

Supporting information

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

Guangzhou Cao, Xiangfeng Guo*, Lihua Jia*, Xuhua Tian

College of Chemistry and Chemical Engineering, Key Laboratory of Fine Chemicals
of College of Heilongjiang Province, Qiqihar University, Qiqihar 161006, China.

*Corresponding author. Email: xfguo@163.com (X. Guo); jlh29@163.com (L. Jia).

Synthesis and Characterization

Synthesis of ethyl phenoxyacetate (1)

Phenol (15.0 g, 160 mmol), ethyl chloroacetate (39.7 g, 324 mmol) and anhydrous K_2CO_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) ν cm^{-1} : 2978(-CH₃), 1760(C=O, ester), 1086(Ar-O-R, ether), 886-694(C-H, aromatic hydrocarbon); ¹H NMR (600 MHz, CDCl₃) δ ppm 6.90-7.28 (m, 5H, C₆H₅OCH₂), 4.61 (s, 2H, C₆H₅OCH₂COOCH₂CH₃), 4.24-4.28 (m, 2H, C₆H₅OCH₂COOCH₂CH₃), 1.28 (t, $J = 7.2$ Hz, 3H, C₆H₅OCH₂COOCH₂CH₃).

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) ν cm^{-1} : 3264(N-H, amide), 2945(-CH₃), 2814(-CH₂-), 1654(C=O, amide), 1053(Ar-O-R, ether), 886-699(C-H, aromatic hydrocarbon); ¹H NMR (600

MHz, CDCl₃): δ ppm 6.94-7.33 (m, 5H, C₆H₅OCH₂), 7.02 (t, $J = 5.2$ Hz, 1H, CH₂CONHCH₂CH₂), 4.50 (s, 2H, CH₂CONHCH₂CH₂), 3.40-3.43 (m, 2H, CH₂CONHCH₂CH₂), 2.45 (t, $J = 6.0$ Hz, 2H, CH₂CONHCH₂CH₂), 2.23 (s, 6H, CONHCH₂CH₂NCH₃).

