Electronic Supplementary Information

Micelle formation of a non-ionic surfactant in non-aqueous molecular solvents and protic ionic liquids (PILs)

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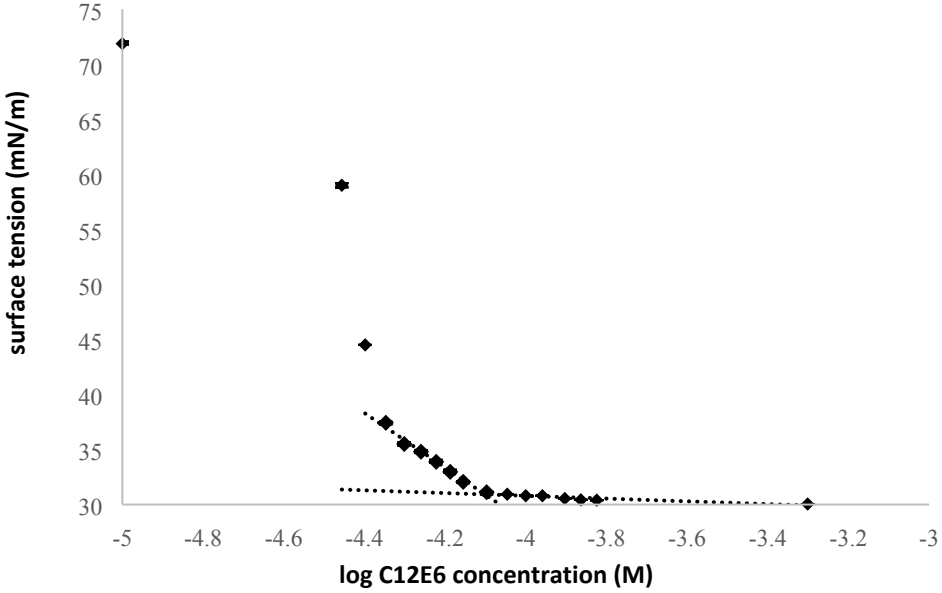


Figure S1. *Change in surface tension with different $C_{12}E_6$ concentrations in water*

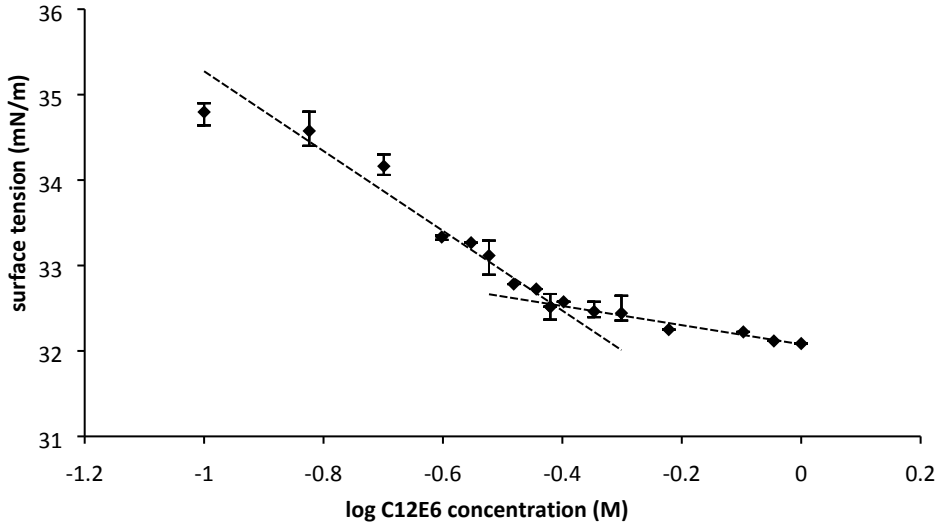


Figure S2. *Change in surface tension with different $C_{12}E_6$ concentrations in 1-amino-2-propanol*

