Supplementary Information

CHARMM36 United-Atom Chain Model for Lipids and Surfactants

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Table S1. Characteristics of micelles in M1-M6.

Simulation	Micelle	# of lipids	I_{max}/I_{min}	r_m [Å]	R_g [Å]
M1	1	54	1.23±0.080	18.88±0.19	17.73±0.19
M2	1	64	1.27±0.11	19.87±0.19	18.88±0.20
M2	2	27	1.32±0.13	15.35±0.27	14.79±0.28
M2	3	17	1.48±0.12	15.05±0.89	13.38±0.34
M3	1	14	1.44±0.15	12.68±0.46	12.71±0.46
M3	2	42	1.23±0.080	17.49±0.20	16.67±0.23
M3	3	45	1.27±0.10	18.62±0.73	16.98±0.28
M3	4	61	1.24±0.092	19.55±0.17	18.55±0.20
M4	1	20	1.39±0.14	14.74±0.64	13.52±0.35
M5	1	17	1.38±0.15	13.04±0.35	13.03±0.36
M5	2	22	1.39±0.16	14.77±0.66	14.13±0.33
M6	1	36	1.25±0.10	16.60±0.22	15.99±0.24

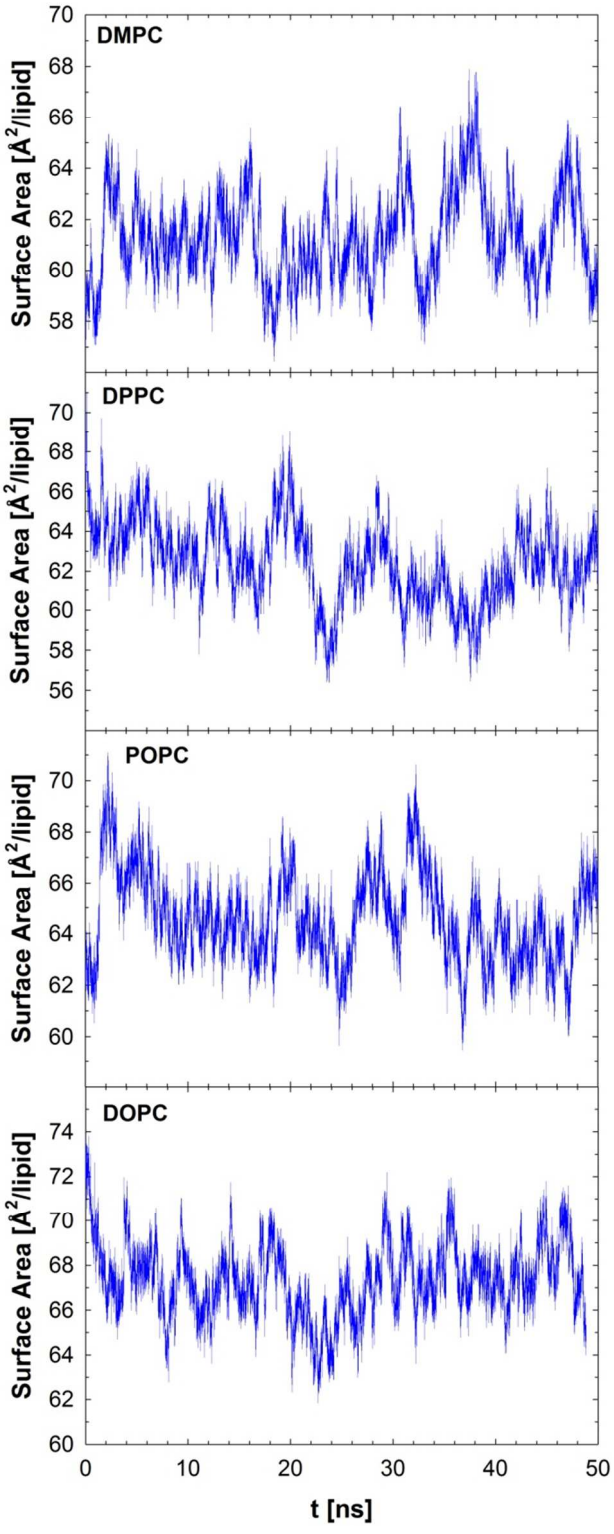

Figure S1. Time series of surface area per lipid for the single-lipid bilayer simulations.