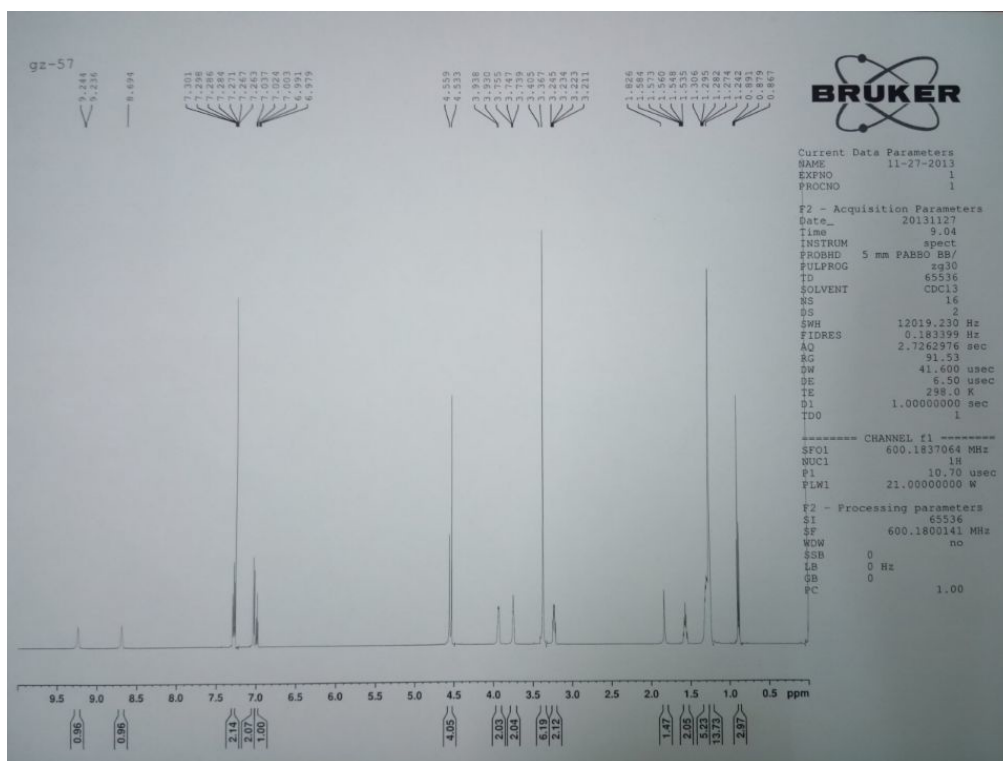


Figure 1 ¹H NMR and ¹³C NMR of C₁₂PDA

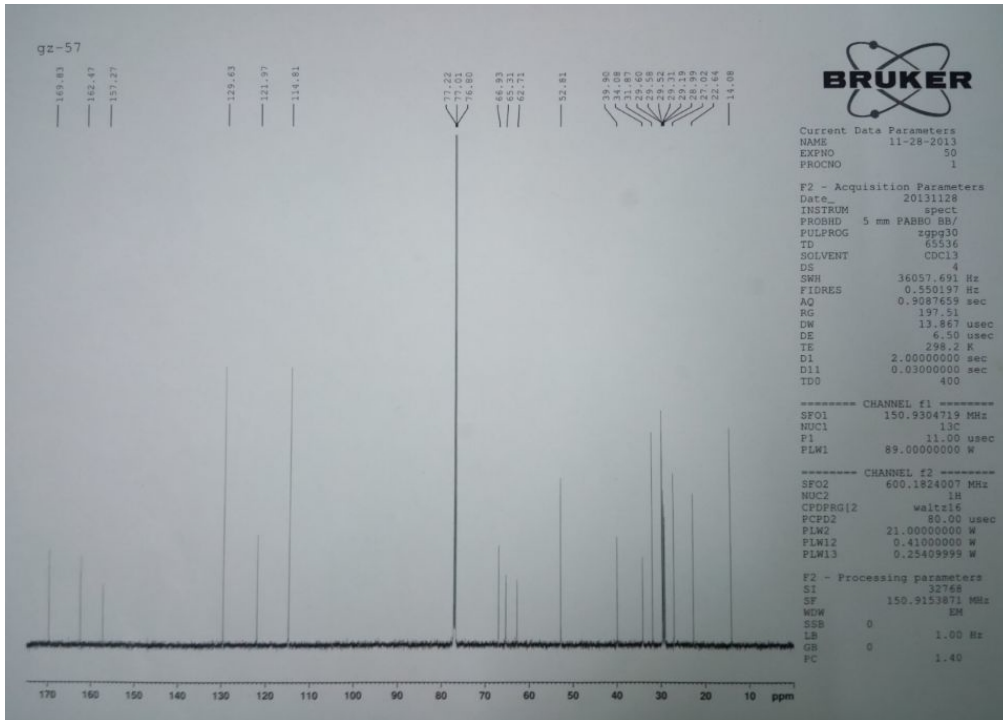


Figure 2 ^{13}C NMR of C_{12}PDA

