molecules

MDPI

# Supporting Information

**Table S1.** Chemical composition, molecular volumes and electron densities of the lipids and detergent components. a is from [34], b is from [35], c was from [36] and d was estimated using the VegaZZ software [37].

| Component | Chemical formula | Molecular volume (Å$^3$) | Electron density (e$^-$/ Å$^3$) |
|---|---|---|---|
| DMPC tails | $C_{26}H_{54}$ | 779.8[a] | 0.269 |
| DMPC heads | $C_{10}H_{18}NO_8P$ | 320.9[a] | 0.489 |
| DMPG heads | $C_8H_{12}O_{10}P$ | 283.0[b] | 0.494 |
| POPC tails | $C_{32}H_{64}$ | 937.2[a] | 0.273 |
| DHPC tails | $C_{10}H_{22}$ | 330.2[a] | 0.248 |
| CHAPS | $C_{32}H_{58}N_2O_7S$ | 830.3[c] | 0.405 |
| Cholate | $C_{24}H_{39}O_5$ | 473.0[d] | 0.471 |

**Table S2.** Complete list of the values describing the fits obtained for the curves shown in Figure 3, Figure 5 and Figure S2 and plotted in Figure 4B, Figure 5B and Figure S7.

| q | Scale | BKG | Radius | X_core | Thick_rim | Thick_face | Length | SLD_core | SLD_face | SLD_rim | SLD_solvent | Belt_rough | ChiSq |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| DMPC_CHAPS | | | | | | | | | | | | | |
| 0.5 | 1.25E-02 | 6.28E-04 | 19.6 | 0.705 | 10.7 | 6.4 | 19.8 | 7.6 | 11.85 | 11.18 | 9.27 | 3 | 1.27 |
| 1 | 8.69E-03 | 4.32E-04 | 26.0 | 0.667 | 8.8 | 9.5 | 24.1 | 7.6 | 11.74 | 11.29 | 9.27 | 3 | 1.34 |
| 1.5 | 7.35E-03 | 2.61E-04 | 31.4 | 0.685 | 8.0 | 10.3 | 23.3 | 7.6 | 11.80 | 11.25 | 9.27 | 3 | 1.45 |
| 2 | 6.73E-03 | 2.67E-04 | 34.5 | 0.675 | 7.8 | 10.5 | 23.8 | 7.6 | 11.83 | 11.23 | 9.27 | 3 | 1.65 |
| 2.5 | 6.34E-03 | 2.61E-04 | 34.8 | 0.672 | 8.4 | 9.7 | 24.5 | 7.6 | 11.89 | 11.27 | 9.27 | 3 | 1.90 |
| 3 | 6.13E-03 | 2.60E-04 | 37.3 | 0.654 | 8.3 | 10.0 | 24.7 | 7.6 | 11.84 | 11.26 | 9.27 | 3 | 1.73 |
| 5 | 5.67E-03 | 2.16E-04 | 39.0 | 0.688 | 8.6 | 9.9 | 25.0 | 7.6 | 11.88 | 11.23 | 9.27 | 3 | 1.82 |
| DMPC_Chol | | | | | | | | | | | | | |
| 0.5 | 8.89E-03 | 1.00E-03 | 12.4 | 0.884 | 12.2 | 4.0 | 14.9 | 7.6 | 11.00 | 11.27 | 9.27 | 3 | 1.46 |
| 1 | 7.69E-03 | 7.00E-04 | 15.8 | 0.832 | 10.4 | 4.5 | 20.8 | 7.6 | 11.17 | 11.43 | 9.27 | 3 | 1.46 |
| 1.5 | 6.33E-03 | 7.00E-04 | 22.2 | 0.920 | 4.2 | 11.5 | 17.6 | 7.6 | 11.69 | 11.42 | 9.27 | 3 | 1.46 |
| 2 | 5.92E-03 | 7.50E-04 | 23.0 | 0.877 | 4.4 | 11.5 | 18.2 | 7.6 | 11.72 | 11.40 | 9.27 | 3 | 1.38 |
| 2.5 | 5.83E-03 | 6.00E-04 | 24.0 | 0.919 | 4.3 | 10.8 | 18.9 | 7.6 | 11.97 | 11.22 | 9.27 | 3 | 1.37 |
| 3 | 5.38E-03 | 6.80E-04 | 25.6 | 0.843 | 4.0 | 10.3 | 19.9 | 7.6 | 12.09 | 11.54 | 9.27 | 3 | 1.36 |
| 5 | 5.38E-03 | 6.80E-04 | 25.6 | 0.843 | 4.0 | 10.3 | 19.9 | 7.6 | 12.09 | 11.54 | 9.27 | 3 | 1.36 |
| DMPC_DHPC | | | | | | | | | | | | | |
| 0.5 | 1.07E-02 | 5.45E-04 | 30.1 | 0.694 | 4.5 | 8.3 | 24.4 | 7.6 | 11.63 | 11.97 | 9.27 | 3 | 1.52 |
| 1 | 8.02E-03 | 3.96E-04 | 41.2 | 0.738 | 4.3 | 9.6 | 24.2 | 7.6 | 11.60 | 11.78 | 9.27 | 3 | 1.43 |