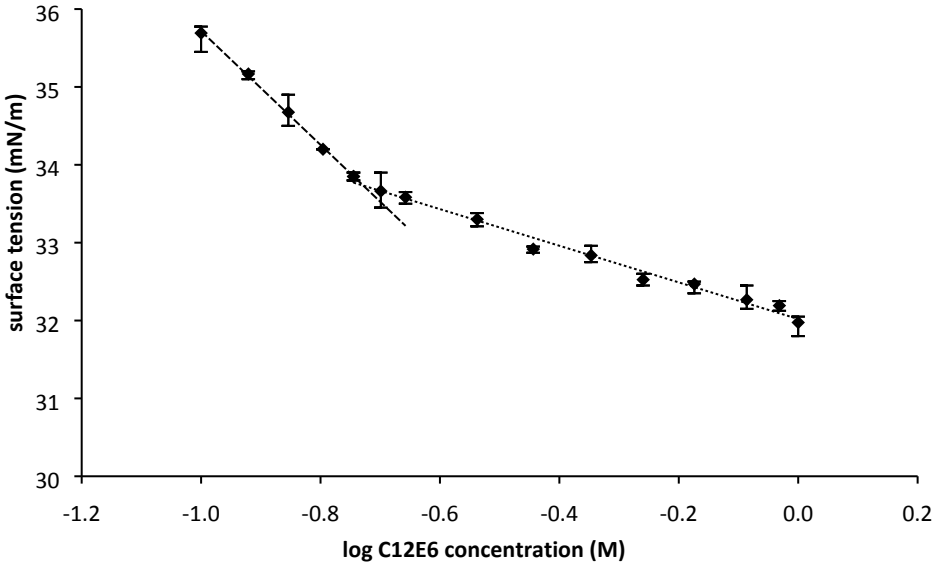


***Figure S3**. Change in surface tension with different $C_{12}E_6$ concentrations in 2-amino-1-propanol*

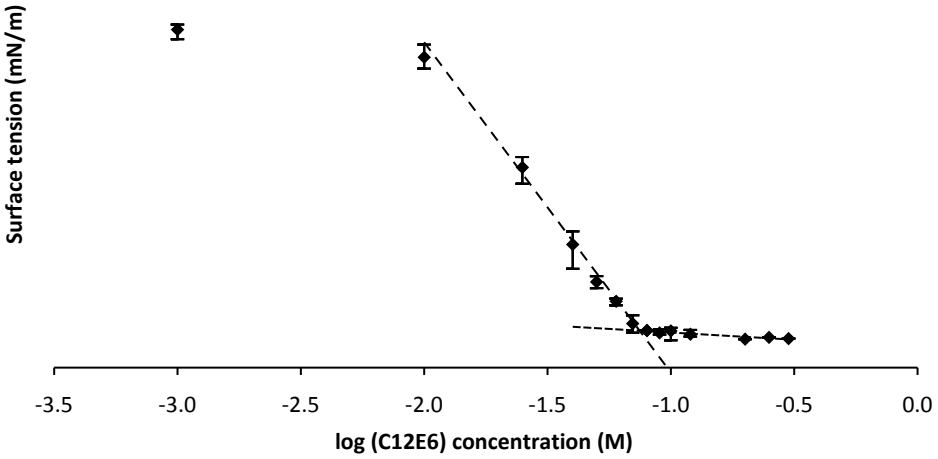


***Figure S4**. Change in surface tension with different $C_{12}E_6$ concentrations in 3-amino-1-propanol*

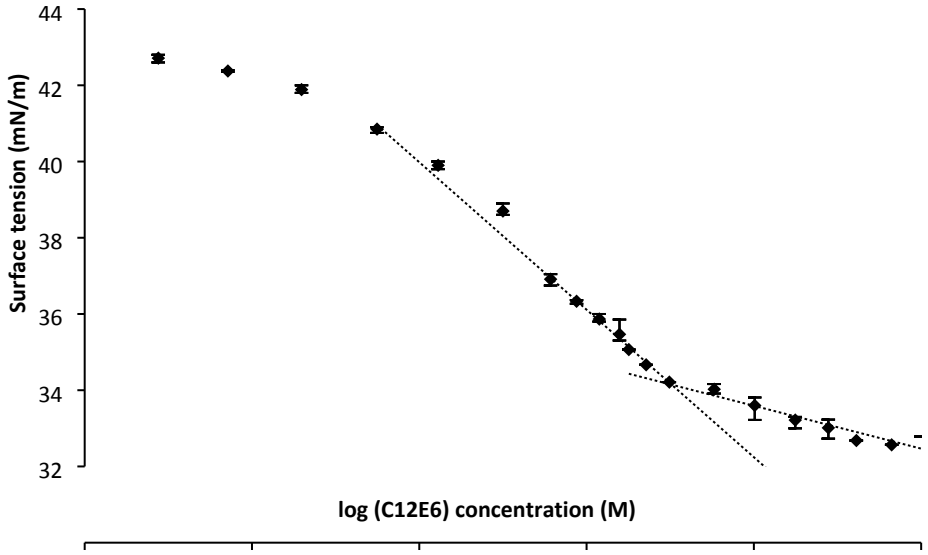


***Figure S5**. Change in surface tension with different $C_{12}E_6$ concentrations in 4-amino-1-butanol*

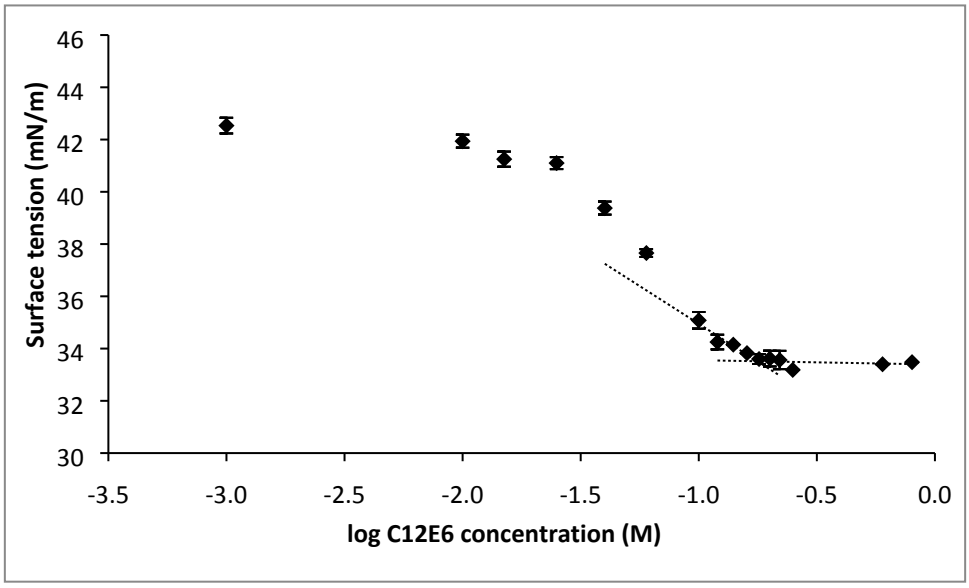