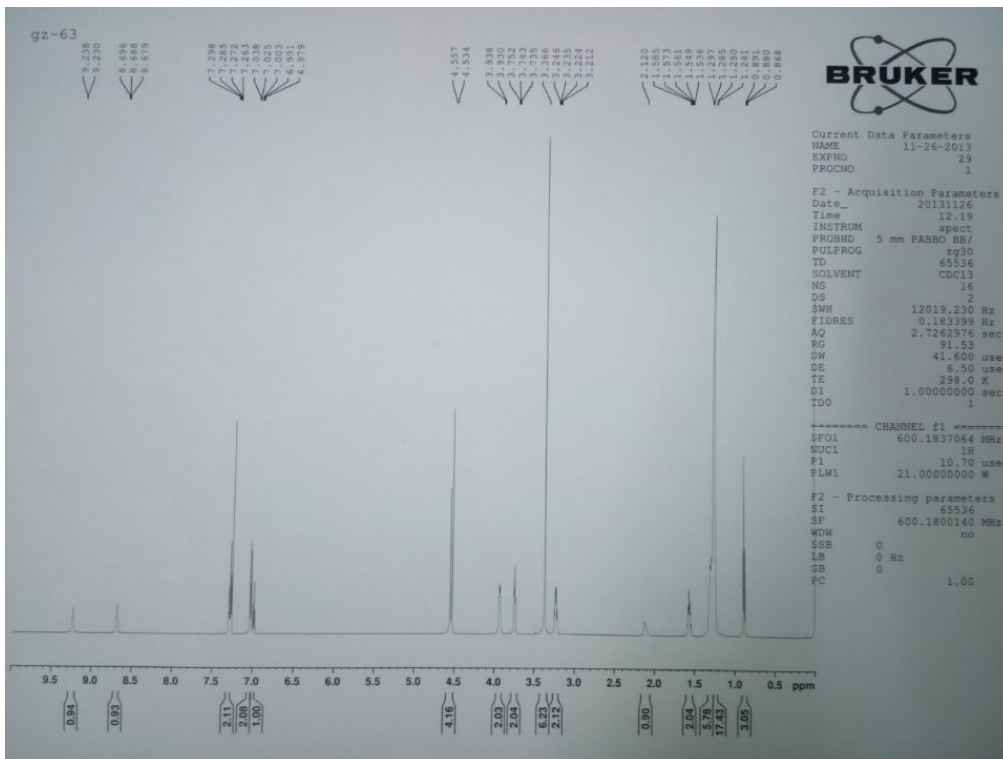


Figure 3 ^1H NMR of C_{14}PDA

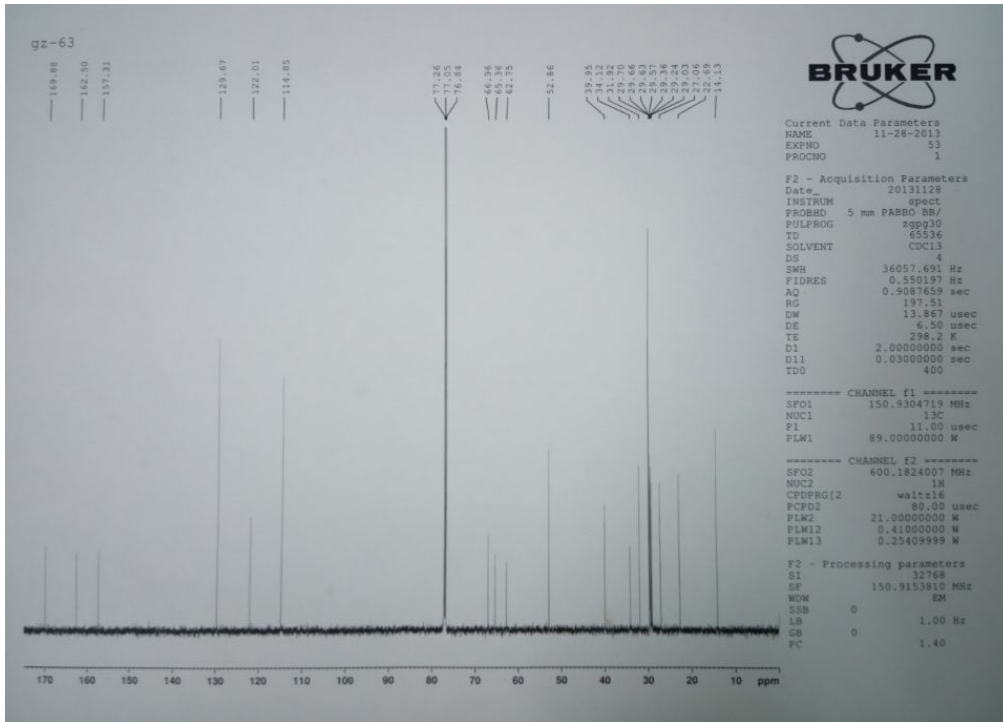


Figure 4 ^{13}C NMR of C_{14}PDA

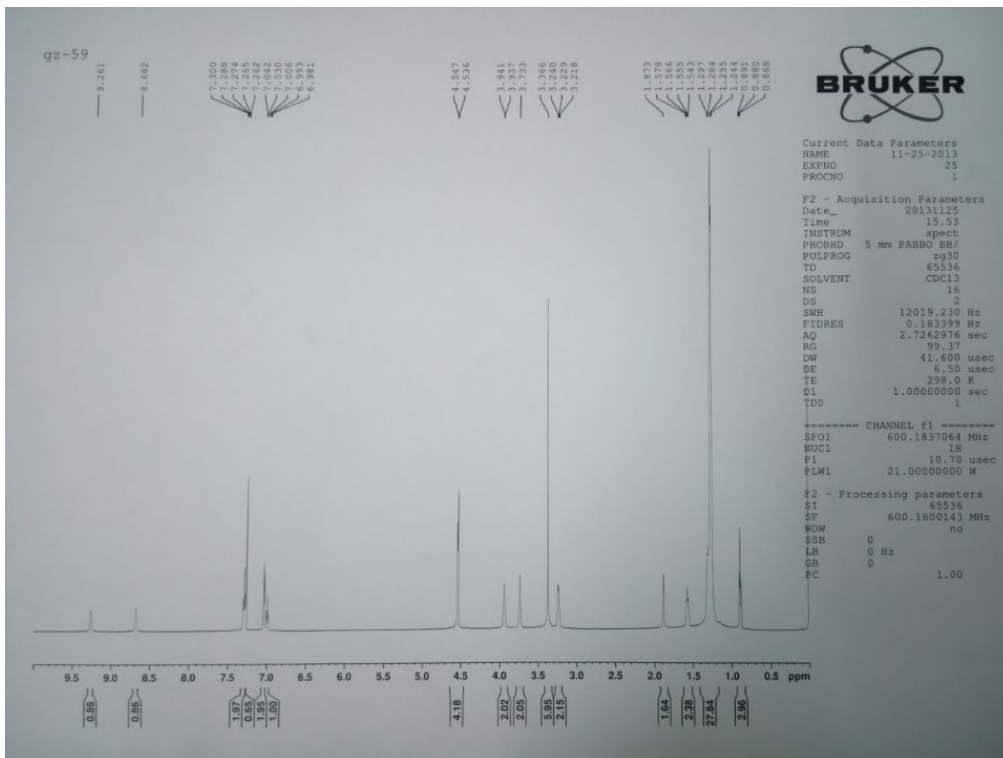


