-CH}_2\text{-CH-CH}_2\text{-CH}_2\text{-N}^+$, 4H); 3.11-3.16 m ($\text{NH-CH}_2\text{-(CH}_2)_2\text{-CH}_3$, 4H); 3.39 m ($\text{N}^+\text{-CH}_2\text{-CH}_2\text{-O-CO-}$, 2H); 3.54 m ($\text{N}^+\text{-CH}_2\text{-Alk}$, 2H); 4.09-4.23 m ($\text{N}^+\text{-CH}_2\text{-CH}_2\text{-CH-CH}_2\text{-CH}_2\text{-N}^+$, 4H); 4.55 m ($\text{N}^+\text{-CH}_2\text{-CH}_2\text{-O-CO-}$, 2H); 5.01 m ($\text{N}^+\text{-(CH}_2)_2\text{-CH-(CH}_2)_2\text{-N}^+$, 1H). IR (KBr) ν : 3329, 2958, 2925, 2855, 1728, 1704, 1539, 1465, 1378, 1251, 1145, 1035, 982, 896, 776, 722, 639 cm^{-1} . Elemental analysis calcd for $\text{C}_{33}\text{H}_{66}\text{BrN}_3\text{O}_4$ (%): C 61.09; H 10.25; Br 12.32; N 6.48. Found (%): C 61.15; H 10.22; Br 12.26; N 6.39. ESI mass spectrum, m/z : $[\text{M}]^+$ 568.6 (calc m/z for $\text{C}_{33}\text{H}_{66}\text{BrN}_3\text{O}_4$ 648.8).