| 1.5 | 6.71E-03 | 2.14E-04 | 45.6 | 0.728 | 4.3 | 9.4 | 25.3 | 7.6 | 11.81 | 11.81 | 9.27 | 3 | 1.31 |
| 2 | 6.45E-03 | 2.00E-04 | 46.5 | 0.769 | 4.3 | 9.7 | 25.6 | 7.6 | 11.83 | 11.78 | 9.27 | 3 | 1.51 |
| 2.5 | 6.06E-03 | 2.66E-04 | 46.6 | 0.802 | 4.1 | 10.0 | 25.7 | 7.6 | 11.77 | 11.81 | 9.27 | 3 | 1.70 |
| 3 | 5.89E-03 | 2.16E-04 | 45.1 | 0.888 | 4.1 | 10.1 | 25.7 | 7.6 | 11.83 | 11.59 | 9.27 | 3 | 1.64 |
| 5 | 5.56E-03 | 2.68E-04 | 50.1 | 0.830 | 4.1 | 10.5 | 25.6 | 7.6 | 11.78 | 11.48 | 9.27 | 3 | 1.92 |
| DMPC_PG_CHAPS | | | | | | | | | | | | | |
| 0.5 | 1.07E-02 | 8.85E-04 | 20.2 | 0.627 | 10.9 | 7.4 | 22.0 | 7.6 | 11.79 | 11.28 | 9.27 | 3 | 2.15 |
| 1 | 7.80E-03 | 5.11E-04 | 27.8 | 0.635 | 9.1 | 10.0 | 23.3 | 7.6 | 11.86 | 11.26 | 9.27 | 3 | 1.65 |
| 1.5 | 6.80E-03 | 3.06E-04 | 31.6 | 0.684 | 8.5 | 10.7 | 23.6 | 7.6 | 11.80 | 11.27 | 9.27 | 3 | 1.55 |
| 2 | 6.30E-03 | 3.02E-04 | 35.1 | 0.670 | 8.5 | 10.8 | 23.8 | 7.6 | 11.80 | 11.23 | 9.27 | 3 | 1.33 |
| 2.5 | 6.00E-03 | 3.34E-04 | 37.1 | 0.700 | 8.0 | 10.5 | 24.2 | 7.6 | 11.98 | 11.21 | 9.27 | 3 | 1.40 |
| 3 | 5.80E-03 | 3.00E-04 | 39.8 | 0.667 | 8.1 | 11.0 | 24.0 | 7.6 | 11.83 | 11.24 | 9.27 | 3 | 2.00 |
| 5 | 5.50E-03 | 2.17E-04 | 40.9 | 0.725 | 9.6 | 11.1 | 24.1 | 7.6 | 11.74 | 11.04 | 9.27 | 3 | 1.68 |
| DMPC_PG_Chol | | | | | | | | | | | | | |
| 0.5 | 9.15E-03 | 1.00E-03 | 13.1 | 0.938 | 11.5 | 4.1 | 15.8 | 7.6 | 11.50 | 11.33 | 9.27 | 3 | 2.48 |
| 1 | 7.58E-03 | 9.38E-04 | 17.6 | 0.661 | 10.5 | 4.1 | 24.8 | 7.6 | 11.82 | 11.32 | 9.27 | 3 | 2.38 |
| 1.5 | 6.11E-03 | 7.50E-04 | 23.4 | 0.869 | 4.1 | 11.6 | 18.0 | 7.6 | 11.85 | 11.39 | 9.27 | 3 | 1.44 |
| 2 | 6.08E-03 | 7.10E-04 | 24.7 | 0.869 | 4.1 | 11.6 | 18.3 | 7.6 | 11.88 | 11.25 | 9.27 | 3 | 1.46 |
| 2.5 | 5.75E-03 | 9.22E-04 | 26.1 | 0.847 | 4.7 | 10.9 | 19.5 | 7.6 | 12.12 | 11.03 | 9.27 | 3 | 1.78 |
| 3 | 5.70E-03 | 7.14E-04 | 25.0 | 0.880 | 4.7 | 10.3 | 19.9 | 7.6 | 12.26 | 11.15 | 9.27 | 3 | 1.42 |
| 5 | 5.55E-03 | 7.00E-04 | 24.3 | 0.976 | 4.5 | 10.8 | 19.6 | 7.6 | 12.08 | 11.16 | 9.27 | 3 | 1.53 |
| DMPC_PG_DHPC | | | | | | | | | | | | | |
| 0.5 | 1.08E-02 | 6.78E-04 | 32.4 | 0.694 | 4.3 | 9.4 | 23.4 | 7.6 | 11.57 | 11.85 | 9.27 | 3 | 1.25 |
| 1 | 7.67E-03 | 4.41E-04 | 45.6 | 0.630 | 4.3 | 9.7 | 24.7 | 7.6 | 11.69 | 11.86 | 9.27 | 3 | 1.43 |
| 1.5 | 6.78E-03 | 2.17E-04 | 47.2 | 0.661 | 4.9 | 9.9 | 25.7 | 7.6 | 11.69 | 11.87 | 9.27 | 3 | 2.18 |
| 2 | 6.21E-03 | 2.60E-04 | 47.5 | 0.690 | 5.1 | 10.2 | 25.8 | 7.6 | 11.67 | 11.82 | 9.27 | 3 | 1.30 |
| 2.5 | 6.07E-03 | 3.17E-04 | 51.7 | 0.785 | 4.2 | 10.8 | 25.2 | 7.6 | 11.72 | 11.72 | 9.27 | 3 | 1.45 |
| 3 | 6.27E-03 | 2.66E-04 | 48.2 | 0.938 | 4.2 | 11.0 | 24.9 | 7.6 | 11.68 | 11.69 | 9.27 | 3 | 1.33 |
| 5 | 5.58E-03 | 2.61E-04 | 55.3 | 0.885 | 4.1 | 11.9 | 24.9 | 7.6 | 11.64 | 11.33 | 9.27 | 3 | 1.41 |

