

Supplementary Information

Bio-physicochemical analysis of ethylene oxide-linked diester-functionalized green cationic gemini surfactants

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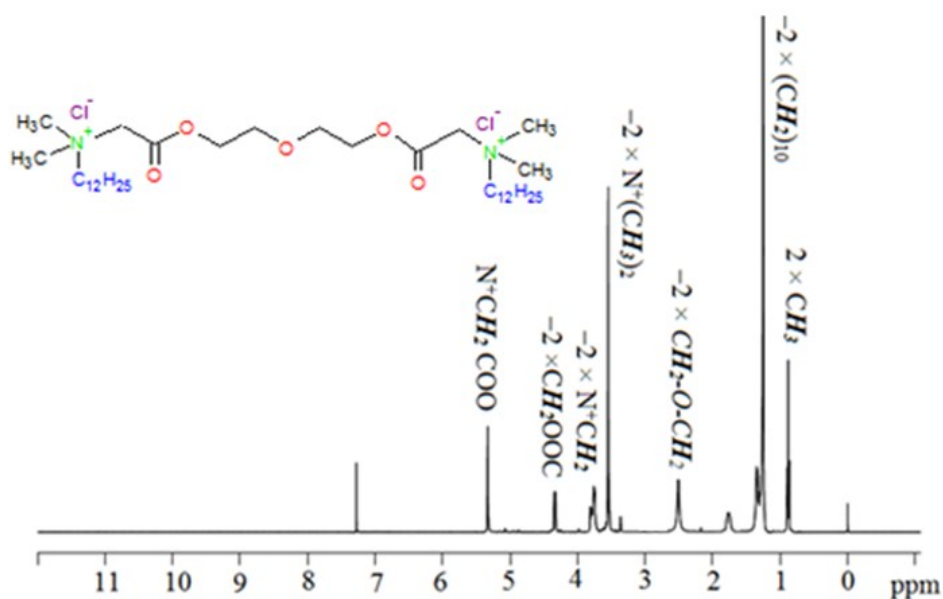
Spectral analysis

The synthesized gemini surfactants were characterized by sophisticated techniques viz. ^1H NMR, FT-IR, LC-MS and elemental analysis. Here, we have taken $\text{C}_{12}\text{-E2O-C}_{12}$ as a prototype, as rest of the two geminis differ only in alkyl chain length. The signal assignments for $\text{C}_{12}\text{-E2O-C}_{12}$ are well represented in Fig. S1 (a) (Supplementary Information).

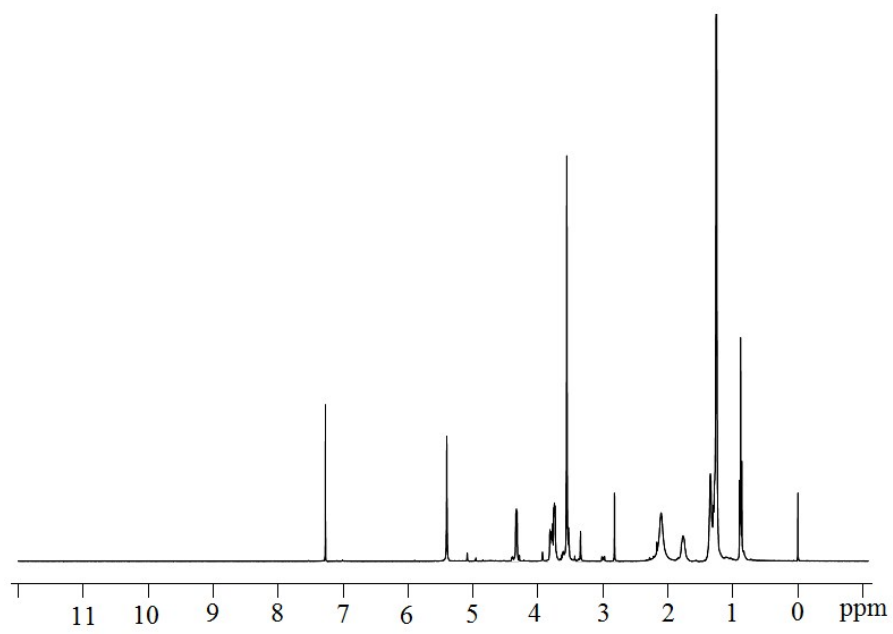
It can be seen (Fig. S1(a)) that $2 \times \text{CH}_3$, $-2 \times (\text{CH}_2)_{10}$ and $-2 \times \text{CH}_2\text{-O-CH}_2$ protons resonate at lower delta (δ) values which may be attributed to higher shielding experienced by them. Due to this shielding effect, the concerned protons experienced less applied magnetic field and hence the signals for these protons have appeared on the lower side of δ scale. Inverse is true for the other protons (i.e., $-2 \times \text{N}^+(\text{CH}_3)_2$, $-2 \times \text{N}^+\text{CH}_2$, $-2 \times \text{CH}_2\text{OOC}$ and $\text{N}^+\text{CH}_2\text{COO}$ protons) which are in close proximity of head groups; reason being the higher deshielding caused by the positive charge located on the nitrogen atoms of the head groups. The positively charged nitrogen pulls the electrons of near head group protons towards itself, which develops a local magnetic field with direction similar to the applied magnetic field, hence the ^1H NMR signals of near head group protons were observed at higher side of δ scale. Similarly, for the corresponding protons of other concerned geminis ($\text{C}_{14}\text{-E2O-C}_{14}$ and $\text{C}_{16}\text{-E2O-C}_{16}$), the above mentioned reasons can be attributive and their spectra are shown in Fig. S1 (b) and (c) (Supplementary Information).