***Figure S6.** Change in surface tension with different $C_{12}E_6$ concentrations in diethylene glycol*

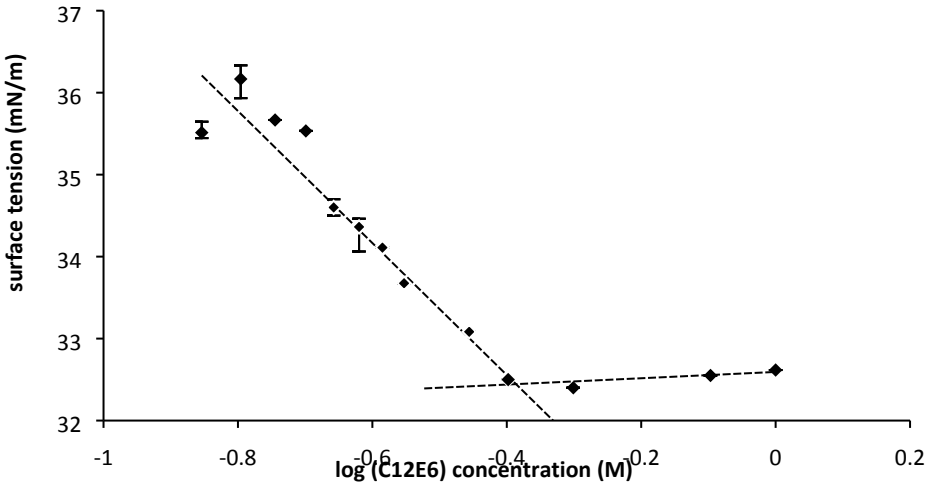


***Figure S7**. Change in surface tension with different $C_{12}E_6$ concentrations in diethylene triamine*

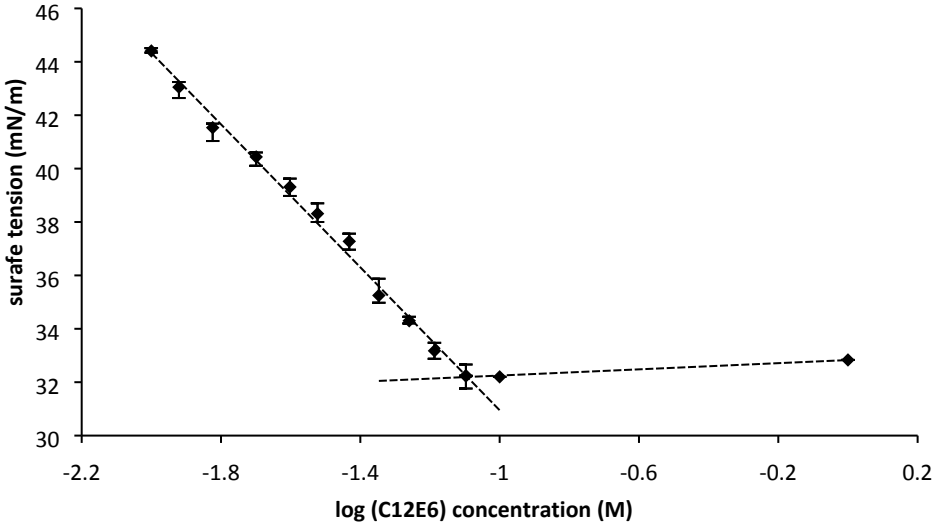


***Figure S8.** Change in surface tension with different $C_{12}E_6$ concentrations in triethanolamine*

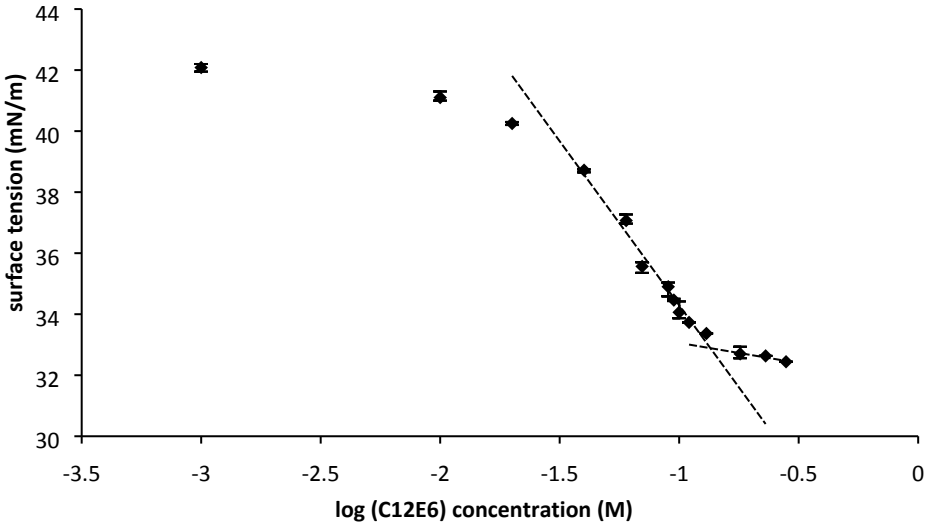


***Figure S9**. Change in surface tension with different $C_{12}E_6$ concentrations in triethylene glycol*

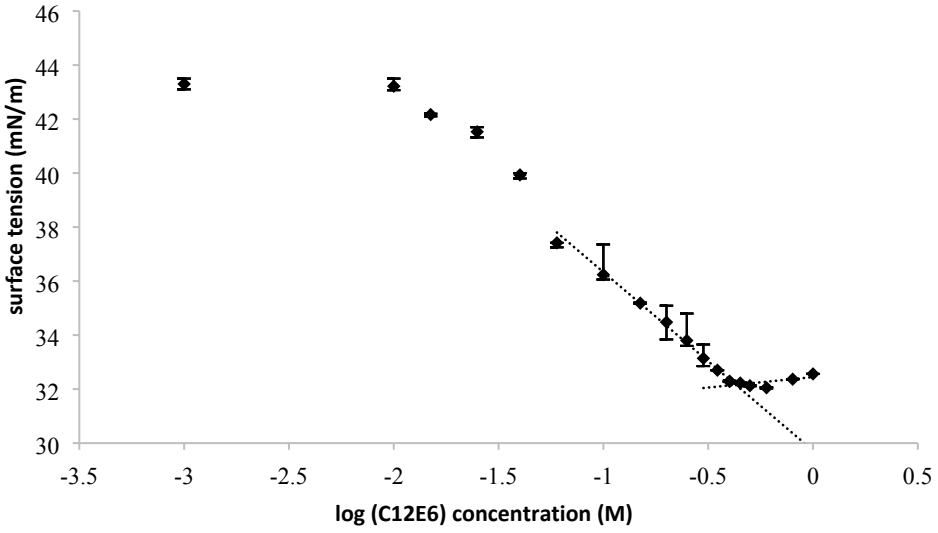