Figure 5 ^1H NMR of C_{16}PDA

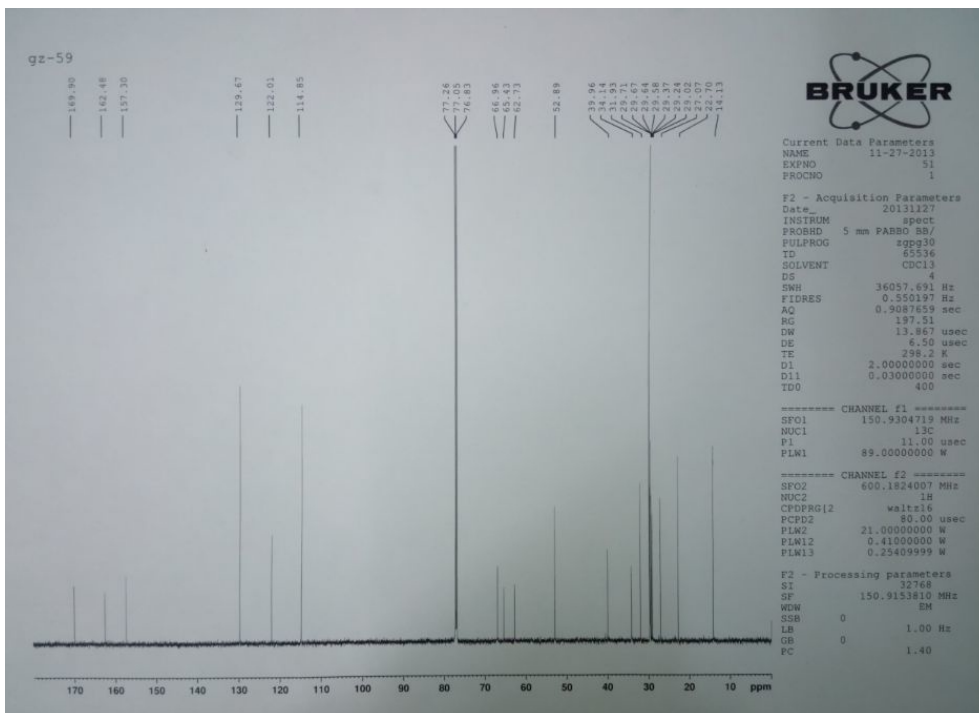


Figure 6 ^{13}C NMR of C_{16}PDA

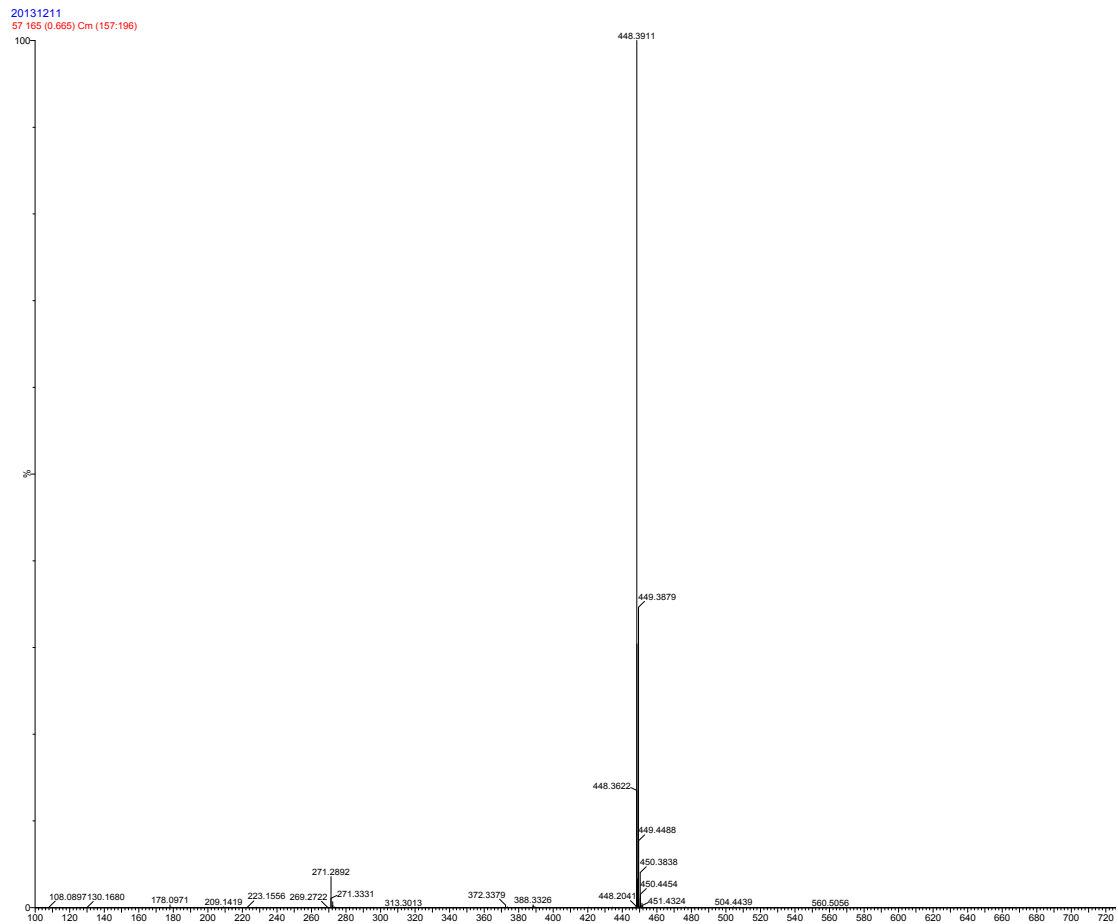