| POPC_DHPC | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.5 | 2.07E-02 | 3.57E-04 | 28.1 | 0.731 | 6.6 | 5.6 | 29.6 | 7.7 | 12.96 | 11.03 | 9.27 | 3 | 3.04 |
| 1 | 1.68E-02 | 1.43E-04 | 38.0 | 0.573 | 6.5 | 5.4 | 29.9 | 7.7 | 12.57 | 11.45 | 9.27 | 3 | 2.88 |
| 1.5 | 1.06E-02 | 1.28E-04 | 137.3 | 0.197 | 7.7 | 11.4 | 24.6 | 7.7 | 11.00 | 11.00 | 9.27 | 3 | 1.45 |
| 2 | 9.94E-03 | 1.20E-04 | 198.9 | 0.136 | 7.6 | 11.5 | 24.6 | 7.7 | 11.00 | 11.02 | 9.27 | 3 | 1.39 |
| 2.5 | 7.39E-03 | 1.12E-04 | 245.7 | 0.124 | 6.1 | 11.3 | 24.2 | 7.7 | 11.00 | 11.61 | 9.27 | 3 | 1.52 |
| 3 | 6.47E-03 | 1.13E-04 | 247.8 | 0.124 | 7.8 | 11.6 | 24.2 | 7.7 | 11.00 | 11.01 | 9.27 | 3 | 1.68 |
| 5 | 4.47E-03 | 8.38E-05 | 943.0 | 0.033 | 4.8 | 10.7 | 24.6 | 7.7 | 11.13 | 12.59 | 9.27 | 3 | 2.38 |

