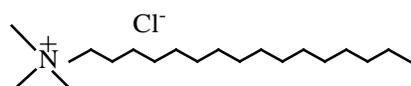
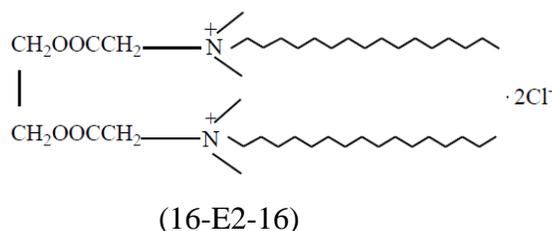
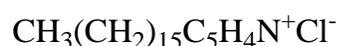


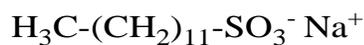
“Supplementary Information”



(CTAC)



(CPC)



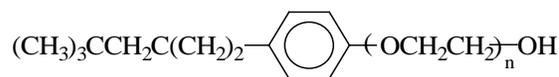
(SDS)



(SDBS)

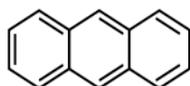


(Brij 58)



(TX-100)

Scheme S2. Structure of surfactant molecules used in this study: Ethane-1,2-diyl bis(*N,N*-dimethyl-*N*-hexadecylammoniumacetoxo) dichloride (16-E2-16), Hexadecyltrimethylammonium Chloride (CTAC), Cetylpyridinium Chloride (CPC), Sodium dodecyl sulfate (SDS), Sodium dodecyl benzene sulfonate (SDBS), Polyoxyethylene (20) cetyl ether (Brij 58), *t*-octylphenoxypolyethoxyethanol (TX-100)