Figure 7 MS of C₁₂PDA

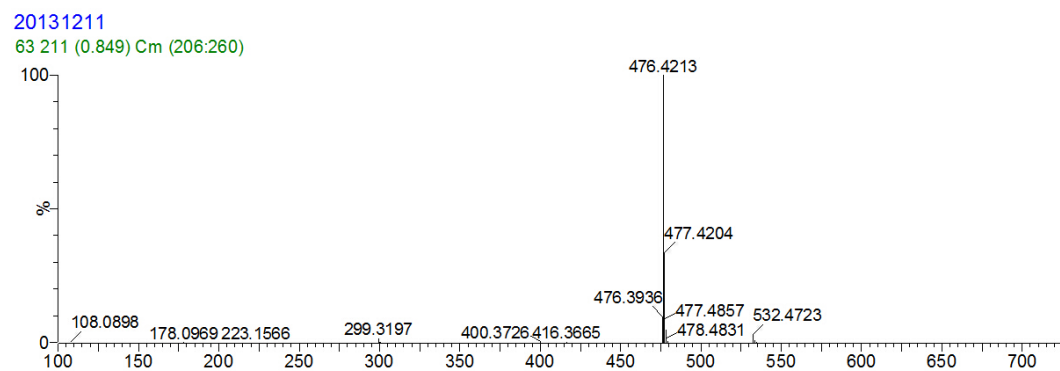


Figure 8 MS of C₁₄PDA

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59 277 (1.105) Cm (264:345)