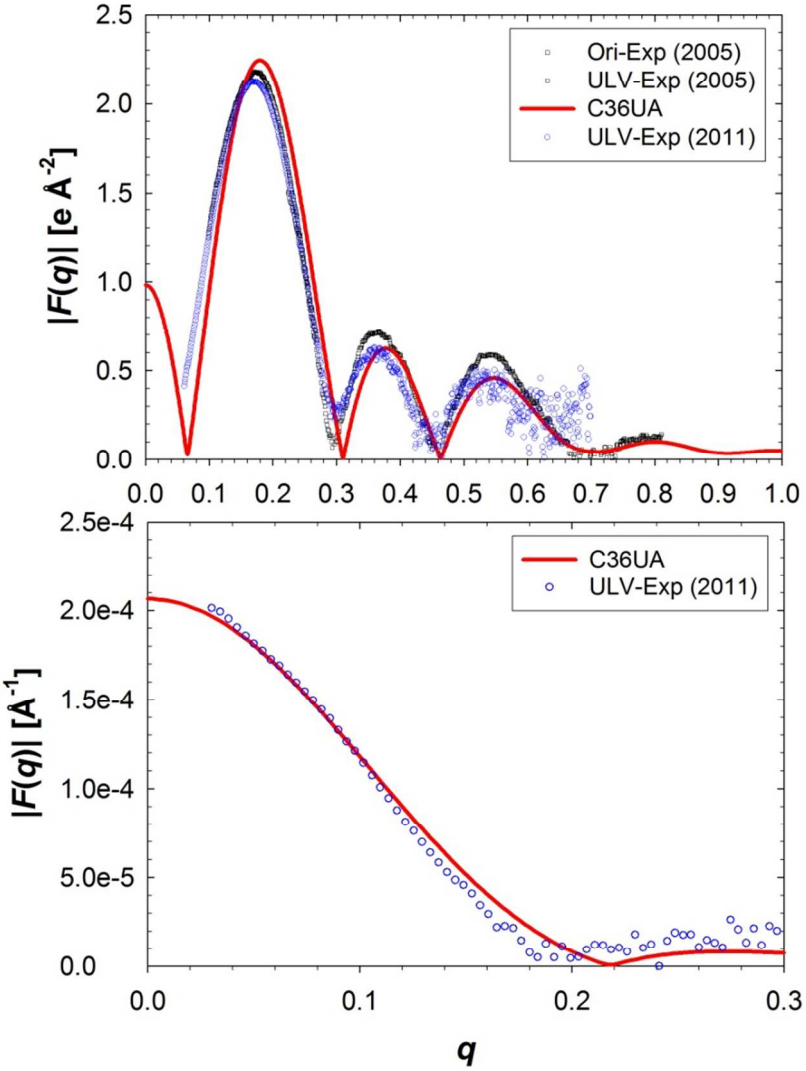

Figure S2. DMPC form factors from x-ray (top) and neutron (bottom) scattering from Kučerka et al. in 2005[1] and 2011.[2] Ori-Oriented stacks and ULV-unilamellar vesicles. Results from our C36-UA are shown in red.

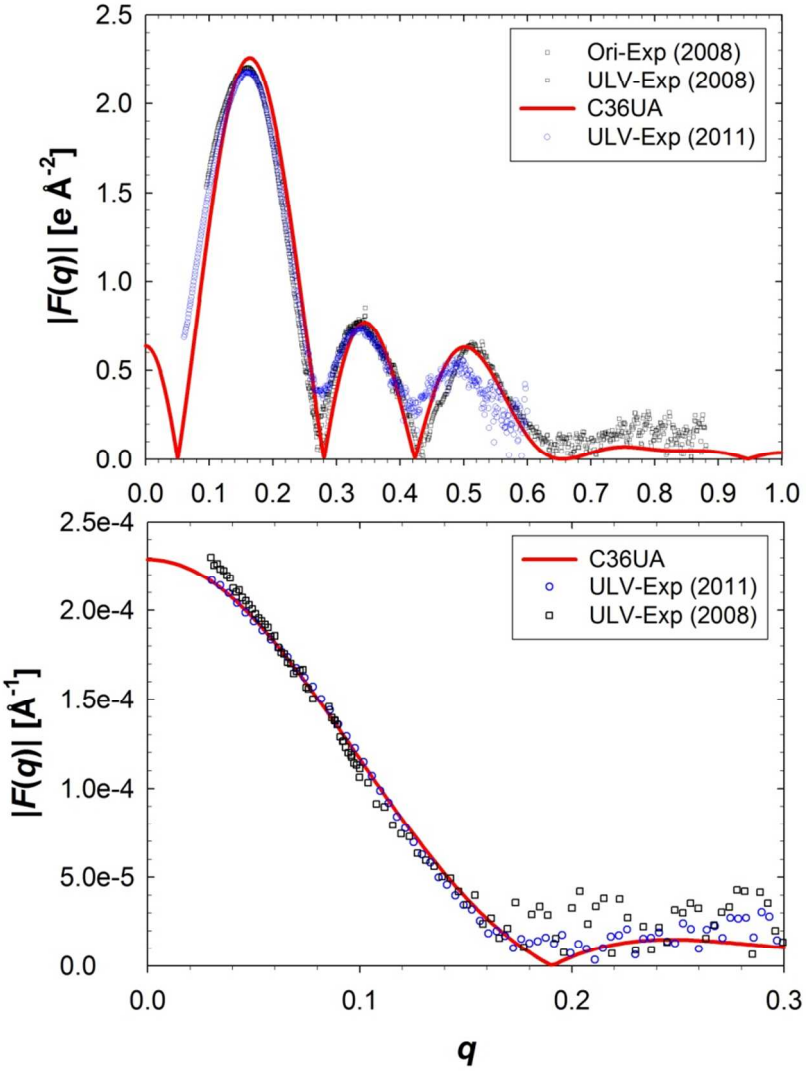

Figure S3. DPPC form factors from x-ray (top) and neutron (bottom) scattering from Kučerka et al. in 2008[3] and 2011.[2] Ori-Oriented stacks and ULV-unilamellar vesicles. Results from our C36-UA are shown in red.

