Supporting information

Aggregation Behavior and Bactericidal Activities of Novel Cationic Surfactants Functionalized with Amides and Ether Groups

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Synthesis and Characterization

Synthesis of ethyl phenoxyacetate (1)

Phenol (15.0 g, 160 mmol), ethyl chloroacetate (39.7 g, 324 mmol) and anhydrous K$_2$CO$_3$ (46.3 g, 336 mmol) were added in 100 mL of dry acetonitrile, and refluxed for 1 h. After filtration, the solvent was evaporated under reduced pressure. Then the residue was separated by column chromatography using the mixture of petroleum ether/dichloromethane (2:1 by volume) as eluent, and then compound 1 as a gummy liquid (25.6 g, 88 % yield) was obtained.

FT-IR (KBr pellet) $\nu$ cm$^{-1}$: 2978(-CH$_3$), 1760(C=O, ester), 1086(Ar-O-R, ether), 886-694(C-H, aromatic hydrocarbon); $^1$H NMR (600 MHz, CDCl$_3$) $\delta$ ppm 6.90-7.28 (m, 5H, C$_6$H$_5$OCH$_2$), 4.61 (s, 2H, C$_6$H$_5$OCH$_2$COOCH$_2$CH$_3$), 4.24-4.28 (m, 2H, C$_6$H$_5$OCH$_2$COOCH$_2$CH$_3$), 1.28 (t, $J$ = 7.2 Hz, 3H, C$_6$H$_5$OCH$_2$COOCH$_2$C$_6$H$_5$).

Synthesis of N’-(2-phenoxyacetyl)-N,N-dimethylethylenediamine (2)

Compound 1 (16.8 g, 93.4 mmol) and N,N-Dimethylethylene-diamine (10.1 g, 114.9 mmol) were dissolved in 60 mL ethanol, refluxed for 5 h. After evaporation of the solvent, distilled water (20 mL) was added to the mixture, and the pH of the mixture was adjusted to 8 by 6 mol L$^{-1}$ HCl solution. The mixed solution was then extracted with 3×20 mL dichloromethane. The organic layers were collected, dried over anhydrous magnesium sulfate, and concentrated under reduced pressure to give compound 2 as a yellow liquid (15.4 g, yield 74 %).

FT-IR (KBr pellet) $\nu$ cm$^{-1}$: 3264(N-H, amide), 2945(-CH$_3$), 2814(-CH$_2$-), 1654(C=O, amide), 1053(Ar-O-R, ether), 886-699(C-H, aromatic hydrocarbon); $^1$H NMR (600
MHz, CDCl$_3$): $\delta$ ppm 6.94-7.33 (m, 5H, C$_6$H$_5$OCH$_2$), 7.02 (t, $J = 5.2$ Hz, 1H, CH$_2$CONHCH$_2$CH$_2$), 4.50 (s, 2H, CH$_2$CONHCH$_2$CH$_2$), 3.40-3.43 (m, 2H, CH$_2$CONHCH$_2$CH$_2$), 2.45 (t, $J = 6.0$ Hz, 2H, CH$_2$CONHCH$_2$CH$_2$), 2.23 (s, 6H, CONHCH$_2$CH$_2$NCH$_3$).

Figure 1 $^1$H NMR and $^{13}$C NMR of C$_{12}$PDA
Figure 2 $^{13}$C NMR of C$_{12}$PDA

Figure 3 $^1$H NMR of C$_{14}$PDA
Figure 4 $^{13}$C NMR of C$_{14}$PDA

Figure 5 $^1$H NMR of C$_{16}$PDA
Figure 6 $^{13}$C NMR of C$_{16}$PDA
Figure 7 MS of C\textsubscript{12}PDA

Figure 8 MS of C\textsubscript{14}PDA
Figure 12 FT-IR of C$_{16}$PDA

Figure 13 $^{13}$C/DEPT spectra of C$_{12}$PDA
Figure 14 $^{13}$C/DEPT spectra of C$_{14}$PDA

Figure 15 $^{13}$C/DEPT spectra of C$_{16}$PDA
Figure 16 Pyrene emission spectra with the concentration of quencher for $C_{12}$PDA(A), $C_{14}$PDA(B) and $C_{16}$PDA(C).