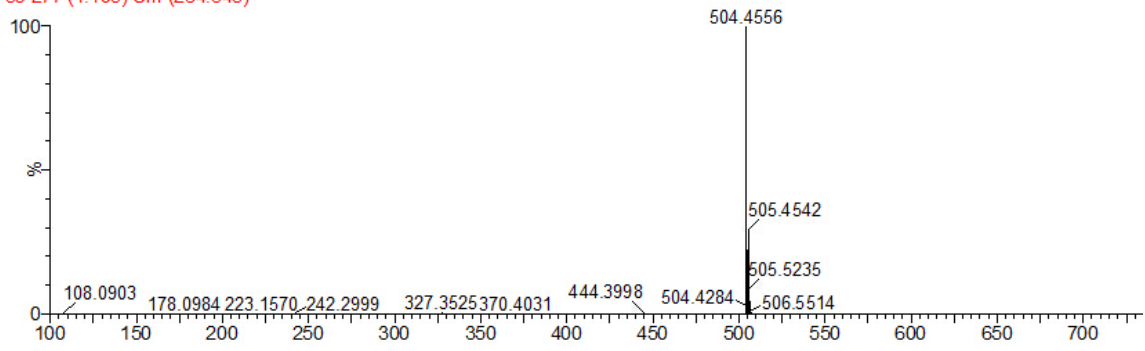


Figure 9 MS of C₁₆PDA

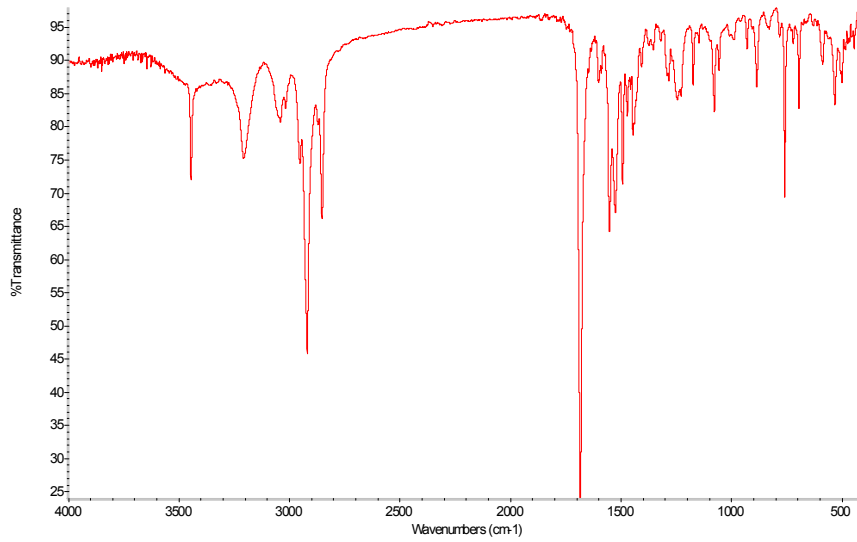


Figure 10 FT-IR of C₁₂PDA

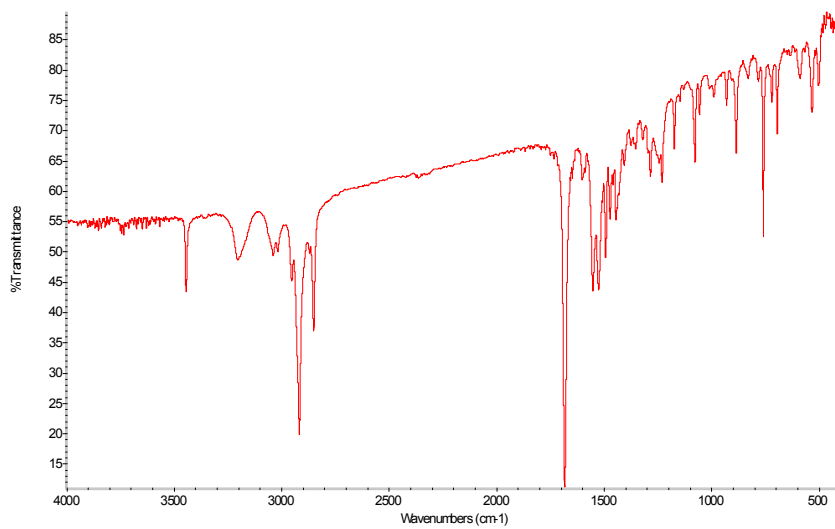


Figure 11 FT-IR of C₁₄PDA

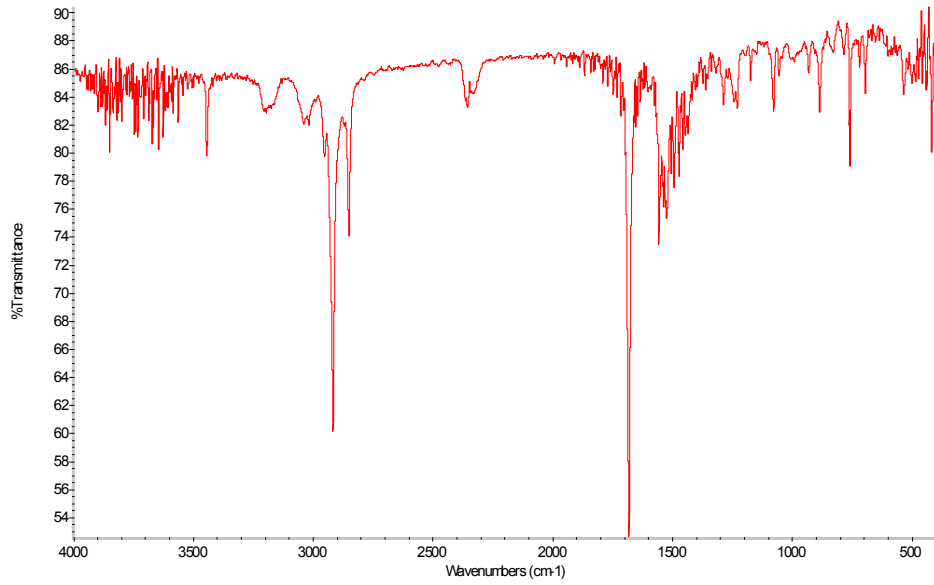