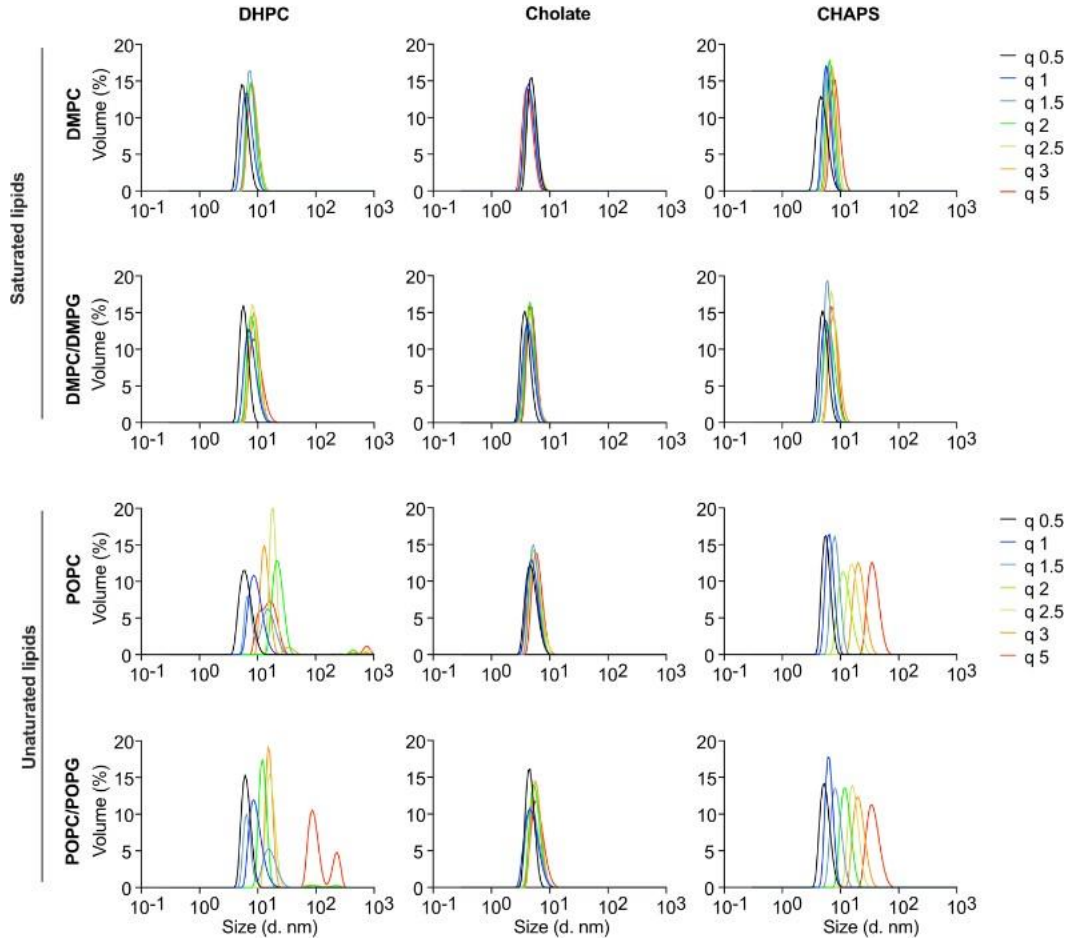


**Figure S1.** DLS size distributions of the lipid-detergent mixtures measured in this study. The curves are representative of one to three independent experiments.