***Figure S10.** Change in surface tension with different $C_{12}E_6$ concentrations in triethylene tetramine*

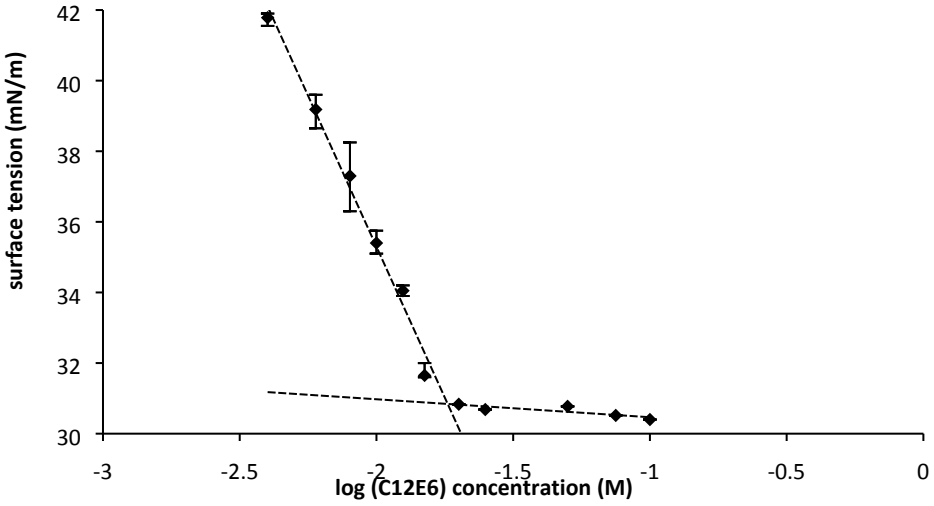


Figure S11. *Change in surface tension with different $C_{12}E_6$ concentrations in ethylammonium formate (EAF)*

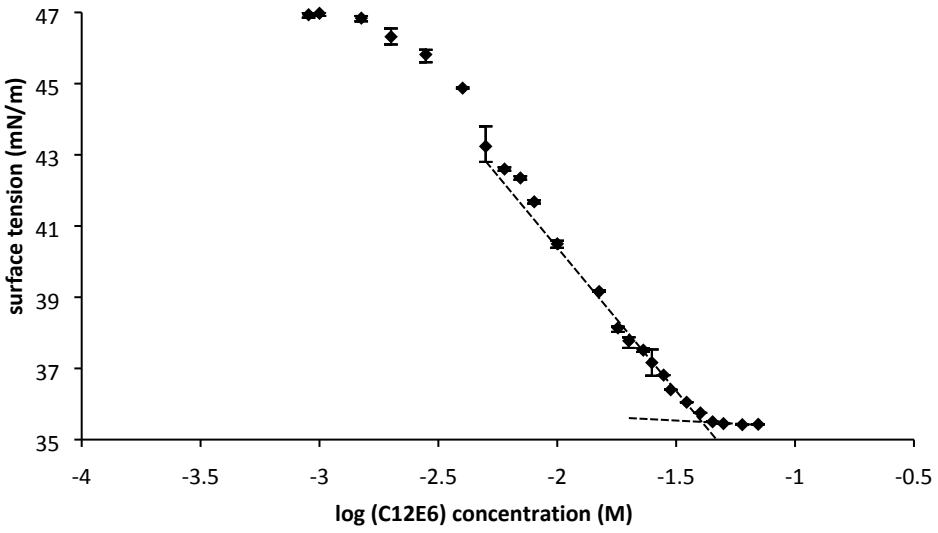


Figure S12. *Change in surface tension with different $C_{12}E_6$ concentrations in ethylammonium nitrate (EAN)*

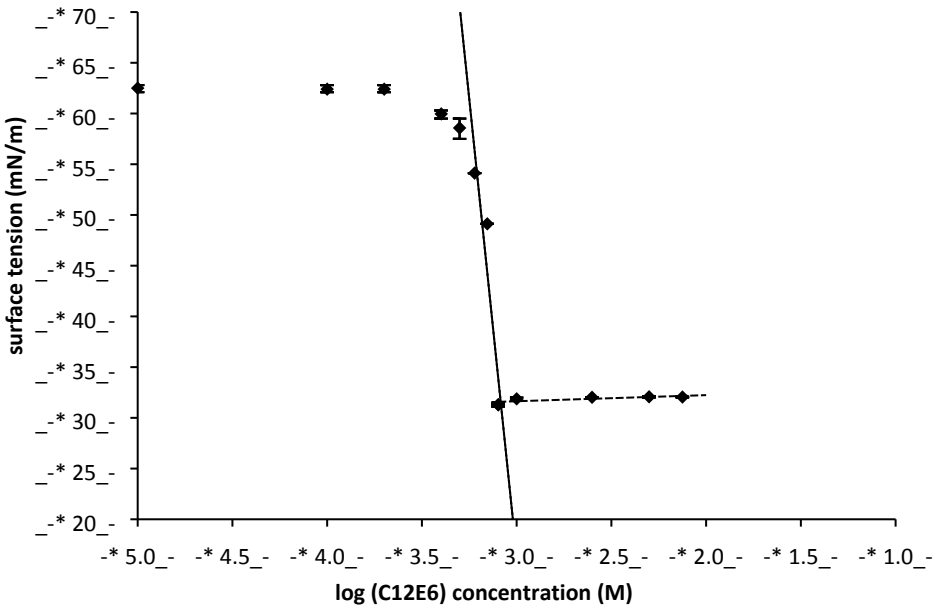


Figure S13. *Change in surface tension with different $C_{12}E_6$ concentrations in ethanolammonium formate (EOAF)*