Further structure elucidation was achieved by the analysis of FT-IR and mass spectra (LC-MS). In FT-IR spectra (Fig. S2 (a), Supplementary Information) the main peaks related to functional groups of $\text{C}_{12}\text{-E2O-C}_{12}$ gemini surfactant were observed at 2921 (C-H), 2852 (C-H), 1749 (C=O), 1466 (C-O) and 1127 (C-N). The vibrational frequencies at 2921 cm^{-1} and 2852 cm^{-1} were assigned respectively, to symmetrical and asymmetrical vibrations of $-\text{CH}_2$ and $-\text{CH}_3$ groups of $\text{C}_{12}\text{-E2O-C}_{12}$ and the 1749 cm^{-1} , 1466 cm^{-1} , 1127 cm^{-1} frequencies were

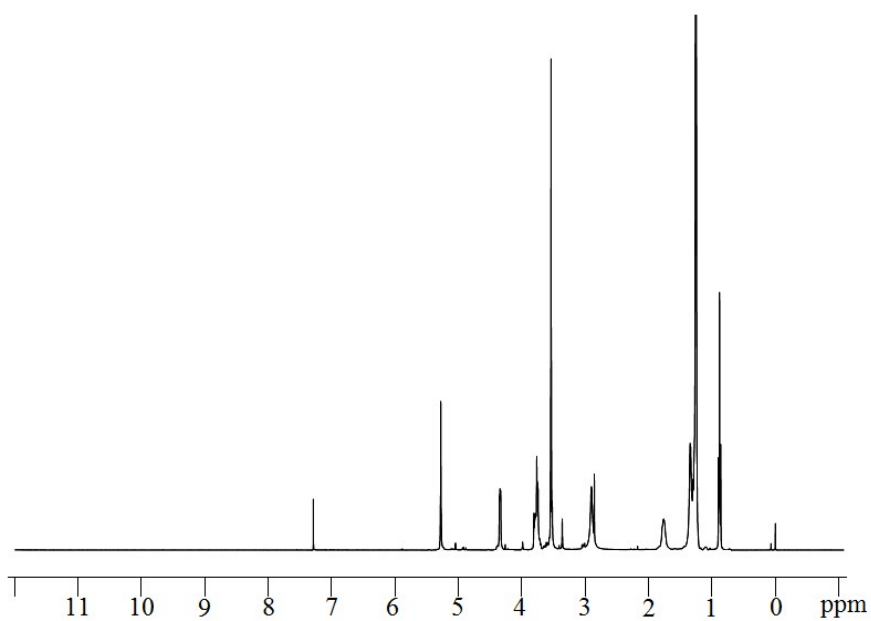
attributed to C=O (ester), C-O and C-N groups, respectively. Thus, the FT-IR spectra further ascertain and validate the structure of C₁₂-E2O-C₁₂. Moreover, further authentication for the formation of C₁₂-E2O-C₁₂ was provided by molecular ion peak (for C₃₆H₇₄N₂O₅²⁺/2) at 308.1; which is in close agreement with the calculated value (307). Similar reasons can explain the spectra of C₁₄-E2O-C₁₄ and C₁₆-E2O-C₁₆ (Fig. S2 (b) and (c), Supplementary Information). On the whole, our spectroscopic characterizations confirm the formation of C_m-E2O-C_m gemini surfactants.