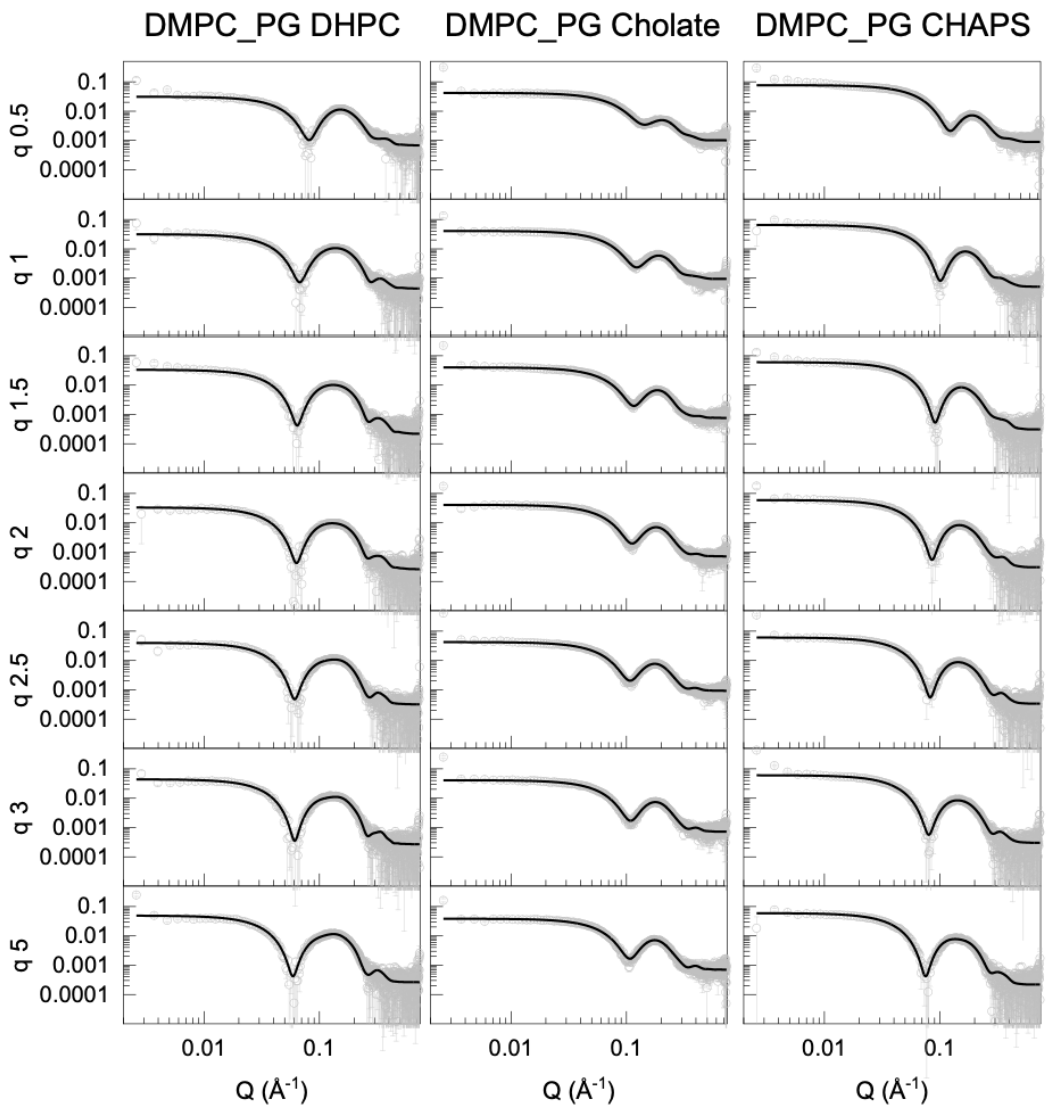


**Figure S2.** SAXS curves and best fit to the data for the systems containing DMPC-DMPG (80:20) and the three detergents.

