

Supporting Information

Synthesis and pH-stimuli responsive research of gemini amine-oxide surfactants containing amides

Hanyu Chen, Duoqiao Fu, Xiqin Zhou, Hongqin Liu* and Baocai Xu*

School of Food and Chemical Engineering, Beijing Key Laboratory of Flavor Chemistry, Beijing Higher Institution Engineering Research Center of Food Additives and Ingredients, Beijing Technology and Business University, No. 11 Fucheng Road, Beijing 100048, People's Republic of China

Email: liuhongqin@th.btbu.edu.cn, xubaoc@btbu.edu.cn

11-3-11-OA: Mass Spectra: Cationic scanning M/E : 585.0 [M+1]⁺, 607.0 [M+Na⁺]; FTIR Spectra (KBr, v, cm⁻¹): 3337.76, 3277.43 (N-H), 3000~2843 (C-H), 1639.52 (C=O), 1558.54 (N-H), 1490~1350 (C-H), 1310~1200 (C-N), 1036.95 (N-O), 716.41 (-(CH₂)n-); ¹H-NMR Spectra [CDCl₃, 600 MHz, δ ppm]: 0.868-0.891 [t, 6H, J=7.2 Hz, CH₃C-of two long alkyl chains], 1.254 [m, methylene in two long alkyl chains, C(CH₂)₈C-], 1.603 [tt, 4H, C-C₈-CH₂-C-], 2.196-2.223 [t, 4H, J=7.8 Hz, -CH₂(C=O)N-], 2.279 [tt, 2H, N⁺-C-CH₂-C-N⁺], 3.321 [s, 6H, CH₃-N⁺], 3.599 [t, 4H, N⁺-CH₂-C-N(C=O)-], 3.667 [t, 4H, -CH₂N(C=O)-], 3.923 [t, 6H, J=5.4 Hz, N⁺-C-C-CH₂-N⁺].

13-3-13-OA: Mass Spectra: Cationic scanning M/E : 641.0 [M+1]⁺, 663.1 [M+Na⁺]; FTIR Spectra (KBr, v, cm⁻¹): 3337.98, 3280.81 (N-H), 3000~2843 (C-H), 1640.10 (C=O), 1558.82 (N-H), 1490~1350 (C-H), 1310~1200 (C-N), 1037.44 (N-O), 722.03 (-(CH₂)n-); ¹H-NMR Spectra [CDCl₃, 600 MHz, δ ppm]: 0.868-0.891 [t, 6H, J=7.2 Hz, CH₃C-of two long alkyl chains], 1.251 [m, methylene in two long alkyl chains, C(CH₂)₁₀C-], 1.602 [tt, 4H, C-C₁₀-CH₂-C-], 2.198-2.222 [t, 4H, J=7.8 Hz, -CH₂(C=O)N-], 2.274 [tt, 2H, N⁺-C-CH₂-C-N⁺], 3.269 [s, 6H, CH₃-N⁺], 3.547-3.568 [t, 4H, J=6.6 Hz, N⁺-CH₂-C-N(C=O)-], 3.632 [t, 4H, -CH₂N(C=O)-], 3.859-3.884 [t, 6H, J=5.4 Hz, N⁺-C-C-CH₂-N⁺].

15-3-15-OA: Mass Spectra: Cationic scanning M/E : 697.0 [M+1]⁺, 720.1 [M+Na⁺]; FTIR Spectra (KBr, v, cm⁻¹): FTIR Spectra (KBr, v, cm⁻¹): 3312.60 (N-H), 3000~2843 (C-H), 1652.95 (C=O), 1548.64 (N-H), 1490~1350 (C-H), 1310~1200 (C-N), 1099.59 (N-O), 719.87 (-(CH₂)n-); ¹H-NMR Spectra [CDCl₃, 600 MHz, δ ppm]: 0.868-0.891 [t, 6H, J=7.2 Hz, CH₃C-of two long alkyl chains], 1.254 [m, methylene in two long alkyl chains, C(CH₂)₁₂C-], 1.601 [tt, 4H, C-C₁₂-CH₂-C-], 2.191-2.217 [t, 4H,

$J=7.8$ Hz, $-\text{CH}_2(\text{C}=\text{O})\text{N}-]$, 2.297 [tt, 2H, $\text{N}^+\text{-C-CH}_2\text{-C-N}^+$], 3.276 [s, 6H, $\text{CH}_3\text{-N}^+$], 3.583-3.605 [t, 4H, $J=6.6$ Hz, $\text{N}^+\text{-CH}_2\text{-C-N}(\text{C}=\text{O})-$], 3.634 [t, 4H, $-\text{CH}_2\text{N}(\text{C}=\text{O})-$], 3.844-3.862 [t, 6H, $J=5.4$ Hz, $\text{N}^+\text{-C-C-CH}_2\text{-N}^+$].