Figure 12 FT-IR of C₁₆PDA

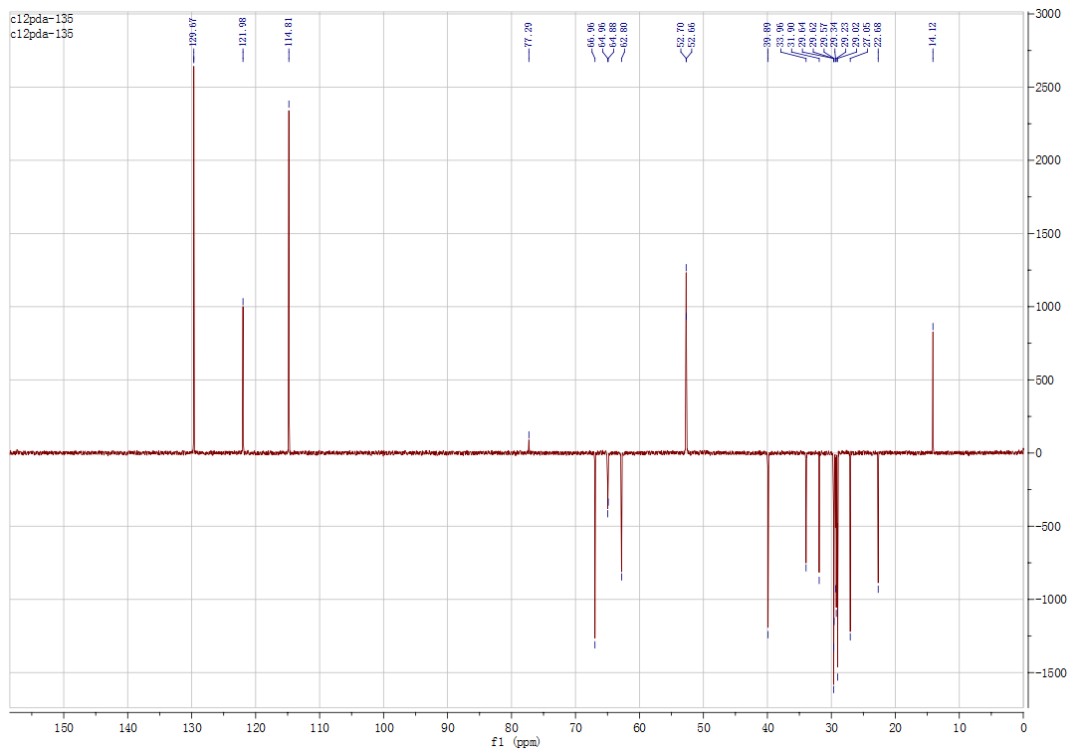


Figure13 ¹³C/DEPT spectra of C₁₂PDA

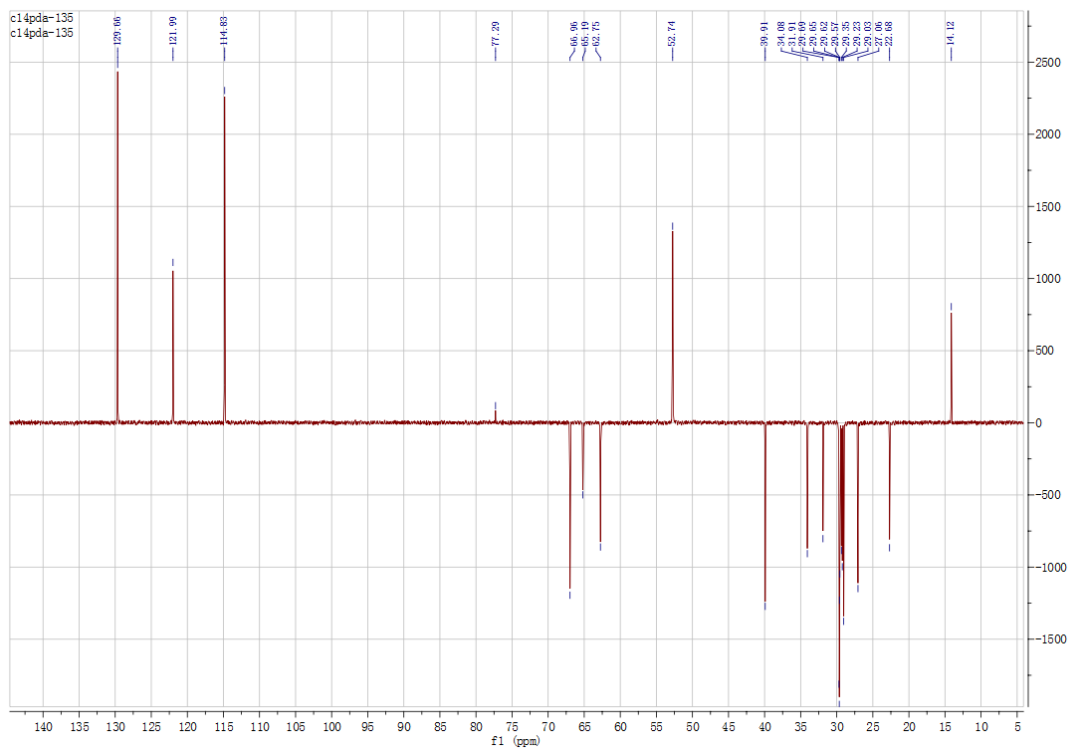


Figure14 $^{13}\text{C}/\text{DEPT}$ spectra of C_{14}PDA