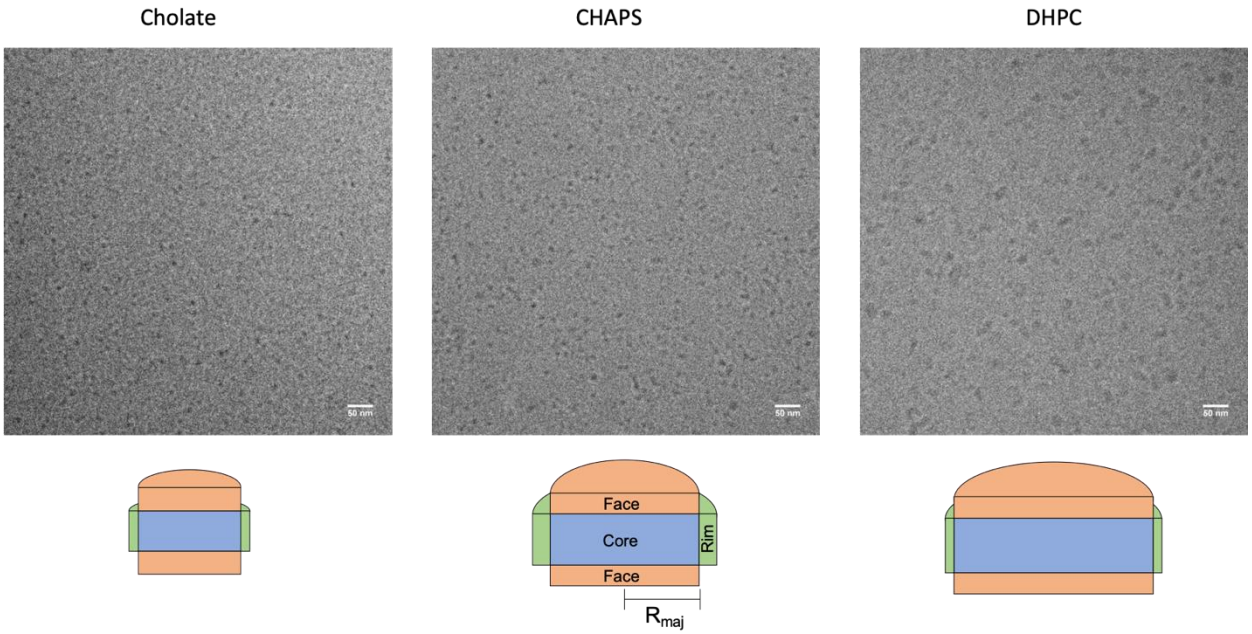


**Figure S3.** Cryo EM images of DMPC mixed with cholate (left) CHAPS (centre) and DHPC (left) at a q ratio of 2.5, scale bar = 50 nm. The schematic cartoons underneath represent the structures obtained from the fitting of the SAXS data drawn to scale using the thickness parameters obtained from the fits.