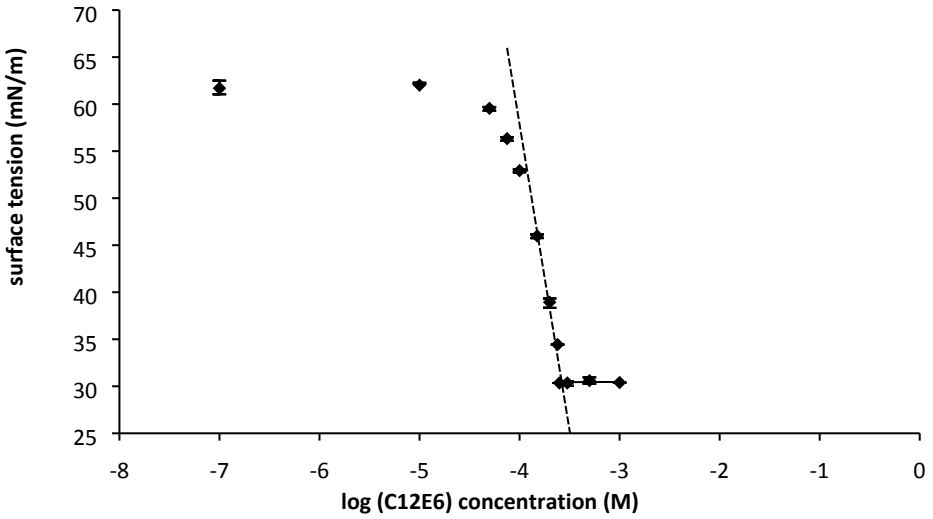


Figure S14. *Change in surface tension with different $C_{12}E_6$ concentrations in ethanolammonium nitrate (EOAN)*

Micelle scattering models

Coreshell spherical model

The spherical shape is the simplest form of micelles, which is usually found at low amphiphile concentrations. The coreshell spherical model was used in this study due to the difference between SLD core and SLD shell, and between SLD shell and SLD solvent. It provides a form factor, $P(q)$, and is expressed by Eg 1 below,

$$P(q) = \frac{scale}{V_s}\left[3V_c(\rho_c - \rho_s)\frac{\left[\sin(qr_c) - qr_c\cos(qr_c)\right]}{(qr_c)^3} + 3V_s(\rho_s - \rho_{solv})\frac{\left[\sin(qr_s) - qr_c\cos(qr_s)\right]}{(qr_s)^3}\right]^2 + bkg$$

(1)

where $scale$ is a scaling factor, V_s is the volume of the outer shell, V_s is the volume of the core, r_s is the radius of the shell, r_c is the radius of the core (the shell thickness is r_s-r_c), ρ_c is the SLD of the core, ρ_s is the SLD of the shell, ρ_{solv} is the solvent SLD, and bkg is the background level.

SLD is calculated by equation

$$\rho = \sum_i^n z_i r_e / V_m$$

where $r_e = 2.81 \times 10^{-13}$ cm, which is the classical radius of the electron, z_i is the atomic number of the i^{th} atom in the molecular volume V_m. SLD core was calculated to be 7.92x10^{-6}

Solvent SLDs were obtained from the SLD calculator provided in *SASview* software, by simply input the chemical formula and the corresponding density. SLD solvents calculated for all solvents used in this fitting are provided in Table S1 below.

Table S1. The chemical formula, density and SLD of solvents used in micelle fitting

Solvent	Chemical formula	Density (g/mL)	SLD solvent
water	H_2O	1	9.47x10^{-06}
ethylene glycol	$C_2H_6O_2$	1.1132	1.04 x10^{-05}
diethylene glycol	$C_4H_{10}O_3$	1.118	1.04 x10^{-05}
triethylene glycol	$C_6H_{14}O_4$	1.1255	1.05 x10^{-05}
3-amino-1-propanol	C_3H_9NO	0.982	9.35 x10^{-06}
triethanolamine	$C_6H_{15}NO_3$	1.124	1.05 x10^{-05}
2-amino-2-ethyl-1,3-propanediol	$C_5H_{13}NO_2$	1.099	1.04 x10^{-05}
ethylammonium nitrate	$C_2H_8N_2O_3$	1.216	1.11 x10^{-05}

ethylammonium formate	$C_3H_9NO_2$	1.039	9.71 x10^{-06}
ethanolammonium nitrate	$C_2H_8N_2O_4$	1.265	1.15 x10^{-05}
ethanolammonium formate	$C_3H_9NO_3$	1.184	1.09 x10^{-05}

Ellipsoid model

The scattering for ellipsoids with radii R_a, R_a and R_b is shown Equations 2-4 below.

$$P(q,\alpha) = \frac{scale}{V} f^2(q) + bkg \qquad (2)$$

$$f(q) = \frac{3(\Delta\rho)V(sin[qr(R_a,R_b,\alpha)] - qr\ cos[qr(R_a,R_b,\alpha)]}{[qr(R_a,R_b,\alpha)]^3} \qquad (3)$$

$$r(R_a,R_b,\alpha) = \left[{R_b}^2 sin^2\alpha + {R_b}^2 cos^2\alpha\right]^{\frac{1}{2}} \qquad (4)$$

α is the angle between the axis of the ellipsoid and the q-vector, V is the volume of the ellipsoid, $R_a$is the radius along the rotation axis of the ellipsoid, R_a is the radius perpendicular to the rotation axis of the ellipsoid, and Δρ is the SLD difference between the scatterer and the solvent.

Coreshell ellipsoid mode

This model provides the form factor, $P(q)$, for a core shell ellipsoid.

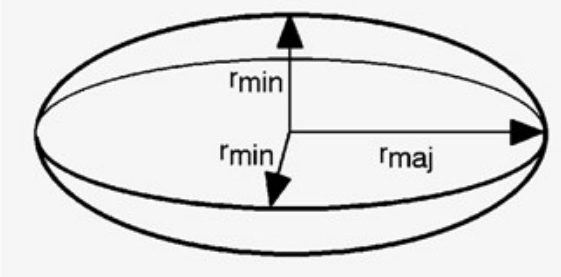
The form factor is calculated by using Equation 5-7 below,

$$P(q) = \frac{scale}{V_s} \int_0^1 |F(q,r_{min},r_{maj},\alpha)|^2 d\alpha + bkg \qquad (5)$$

$$|F(q,r_{min},r_{maj},\alpha)| = V\Delta\rho \times \left(\frac{3j_1(u)}{u}\right) \qquad (6)$$

$$u = q\left[{r_{maj}}^2\alpha^2 + {r_{min}}^2(1-\alpha^2)\right]^{\frac{1}{2}} \qquad (7)$$

where r_{min} is the equatorial outer radius, r_{maj} is the polar outer radius, and $j_1(u) = (sinx - xcosx)/x^2$



Calculation of aggregation number

Volume of micellar core was calculated by

$V_{chain} = (27.4 + 26.9n)$ Å^3

where n is the number of carbon atoms in the alkyl chain, in this case n = 12

For $C_{12}E_6$ amphiphiles, $V_{chain}$was calculated to be 350.2 Å^3

Number of aggregation (N_{agg}) was calculated by

$\frac{V_{micelle}}{V_{chain}}$

where volume of micelle $(V_{micelle})$ was calculated from the dimensions obtained from fitting.