17-3-17-OA: Mass Spectra: Cationic scanning M/E : 753.1 [$\text{M}+1$]⁺, 776.1 [$\text{M}+\text{Na}^+$]; Anion scanning M/E : 45.0; FTIR Spectra (KBr, v, cm^{-1}): 3288.23 (N-H), 3000~2843 (C-H), 1640.85 (C=O), 1558.36 (N-H), 1490~1350 (C-H), 1310~1200 (C-N), 1113.36 (N-O), 720.44 ($-(\text{CH}_2)\text{n}-$); ¹H-NMR Spectra [CDCl_3 , 600 MHz, δ ppm]: 0.868-0.891 [t, 6H, $J=7.2$ Hz, CH_3C -of two long alkyl chains], 1.254 [m, methylene in two long alkyl chains, $\text{C}(\text{CH}_2)_{14}\text{C}-$], 1.602 [tt, 4H, $\text{C-C}_{14}\text{-CH}_2\text{-C}-$], 2.180-2.206 [t, 4H, $J=7.8$ Hz, $-\text{CH}_2(\text{C}=\text{O})\text{N}-]$, 2.304 [tt, 2H, $\text{N}^+\text{-C-CH}_2\text{-C-N}^+$], 3.279 [s, 6H, $\text{CH}_3\text{-N}^+$], 3.570-3.586 [t, 4H, $J=6.0$ Hz, $\text{N}^+\text{-CH}_2\text{-C-N}(\text{C}=\text{O})-$], 3.652 [t, 4H, $-\text{CH}_2\text{N}(\text{C}=\text{O})-$], 3.845-3.862 [t, 6H, $J=5.4$ Hz, $\text{N}^+\text{-C-C-CH}_2\text{-N}^+$].