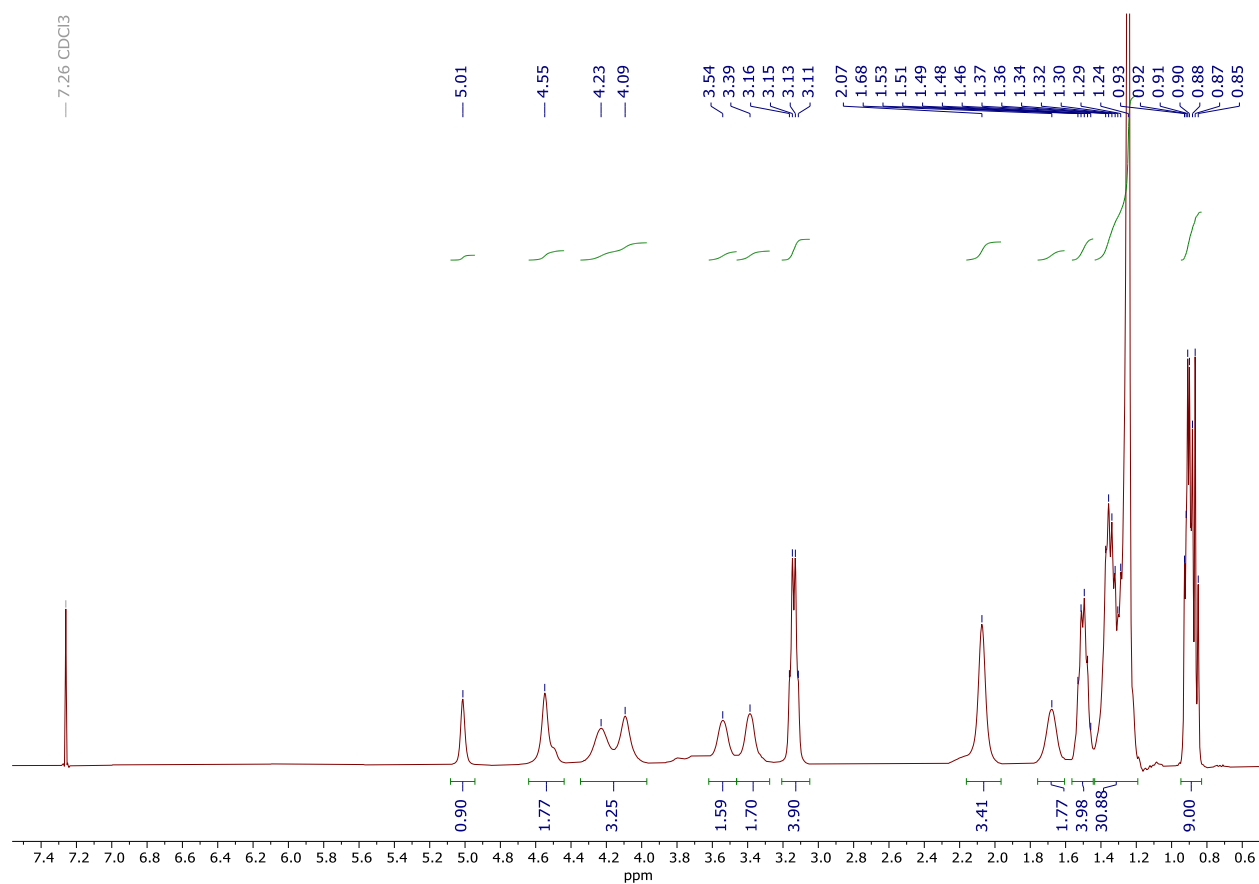


Figure S7. NMR ¹H spectrum of 1,4-CB(Bu)-P-16.

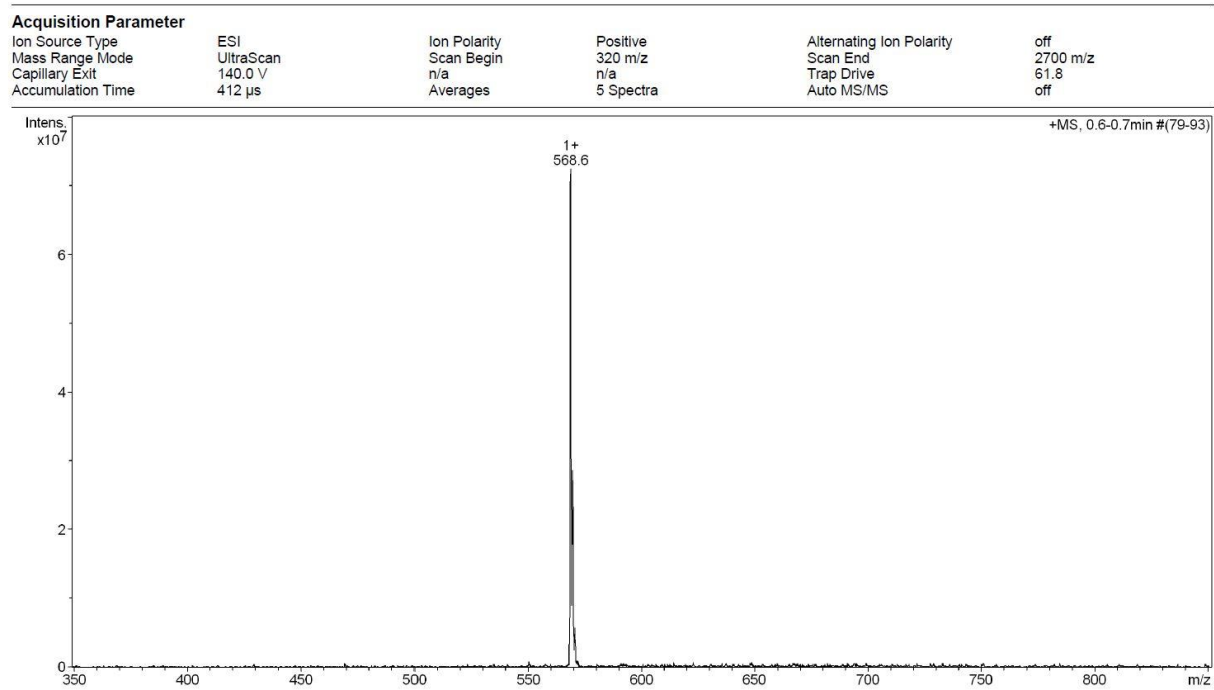


Figure S8. ESI mass spectrum of 1,4-CB(Bu)-P-16.