Table S2. Shell SLD values obtained from the fitting

Solvent	[$C_{12}E_6$] (M)	Shell SLD
water	4.6 x10^{-3}	9.6x10^{-6}
	2.5 x10^{-1}	9.9x10^{-6}
ethylene glycol	1.4 x10^{-1}	
	1	
3-amino-1-propanol	1	1.1x10^{-5}
diethylene glycol	8.8 x10^{-1}	1.0x10^{-5}
	1.5	1.1x10^{-5}
triethylene glycol	7.2 x10^{-1}	8.9x10^{-6}
	1.5	1.1x10^{-5}
triethanolamine	1	-
2-amino-2-ethyl-1,3-	5	1.0x10^{-5}
pronanediol	10	1.0x10^{-5}
EAN	8.5 x10^{-2}	1.7x10^{-5}
	2.1 x10^{-1}	1.1x10^{-5}
EAF	3.6 x10^{-2}	1.4x10^{-5}
	9.0 x10^{-2}	1.0x10^{-5}
	0.5	1.5x10^{-5}

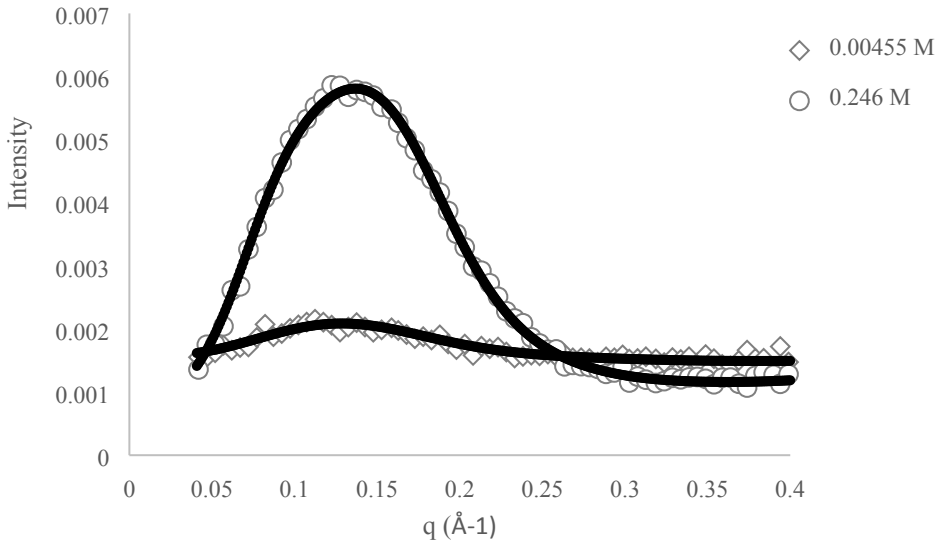


***Figure S15**. Fitted SAXS profiles for 0.00455 and 0.246 M $C_{12}E_6$ in water. Circles and diamonds show experimental data and solid lines shows fits to coreshell spherical model with no structure factor and hardsphere structure factor, respectively.*

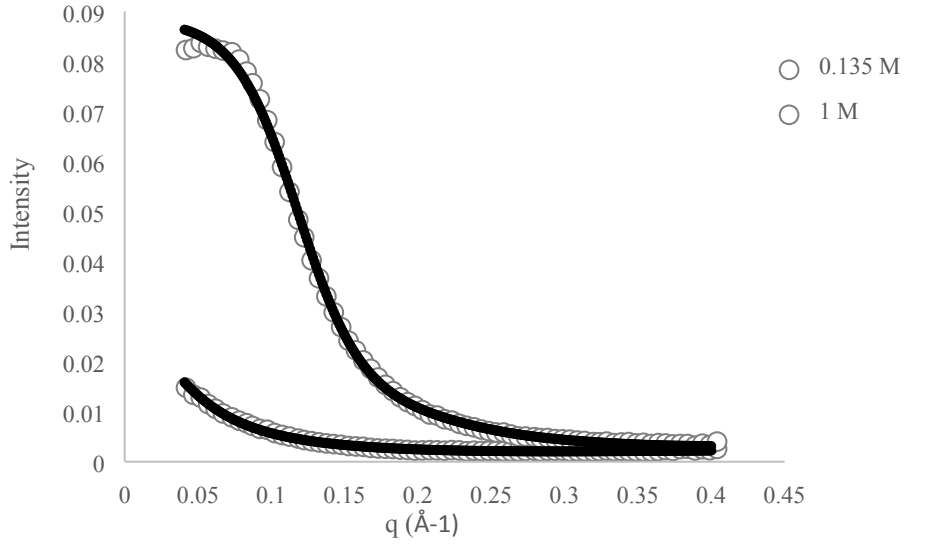


***Figure S16.** Fitted SAXS profiles for 0.135 and 1 M $C_{12}E_6$ in ethylene glycol. Circles and diamonds show experimental data and solid lines shows fits to ellipsoid model with no structure factor and hardsphere structure factor, respectively.*