Anthracene



Pyrene

Molecular weight: 178.2

202.3

Solubility (mol/L): 2.53×10^{-7}

6.57×10^{-7}

log K_{ow} : 4.54

5.18

Molar volume (\AA^3): 157.6

161.9

Scheme S2. Structure and properties of polycyclic aromatic hydrocarbons

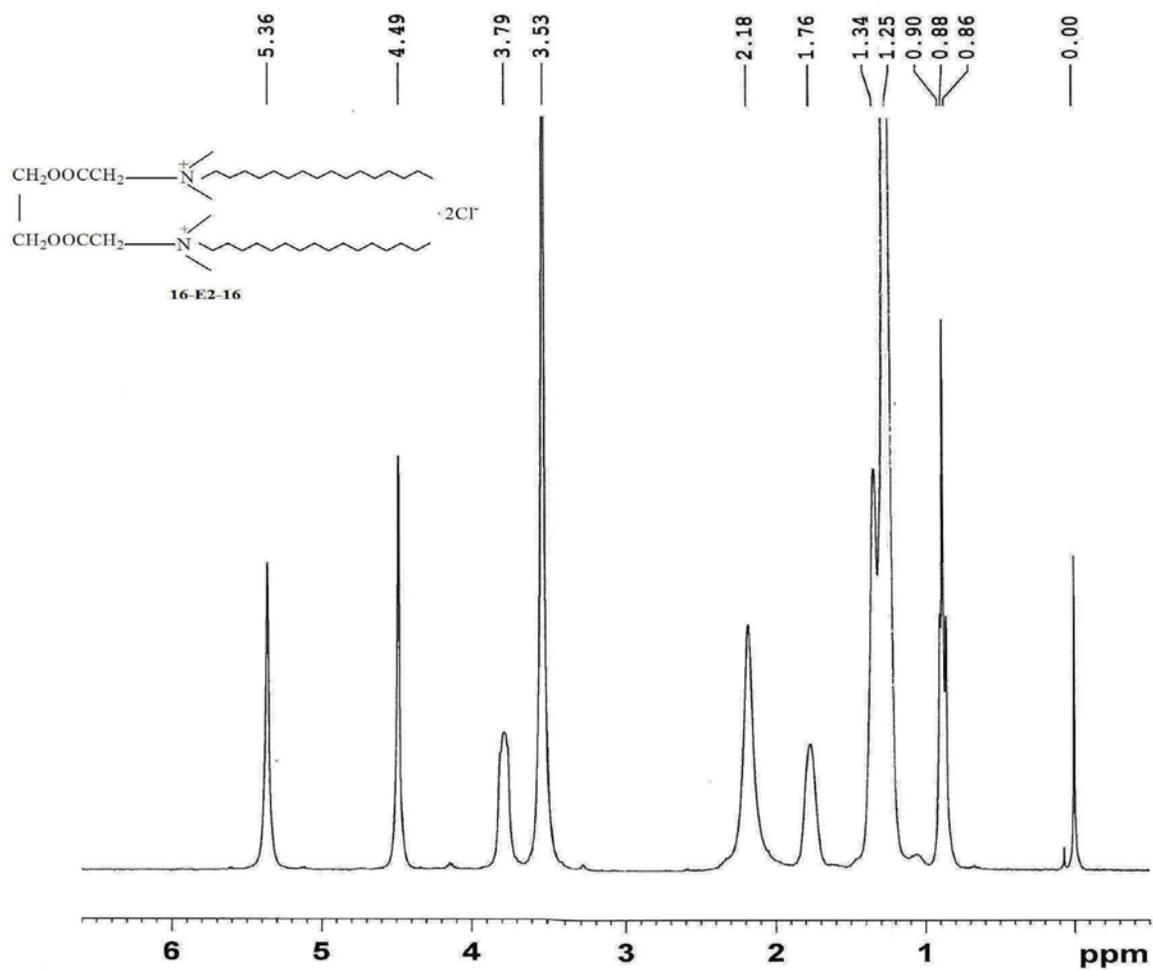


Fig. S1 (A). ¹H-NMR spectrum (300MHz) of Ethane-1,2-diyl bis(*N,N*-dimethyl-*N*-hexadecylammoniumacetoxo) dichloride (16-E2-16) in CDCl₃.

