

SUPPLEMENTARY MATERIAL

PEGylated Assemblies: the Effect of PEG concentration on Self-Assembly Shape as Studied by Coarse-grained Molecular Dynamics

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Supplementary Table 1.

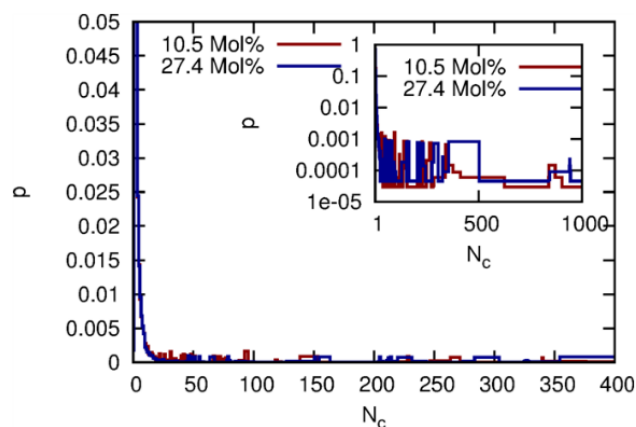
Mol % PEG5-lipid	DPPC	PEG5lipid	water	time	Wt % water
2.2	10269	231	400000	500 ns	73.6
			(838000)	100 ns	85.3
10.5	9400	1100	400000	500 ns	73.1
27.4	7625	2875	400000	500 ns	72.2

Supplementary Table 2.

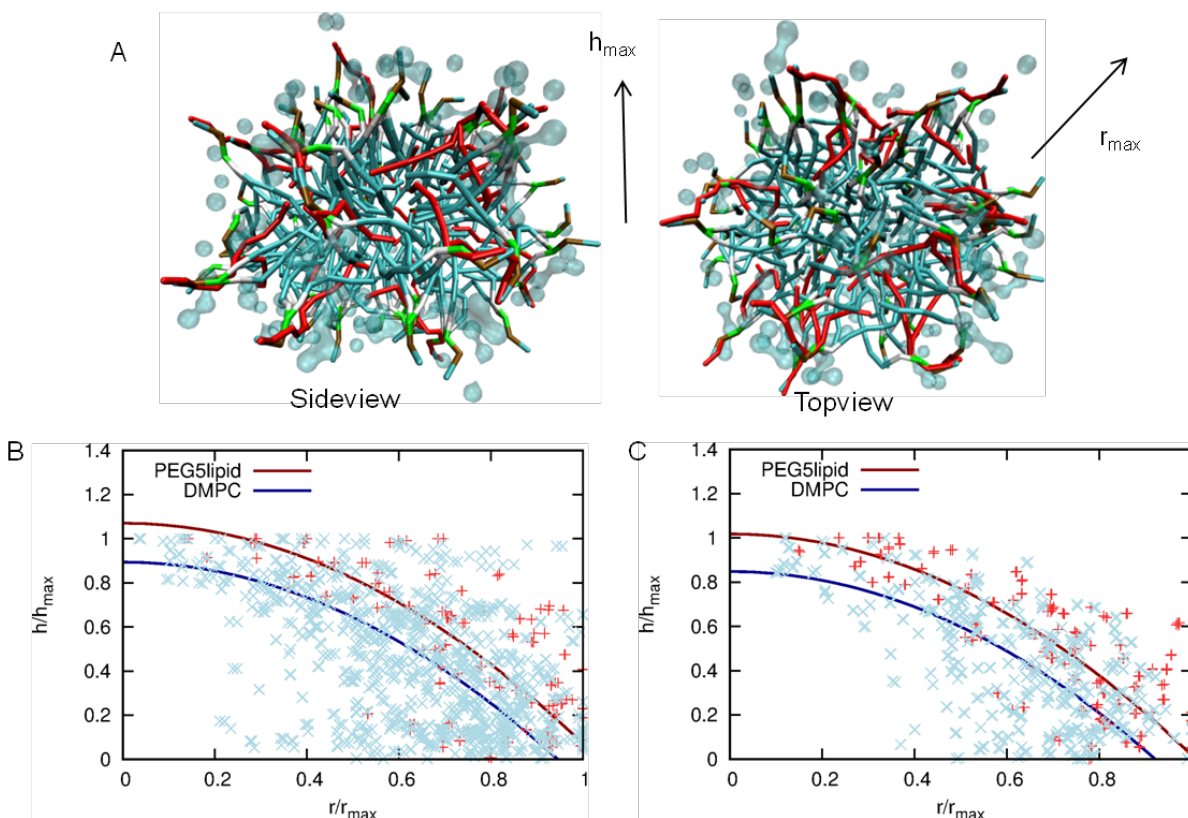
Mol % PEG(5 or13)-lipid	DPPC	PEG-lipid	Water	time
10 Mol %	900	100 (PEG5-lipid)	179313	0.5 μ s
30 Mol %	700	300 (PEG5-lipid)	178391	0.5 μ s
50 Mol %	500	500 (PEG5-lipid)	177728	0.5 μ s
10 Mol %	900	100 (PEG13-lipid)	179313	0.5 μ s
30 Mol %	700	300 (PEG13-lipid)	178391	0.5 μ s
50 Mol %	500	500 (PEG13-lipid)	177728	0.5 μ s