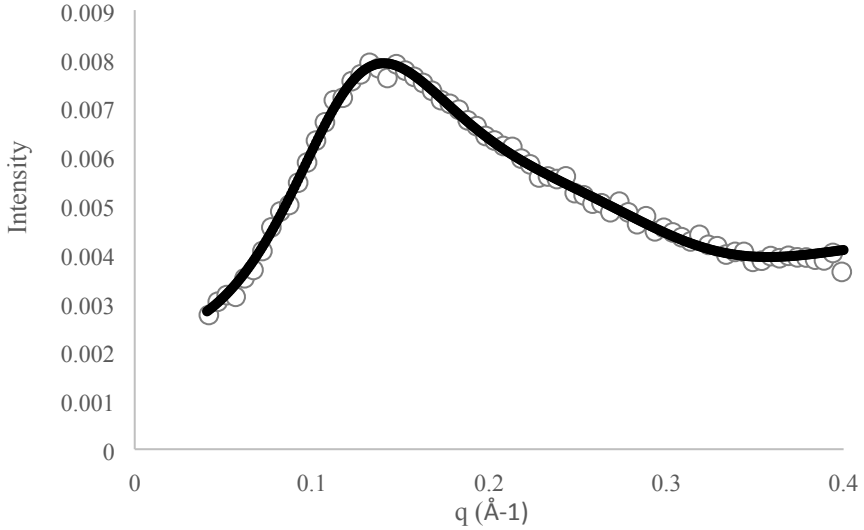


Figure S17. *Fitted SAXS profiles for 1 M $C_{12}E_6$ in 3-amino-1-propanol. Circles show experimental data and solid line shows fits to coreshell spherical model with hardsphere structure factor.*

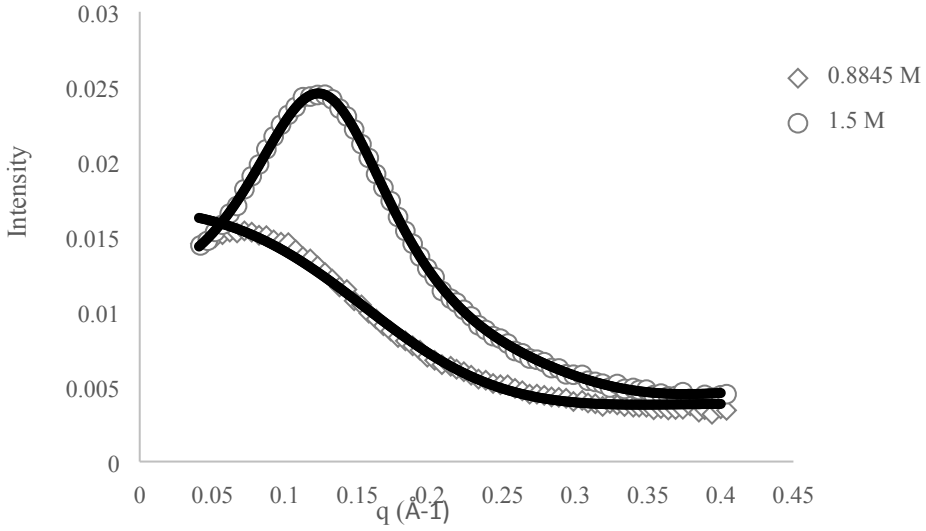


Figure S18. *Fitted SAXS profiles for 0.8845 and 1.5 M $C_{12}E_6$ in diethylene glycol. Circles and diamonds show experimental data and solid lines shows fits to coreshell spherical model with hardsphere structure factor.*

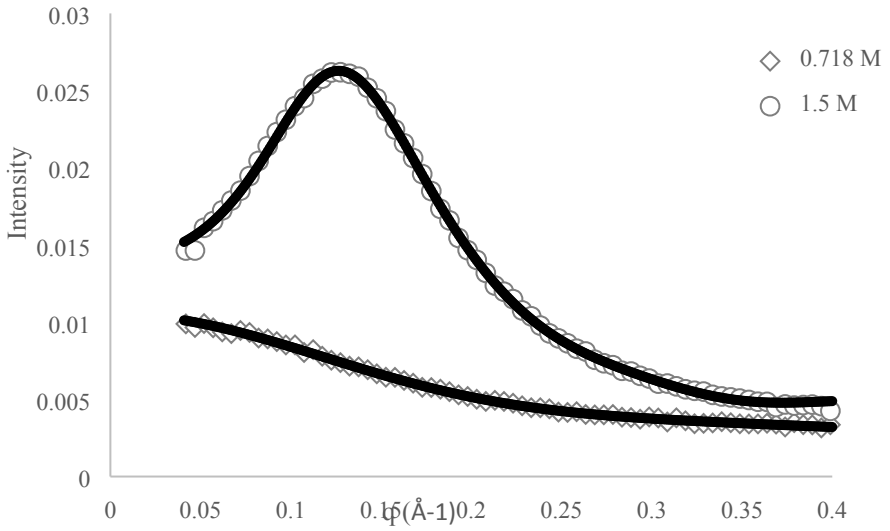


Figure S19. *Fitted SAXS profiles for 0.718 and 1.5 M% $C_{12}E_6$ in triethylene glycol. Circles and diamonds show experimental data and solid lines shows fits to coreshell ellipsoid model with no structure factor and hardsphere structure factor, respectively.*

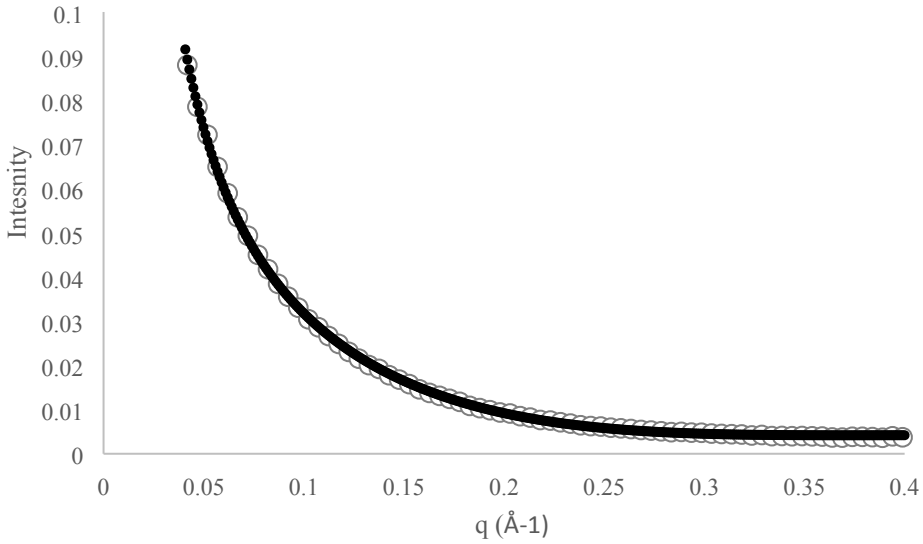


Figure S20. *Fitted SAXS profiles for 1 M $C_{12}E_6$ in triethanolamine. Circles show experimental data and solid lines shows fits to ellipsoid model with no structure factor.*