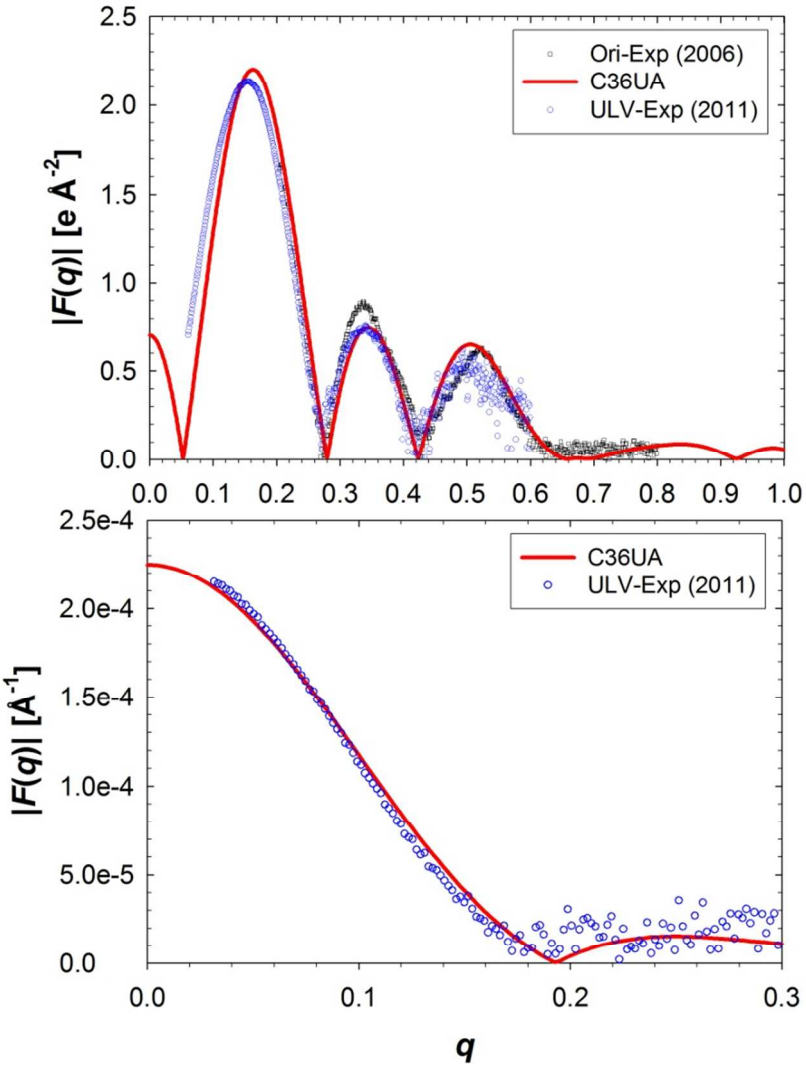

Figure S4. POPC form factors from x-ray (top) and neutron (bottom) scattering from Kučerka et al. in 2006[4] and 2011.[2] Ori-Oriented stacks and ULV-unilamellar vesicles. Results from our C36-UA are shown in red.

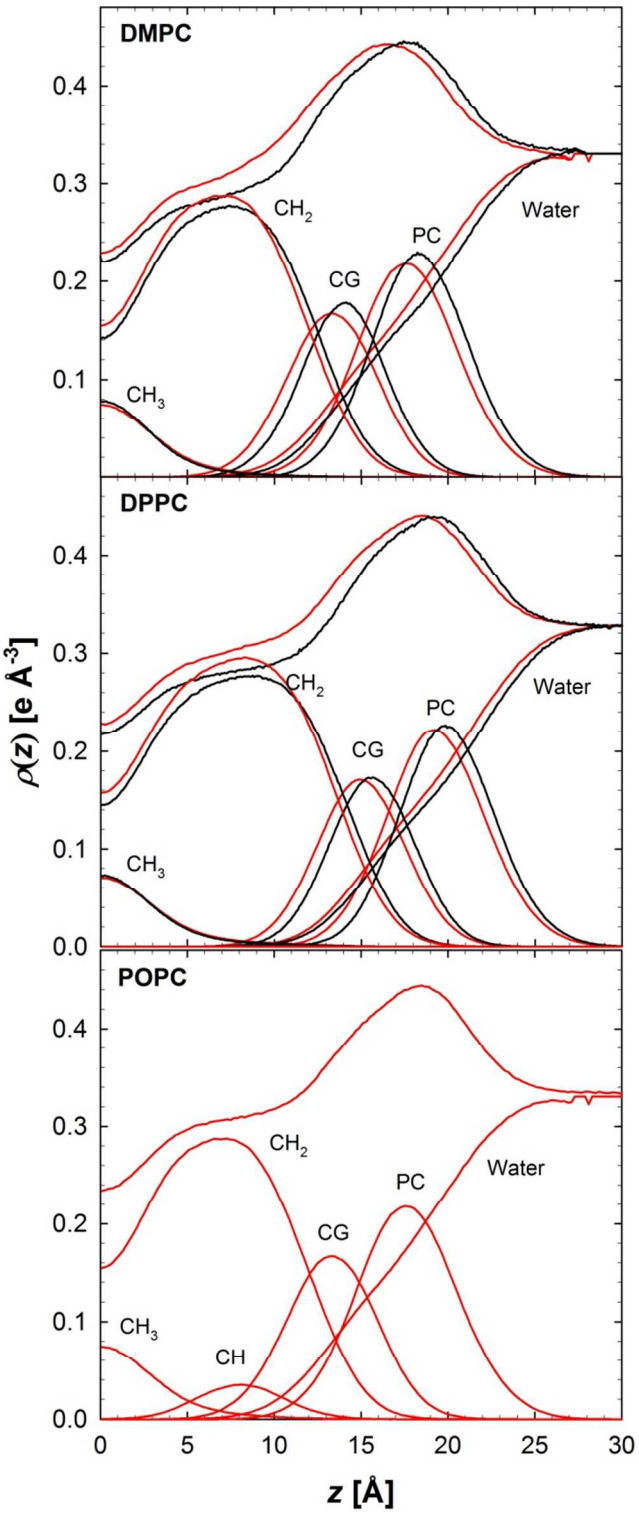

Figure S5. Symmetrized electron density profiles for lipid bilayers for C36-UA (red) and C36 (black).[5]