(a) C₁₂-E2O-C₁₂

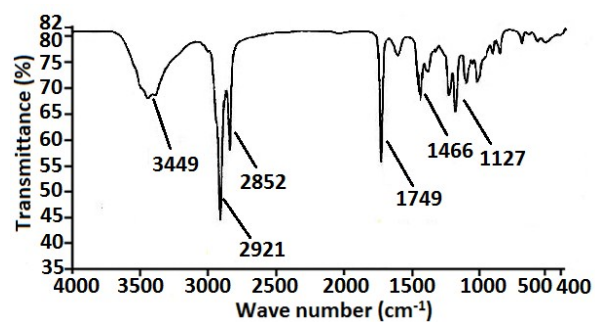


(b) C₁₄-E₂O-C₁₄

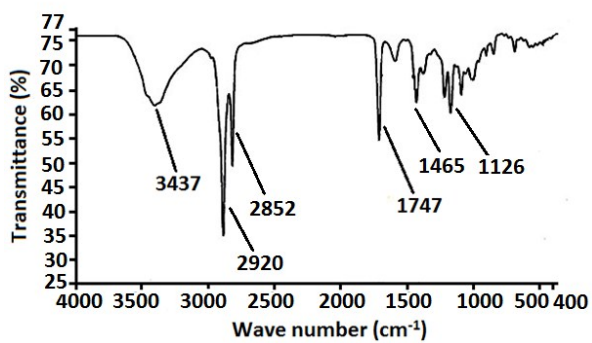


(c) C₁₆-E₂O-C₁₆

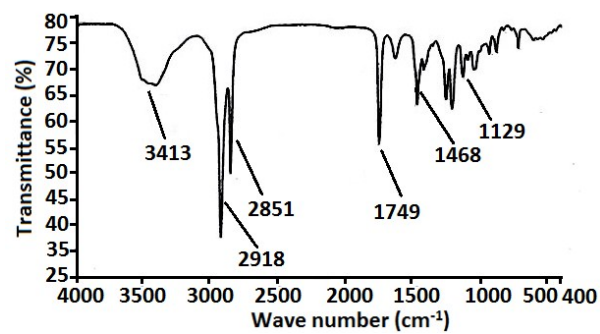
Fig. S1 400 MHz ¹H NMR spectra of (a) C₁₂-E₂O-C₁₂, (b) C₁₄-E₂O-C₁₄ and (c) C₁₆-E₂O-C₁₆ gemini surfactants in deuterated chloroform (CDCl₃) at 23 °C.



(a)



(b)



(c)

Fig. S2 FT-IR spectra of (a) C₁₂-E2O-C₁₂, (b) C₁₄-E2O-C₁₄ and (c) C₁₆-E2O-C₁₆ gemini surfactants.

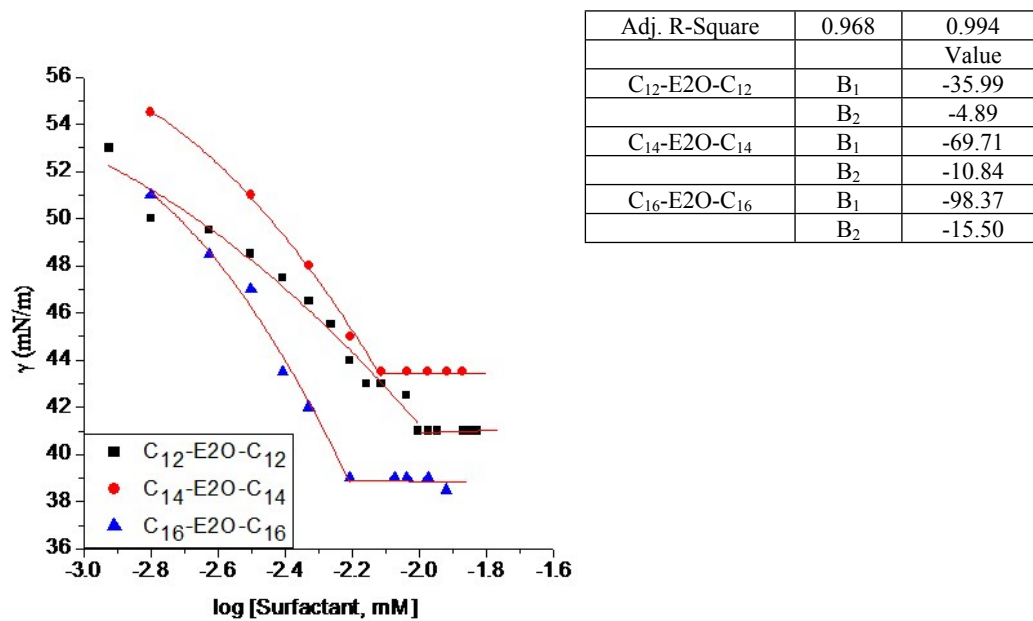


Fig. S3 Second order polynomial fitting of surface tension isotherms for C_m-E2O-C_m gemini surfactants.