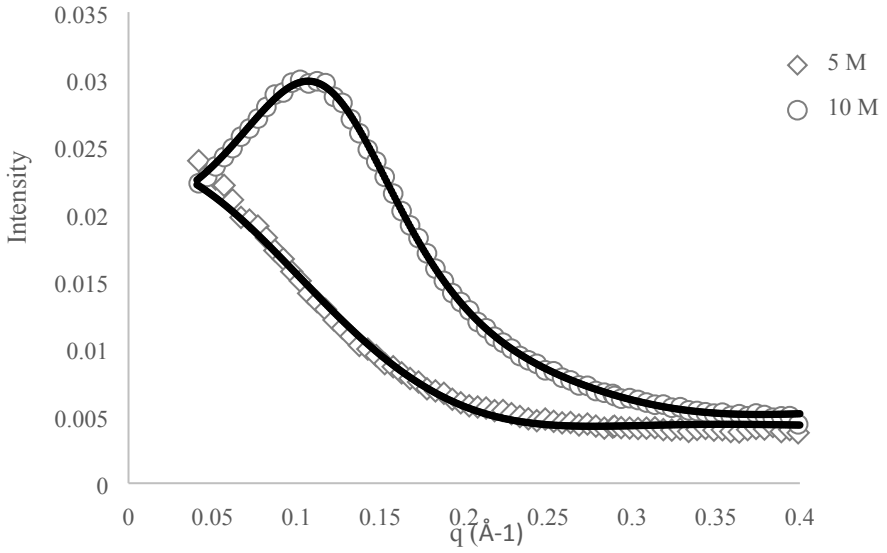


Figure S21. *Fitted SAXS profiles for 5 and 10 M $C_{12}E_6$ in 2-amino-2-ethyl-1,3-propanediol. Circles and diamonds show experimental data and solid lines shows fits to coreshell spherical model with no structure factor and hardsphere structure factor, respectively.*

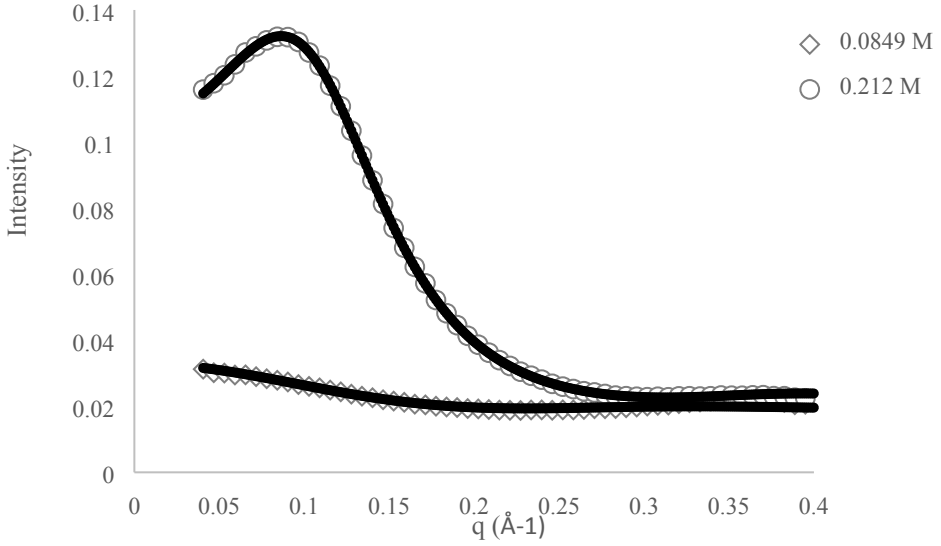


Figure S22. *Fitted SAXS profiles for 0.0849 and 0.212 M $C_{12}E_6$ in ethylammonium nitrate (EAN). Circles and diamonds show experimental data and solid lines shows fits to coreshell spherical model with no structure factor and hardsphere structure factor, respectively.*

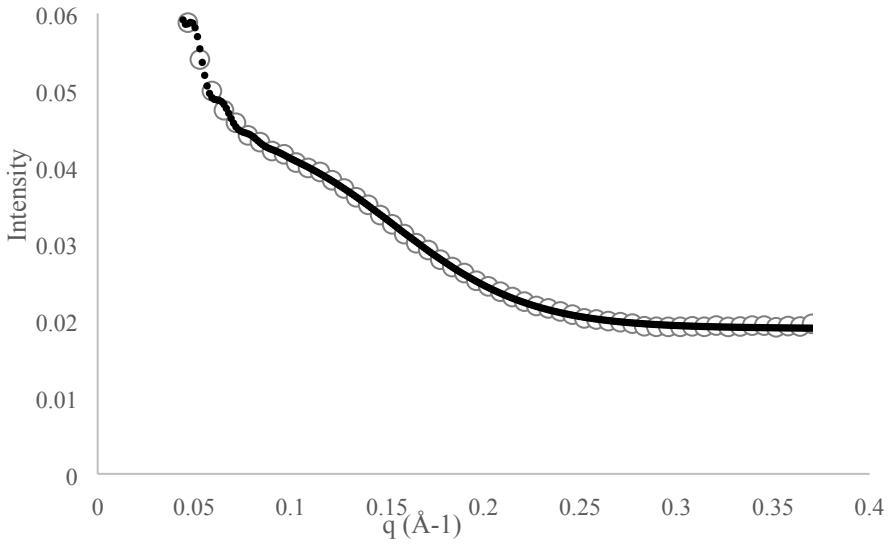


Figure S23. *Fitted SAXS profiles for 0.5 M $C_{12}E_6$ in ethylammonium formate (EAF). Circles, diamonds, and squares show experimental data and solid lines shows fits to coreshell ellipsoid model with no structure factor.*