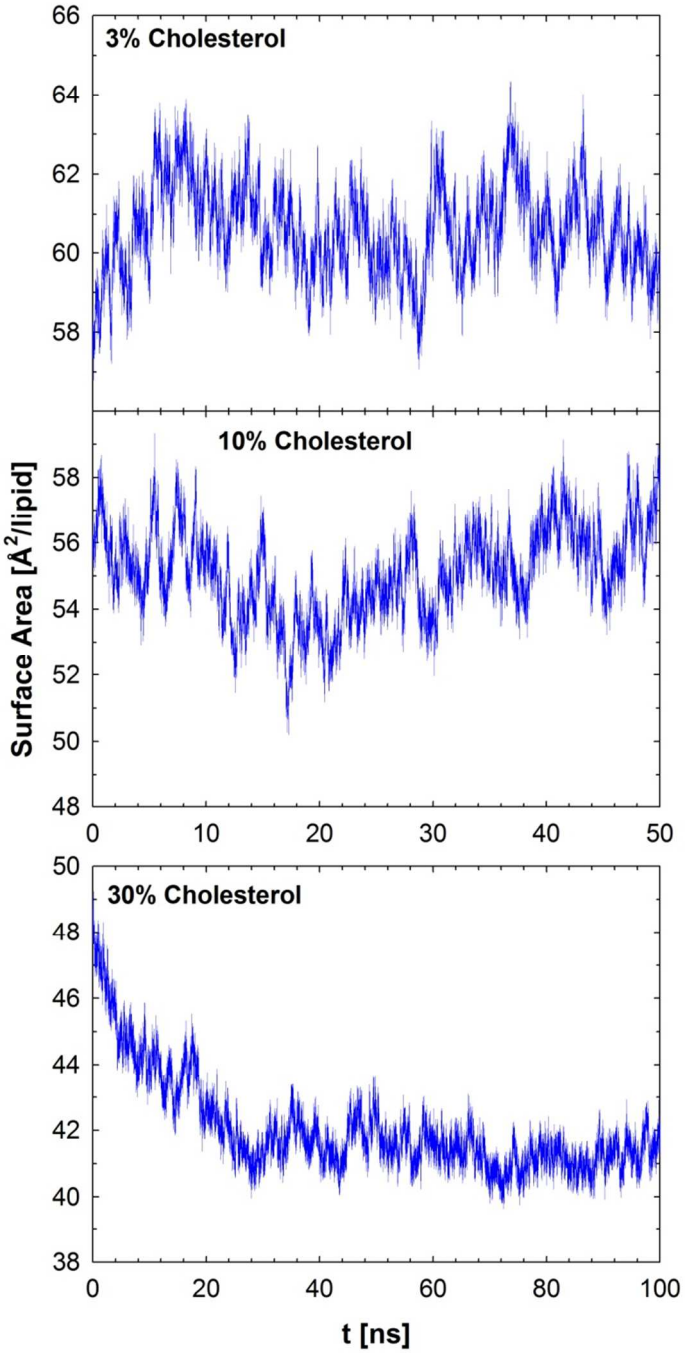

Figure S6. Time series of surface area per lipid for the DMPC-cholesterol bilayer simulations.

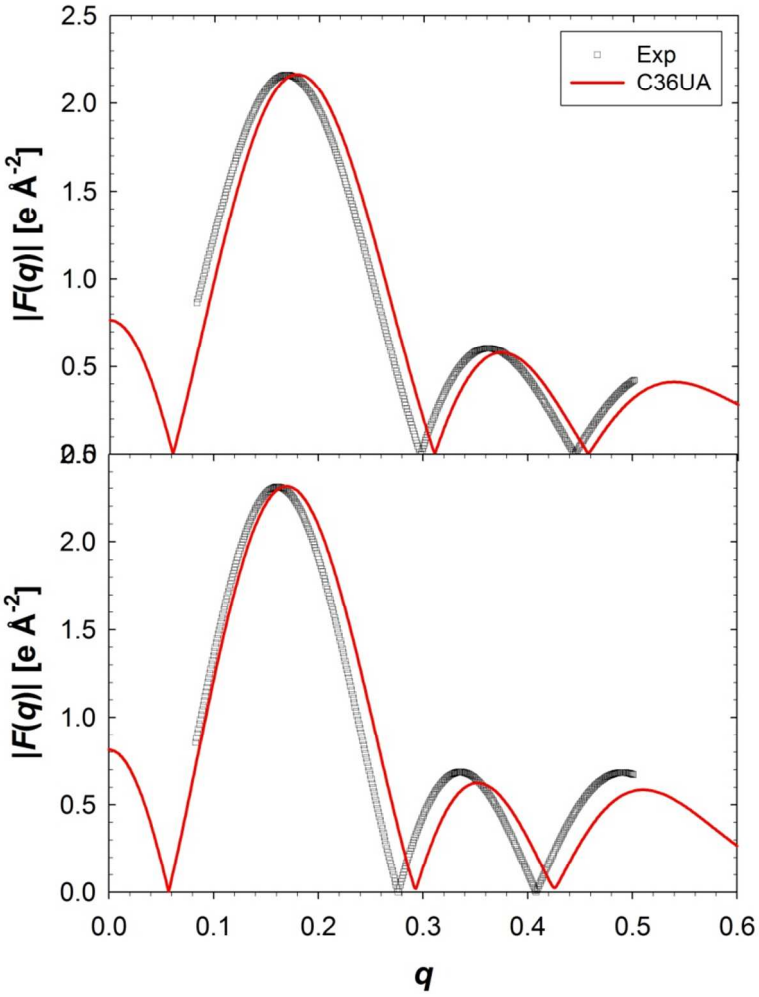

Figure S7. X-ray form factors from experiments on 3% (top) and 10% (bottom) cholesterol[6] scaled to agree with simulations. Results from our C36-UA are shown in red.