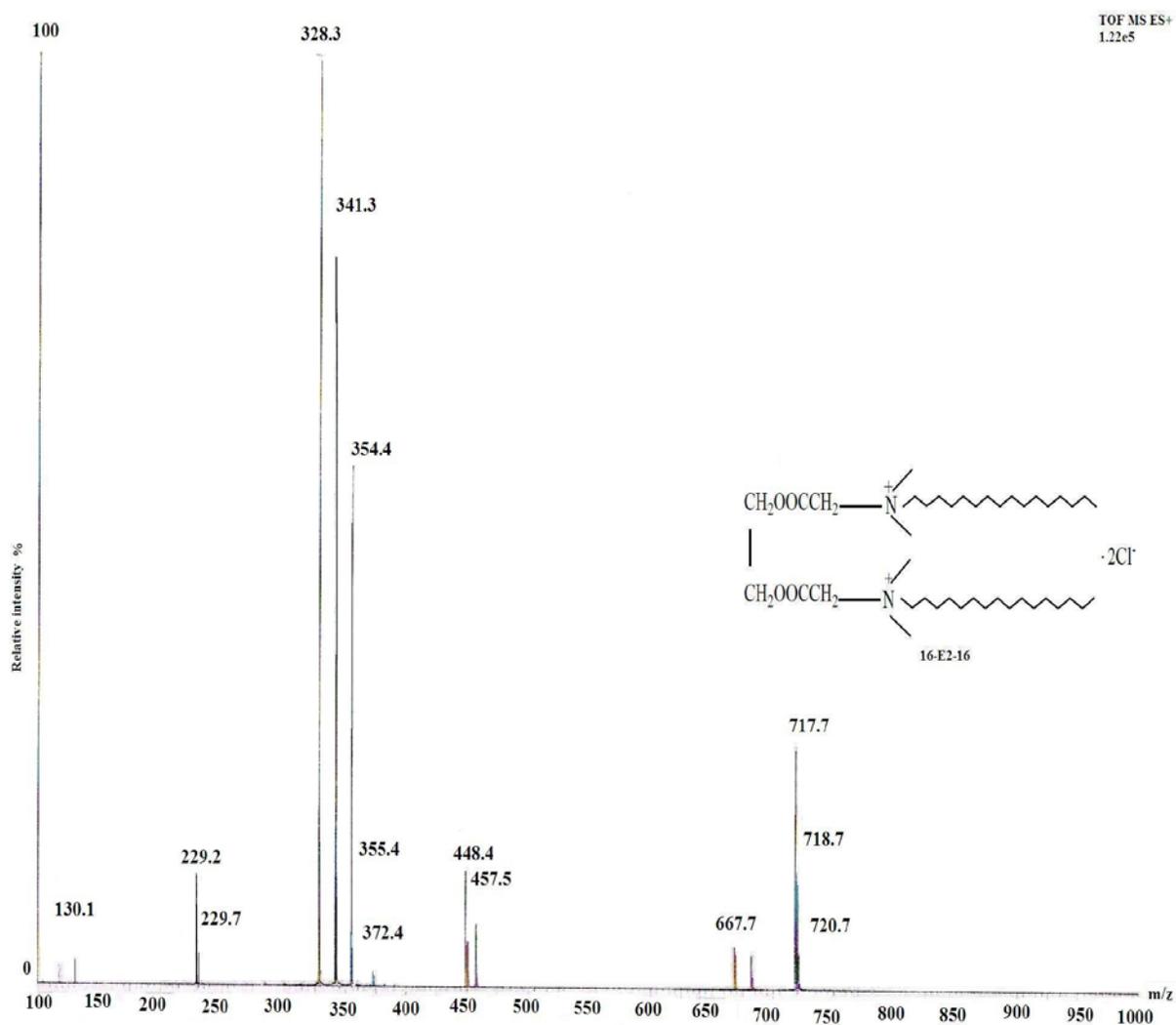


Fig. S1(B). MS-ESI (+) spectrum (relative intensity vs. m/z) of Ethane-1,2-diyl bis(*N,N* dimethyl-*N*-hexadecylammoniumacetoxo) dichloride (16-E2-16).

Table S1 Physicochemical parameters evaluated with the average conductometric and tensiometric cmc values determined at 30 °C

| <i>System</i> | X_1^m | X_1^{ideal} | f_1^m | f_2^m | ΔG_{ex}^m (kJmol^{-1}) |
|------------------|---------|---------------|---------|---------|--|
| 16-E2-16 | | | | | |
| CPC | | | | | |
| CTAC | | | | | |
| SDS | | | | | |
| SDBS | | | | | |
| Brij 58 | | | | | |
| TX-100 | | | | | |
| 16-E2-16+CPC | 0.7899 | 0.9983 | 0.6788 | 0.0041 | -3.668 |
| 16-E2-16+ CTAC | 0.7932 | 0.9988 | 0.6714 | 0.0028 | -3.848 |
| 16-E2-16+SDS | 0.8788 | 0.9998 | 0.8781 | 0.0010 | -2.372 |
| 16-E2-16+SDBS | 0.8742 | 0.9995 | 0.8869 | 0.0030 | -2.100 |
| 16-E2-16+Brij 58 | 0.6856 | 0.7692 | 0.8931 | 0.5841 | -0.621 |
| 16-E2-16+TX-100 | 0.7479 | 0.9923 | 0.6152 | 0.0139 | -3.630 |

Table S2 The Solubilization parameters $\ln K_m$, ΔG_s^0 , R and B for single and binary (1:1) surfactant systems

| <i>System</i> | Anthracene | | | | Pyrene | | | |
|------------------|------------|-------|-------|--|-----------|-------|-------|--|
| | $\ln K_m$ | R | B | ΔG_s^0 (kJmol ⁻¹) | $\ln K_m$ | R | B | ΔG_s^0 (kJmol ⁻¹) |
| 16-E2-16 | 12.64 | | | -31.86 | 15.01 | | | -37.83 |
| CPC | 12.67 | | | -31.94 | 14.77 | | | -37.22 |
| CTAC | 13.91 | | | -35.07 | 14.55 | | | -36.68 |
| SDS | 12.22 | | | -30.80 | 12.77 | | | -32.19 |
| SDBS | 12.01 | | | -30.27 | 9.99 | | | -25.20 |
| Brij 58 | 14.86 | | | -37.46 | 15.75 | | | -39.71 |
| TX-100 | 13.79 | | | -34.77 | 13.92 | | | -35.10 |
| 16-E2-16+CPC | 14.80 | 4.30 | 15.41 | -35.57 | 15.11 | 1.251 | -0.52 | -38.09 |
| 16-E2-16+CTAC | 14.02 | 0.86 | 9.22 | -33.58 | 14.11 | 0.486 | -4.20 | -35.56 |
| 16-E2-16+SDS | 16.15 | 21.15 | 37.42 | -39.02 | 15.36 | 2.560 | 17.38 | -38.73 |
| 16-E2-16+SDBS | 16.13 | 22.46 | 36.34 | -39.98 | 15.61 | 3.627 | 40.62 | -39.35 |
| 16-E2-16+Brij 58 | 15.43 | 1.61 | 12.34 | -37.18 | 16.62 | 3.168 | 3.78 | -41.91 |
| 16-E2-16+TX-100 | 14.05 | 0.978 | 7.99 | -33.66 | 14.18 | 0.876 | 4.33 | -35.74 |