Supplementary Table 3.

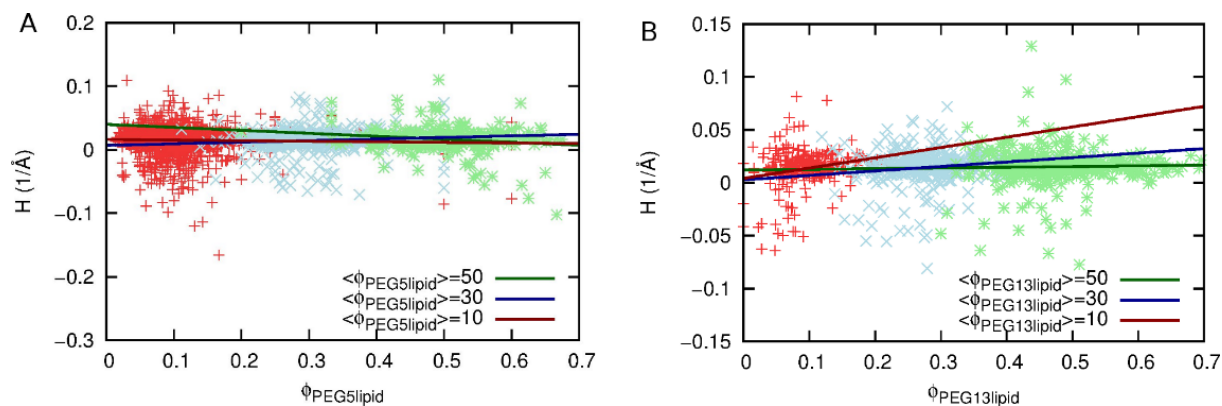
Mol % PEG5- lipid	DMPC	PEG5- lipid	Water	time
30 Mol %	22	10	22288	100 ns
30 Mol %	68	28	22288	100 ns
30 Mol %	140	60	22288	100 ns
30 Mol %	202	86	22288	100 ns
30 Mol %	274	118	22288	100 ns
30 Mol %	358	154	22288	100 ns
50 Mol %	16	16	22288	100 ns
50 Mol %	48	48	22288	100 ns
50 Mol %	100	100	22288	100 ns
50 Mol %	144	144	22288	100 ns
50 Mol %	196	196	22288	100 ns
50 Mol %	256	256	22288	100 ns
70 Mol %	10	22	22288	100 ns
70 Mol %	28	68	22288	100 ns
70 Mol %	60	140	22288	100 ns
70 Mol %	86	202	22288	100 ns
70 Mol %	118	274	22288	100 ns
70 Mol %	154	358	22288	100 ns