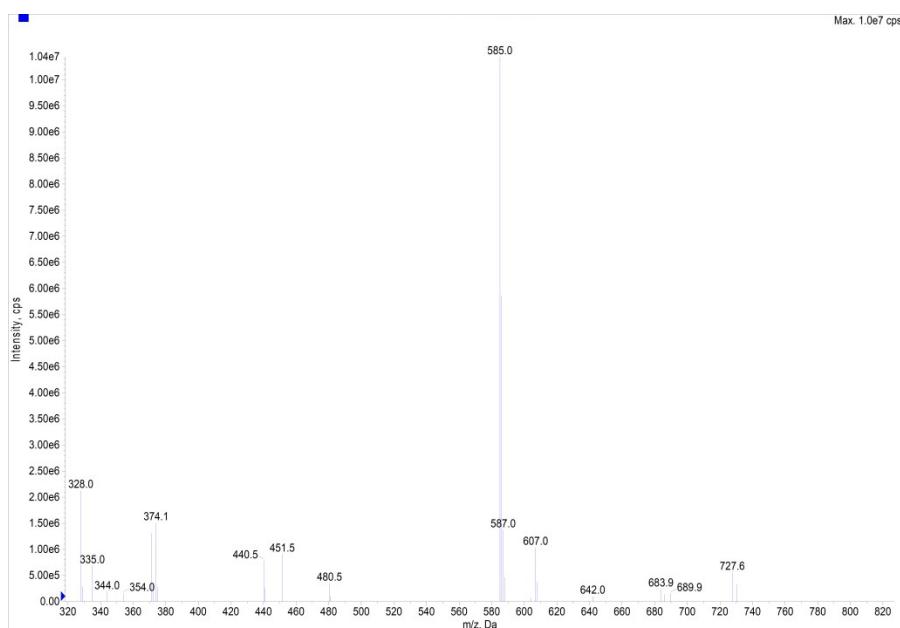


Fig. S1 Cationic scanning mass spectra of 11-3-11-OA

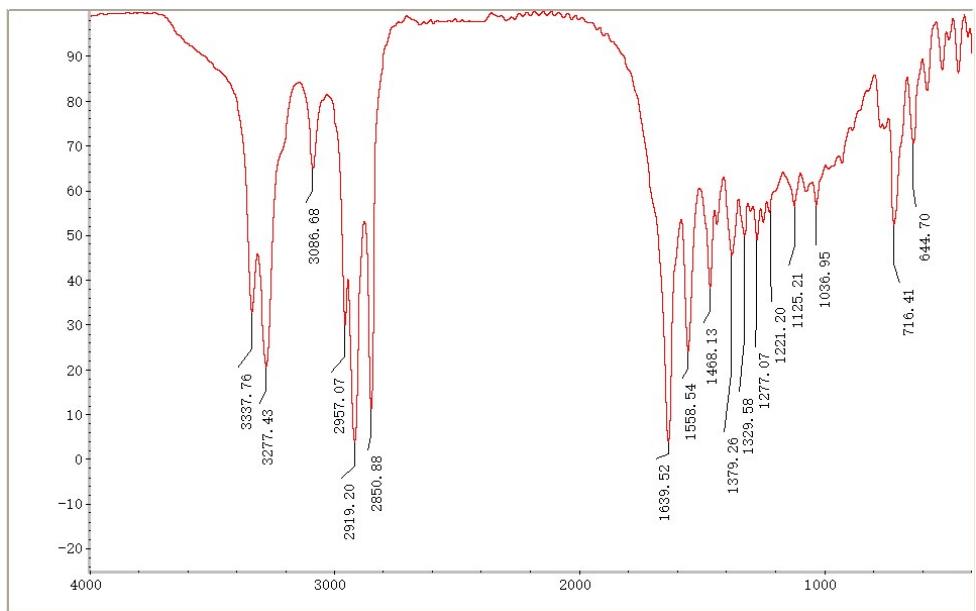


Fig. S2 FTIR spectra of 11-3-11-OA

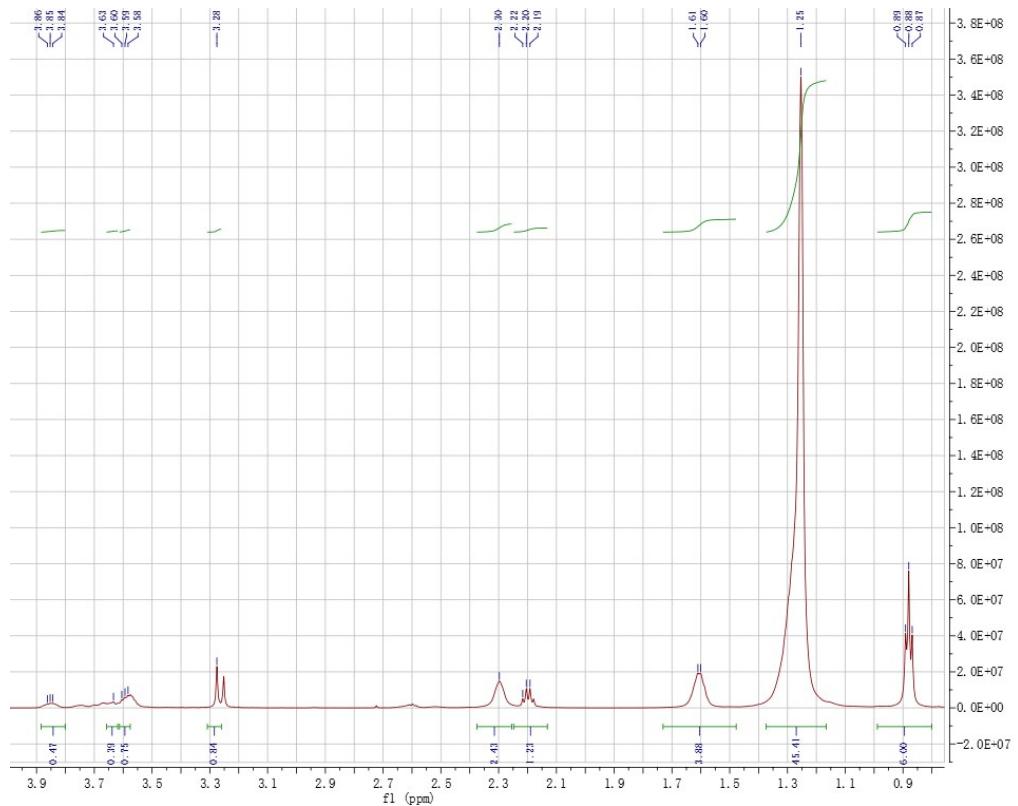


Fig. S3 ¹H-NMR spectra of 16-3-16-AO