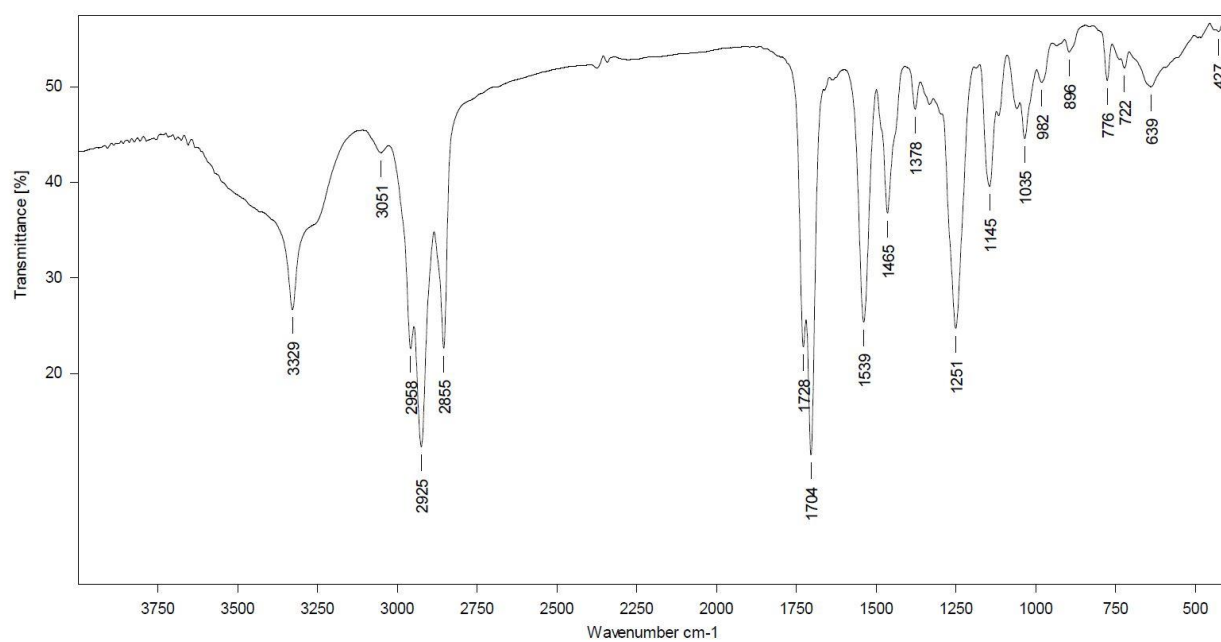


Figure S9. IR spectrum of 1,4-CB(Bu)-P-16.

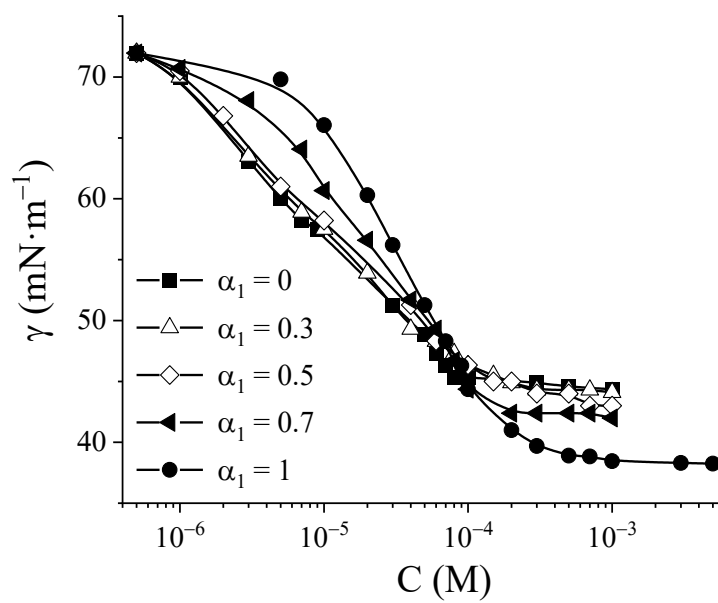


Figure S10. Surface tension isotherms of micellar solutions of 1-CB(Bu)-P-16/Brij®35 at different molar fractions of the cationic surfactant (α_1 – fraction of 1-CB(Bu)-P-16); 25°C.

Table S1. Antimicrobial activity of butylcarbamate-containing piperidinium surfactants and the mixed system 1-CB(Bu)-P-16/Brij®35 at equimolar ratio.

[illegible]