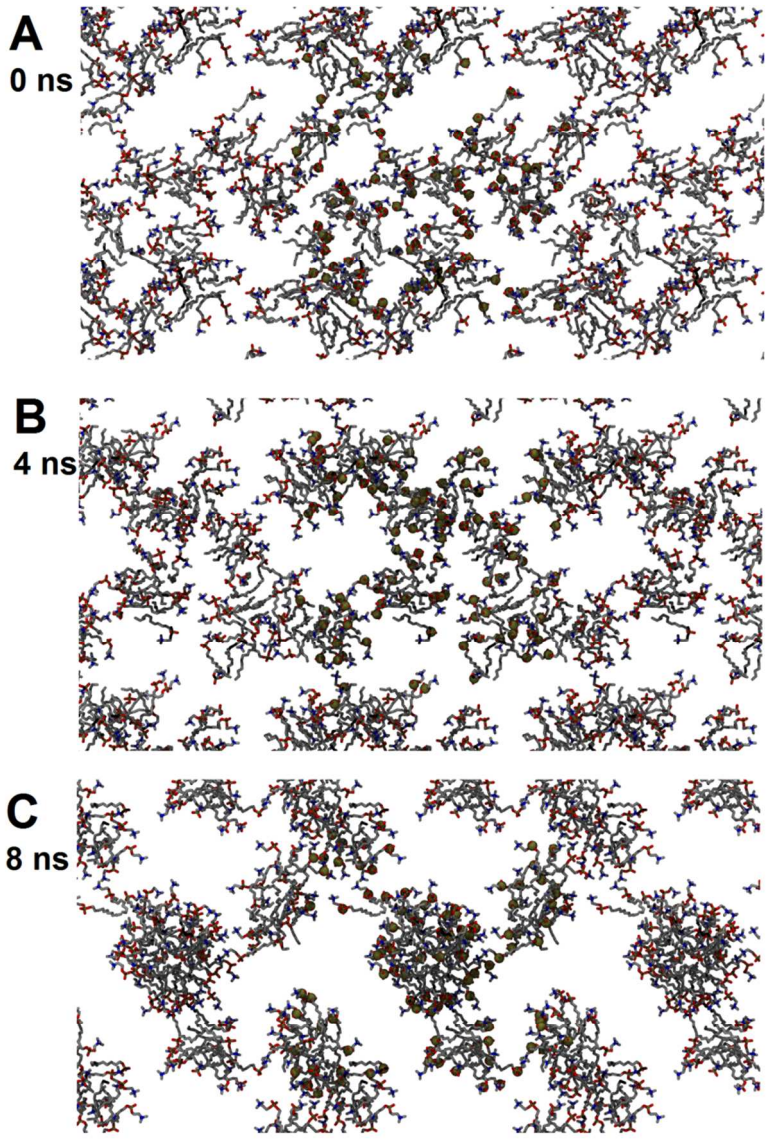

Figure S8. A series of periodic images of M2 showing the very early stages of lipid aggregation and growth. Periodic images are necessary to show aggregations because the simulation is run with multiple copies of the unit cell to simulate a solution much larger than the unit cell. Some aggregations were split across the boundary of the unit cell and require periodic images to be shown in one piece.