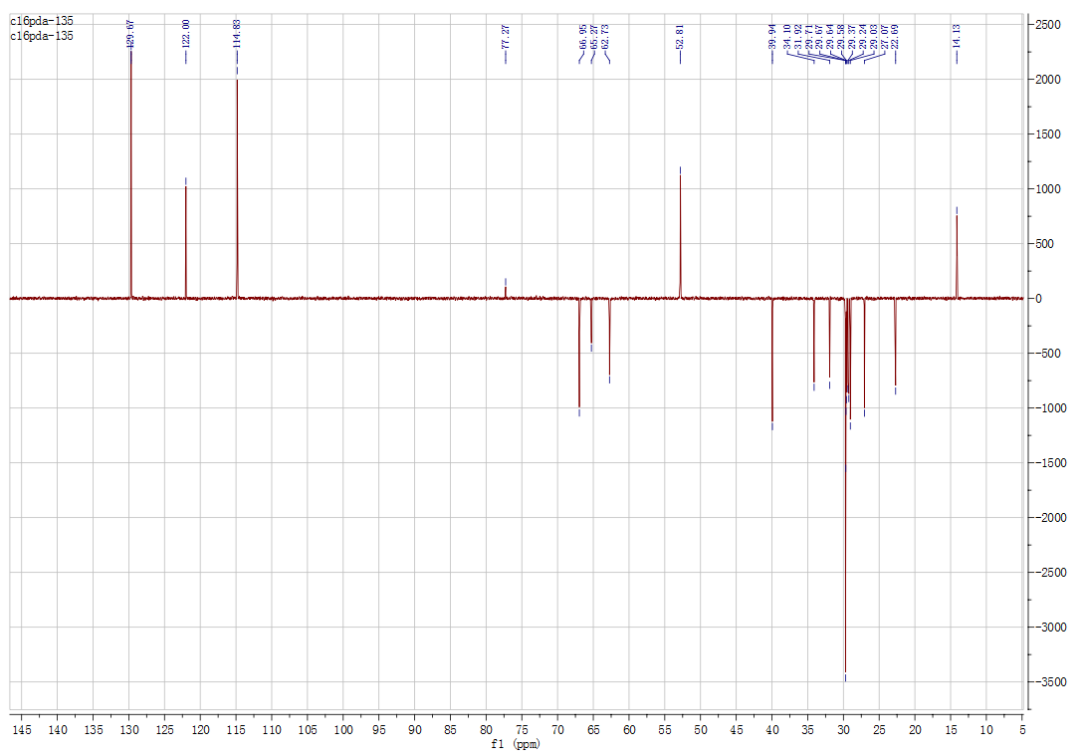


Figure15 $^{13}\text{C}/\text{DEPT}$ spectra of C_{16}PDA

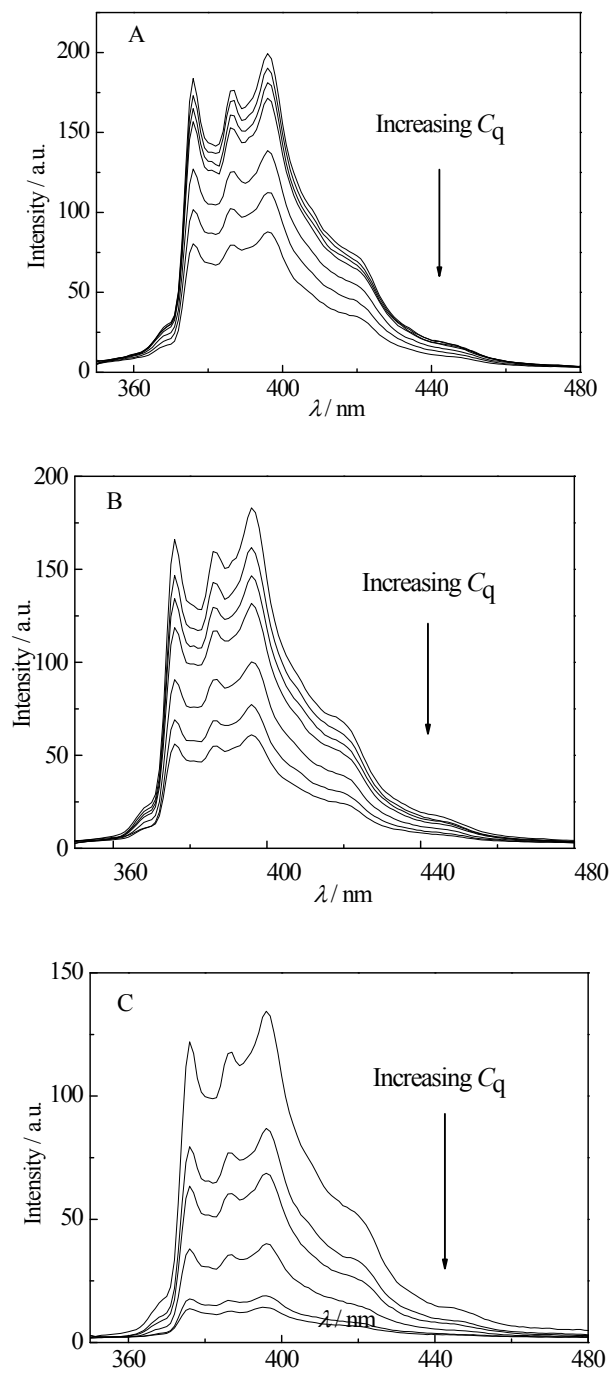


Figure 16 Pyrene emission spectra with the concentration of quencher for C₁₂PDA(A), C₁₄PDA(B) and C₁₆PDA(C).