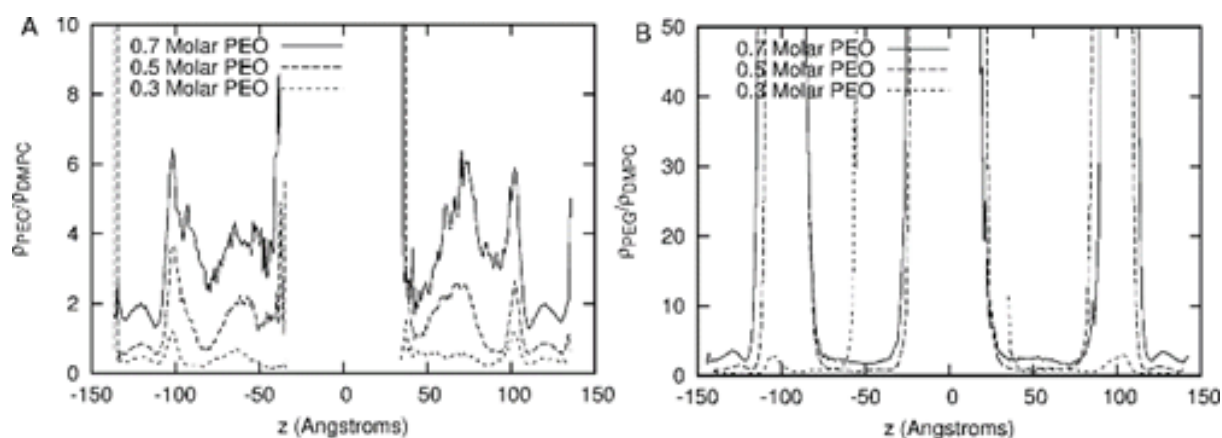
Supplementary Figure 1. There is a wide distribution of cluster sizes, ranging from unimers to a finite probability ($< .0001$) of cluster sizes > 500 . 10.5 and 27.4 Mol % PEG5lipid exhibit similar cluster size distributions after 0.5 microsecond runtime, with a sharp exponential peak that falls off after the unimer concentration, with a small probability of small micelles (< 80 lipids) and larger bicelles (> 80 lipids).



Supplementary Figure 2. A) Sideview and topview of a bicelle nucleus contained 74 lipids. Fluid like blobs represent water within 4.5 \AA of micelle. In the topview, note that PEG5lipids occupy the space towards the outer radius from the center of mass of the micelle. Center of mass location for PEG5lipids and DMPC after 100ns for B) 10.5 Mol % PEG5lipid and C) 27.4 Mol % lipid. PEGylated lipid occupies the positions towards to the outer radius of the bicelle. The bicelle shape can be characterized with a height, h , and radius, r , where h_{\max} and r_{\max} are the outermost and highest lipid locations for each bicelle respectively. (Averaging over size < 80 lipids).



Supplementary Figure 3. Mean curvature, H , of bicelle as a function of the normalized interfacial concentration for two different PEGylated lipid lengths (5,13) and three different concentrations of PEGylated lipid (10, 30, 50 Mol %). A) PEG5lipid does not show a correlation of the mean curvature with interfacial concentration of the PEG5lipid. B) PEG13 lipid also does not show a clear correlation between mean curvature and interfacial concentration.



Supplementary Figure 4. Ratio of PEG5lipid density, ρ_{PEG} , to DMPC lipid density, ρ_{DMPC} , along the normal to the air-water interface. With increasing length of PEG from PEG5lipid (A) to PEG13lipid (B), the density ratio diverges at the micelle buds. PEG13 lipid prefers the micellar bud regions of positive curvature.