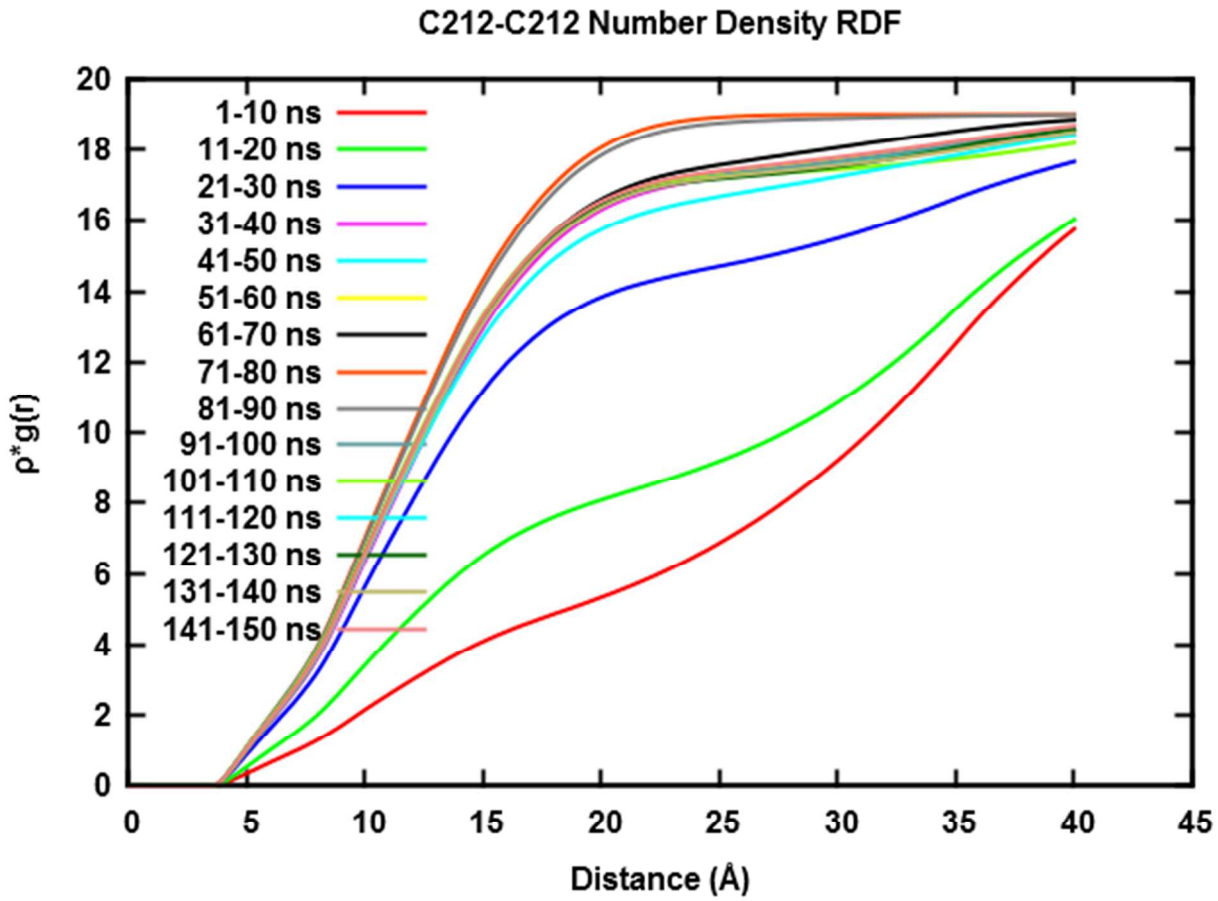

Figure S9. Multiple number density RDFs, from M4, showing the formation of a micelle from an initially random configuration of surfactants and the oscillatory approach to equilibration. The main micelle formation occurred from 1 to 40 ns. The increasing slope of the RDF during this time period corresponded with the surfactants aggregating. After 40 ns, the micelles continued to grow, but with negligible change to its shape. The RDF number of lipids in this simulation approached 20, but then fell until 120 ns. Finally, the RDF increased to its previous height from ~50 ns.

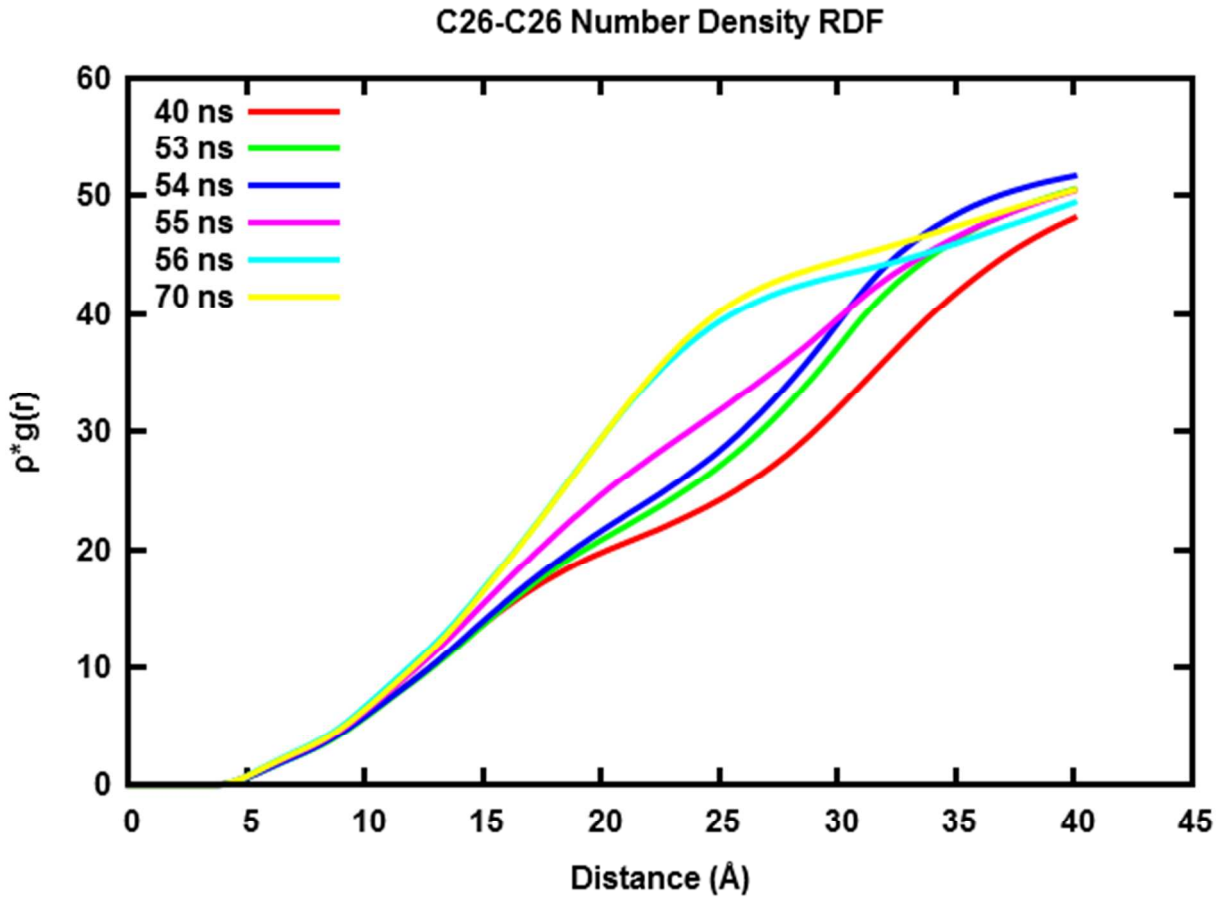

Figure S10. Multiple number density RDFs showing the fusion of two micelles in M1. Notice the difference from 54 to 56 ns, the time period when the micelles fused. As a result, the RDF for 56 ns represents a one-micelle system which corresponded with the greater slope from 20 to 25 Å, compared to the previous RDFs. If, as time increases, the RDFs have a greater slope and more area under the curve, then this signifies that surfactants are moving closer to each other in the system.

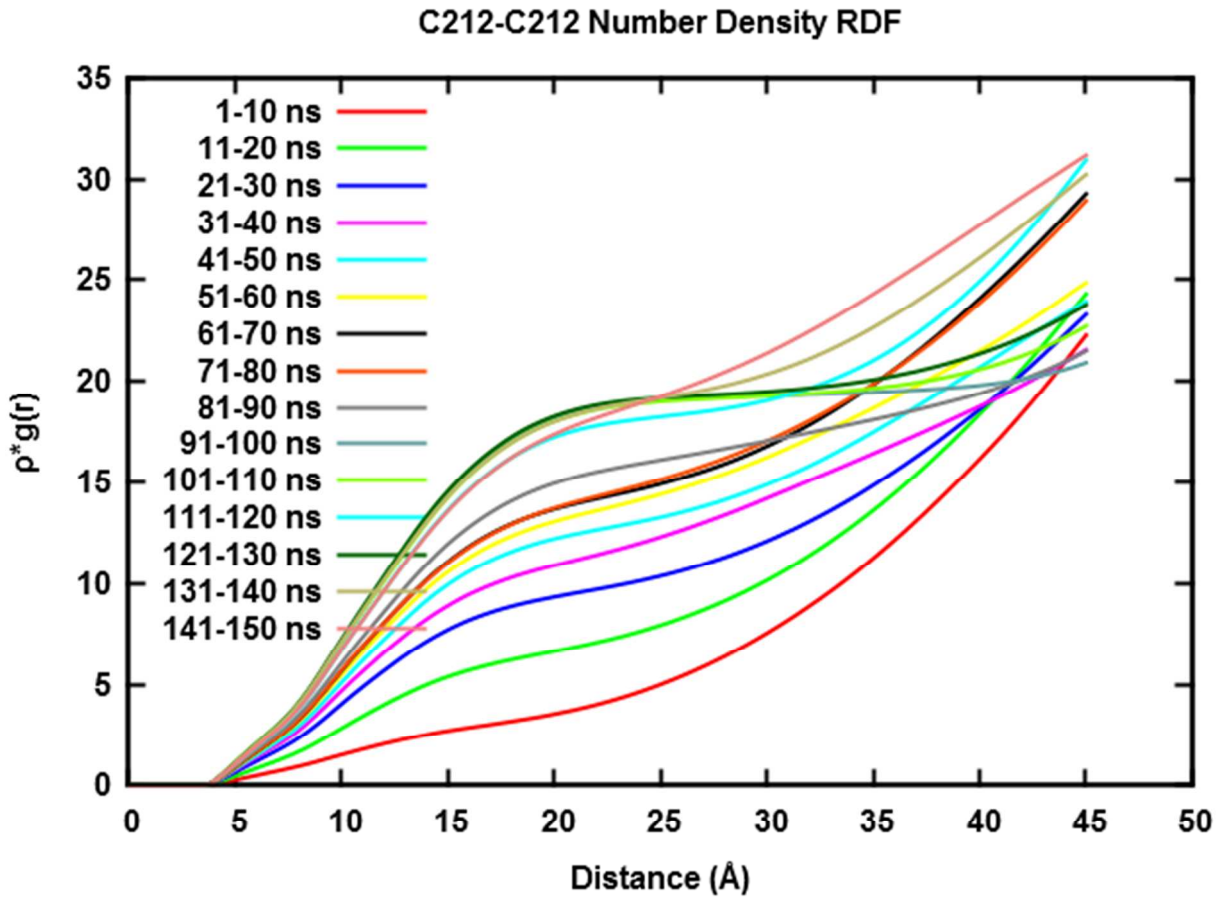

Figure S11. Number density RDF from M5. As time increased and micelles aggregated, the number density RDF gained a height in the 10-40 Å range compared to the RDF plotted using the average of 1-10 ns.

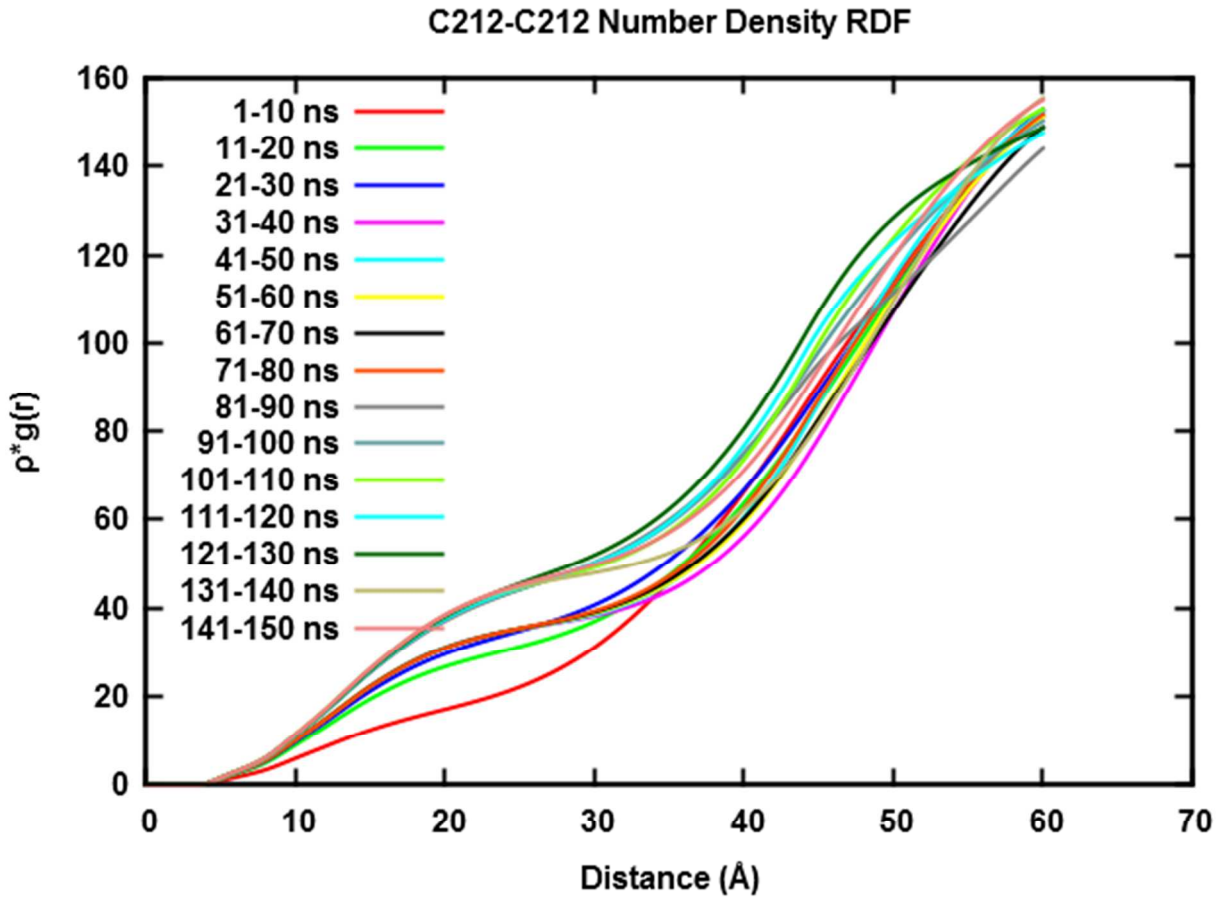

Figure S12. Number density RDF from M3.

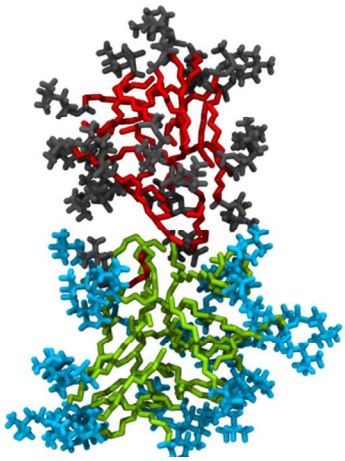

Figure S13. An image of M1 showing the head groups in the way of the micelles, temporarily preventing them from fusing. Additionally, note that several surfactants' tails from the bottom and top micelles reoriented from the normal position in a micelle. Instead of the tail pointing towards the core of the micelle, it pointed to another micelle. At least one head group is between the micelles, which may interfere with interaction of the lipids from different micelles.

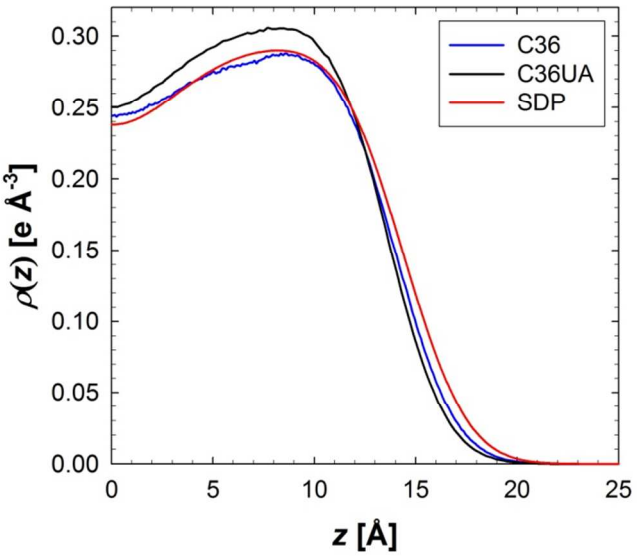

Figure S14. Symmetrized electron density profiles for the lipid chains of DOPC (CH+CH2+CH3) compared to the SDP model fit to experimental x-ray and neutron scattering.[3]

References

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