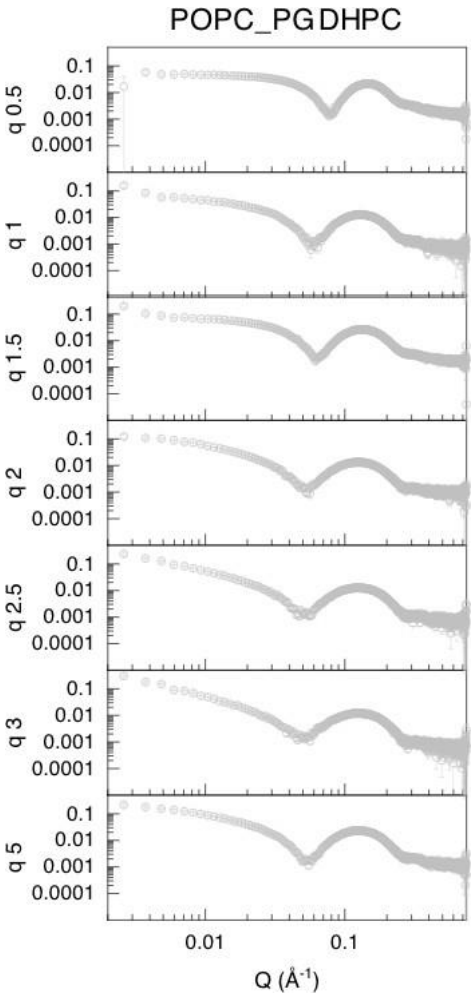


**Figure S4.** SAXS curves for the POPC-POPG (80:20) samples mixed with DHPC.

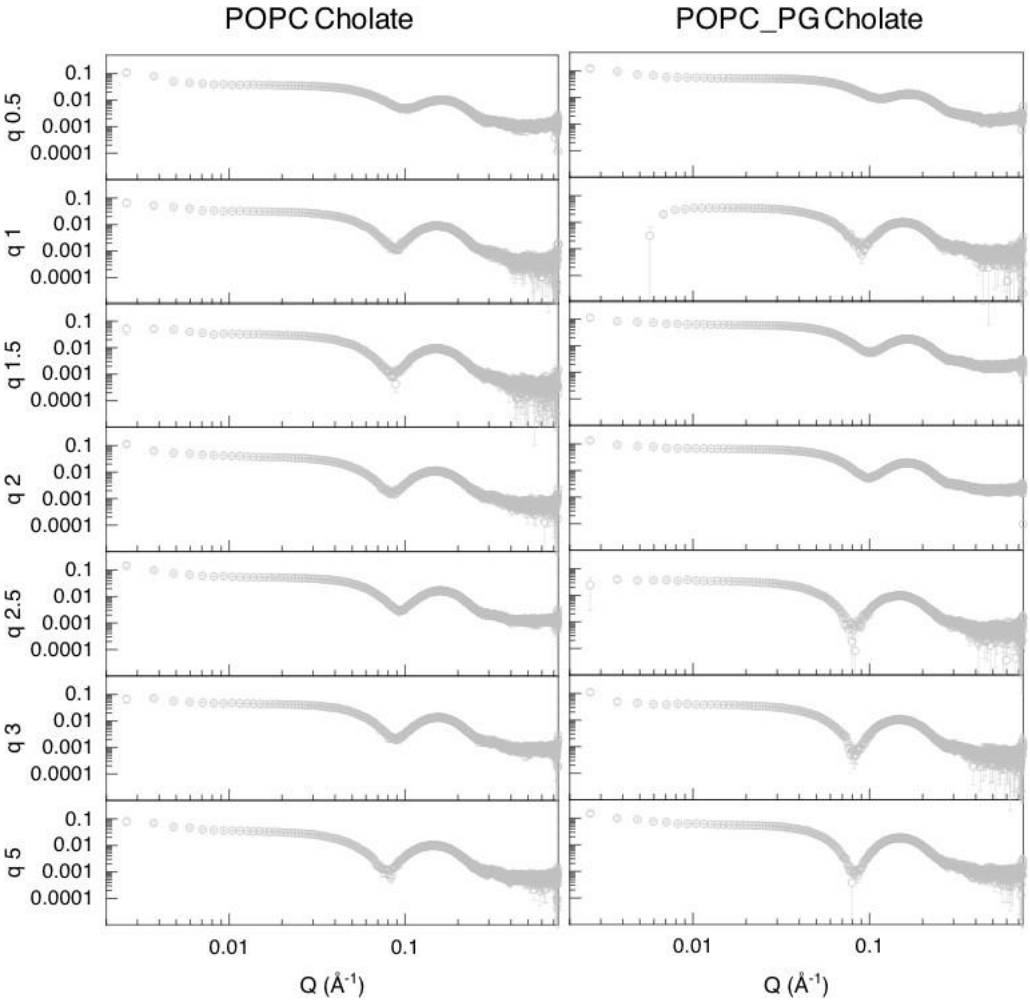


**Figure S5.** SAXS curves for the POPC and POPC-POPG (80:20) samples mixed with sodium cholate.

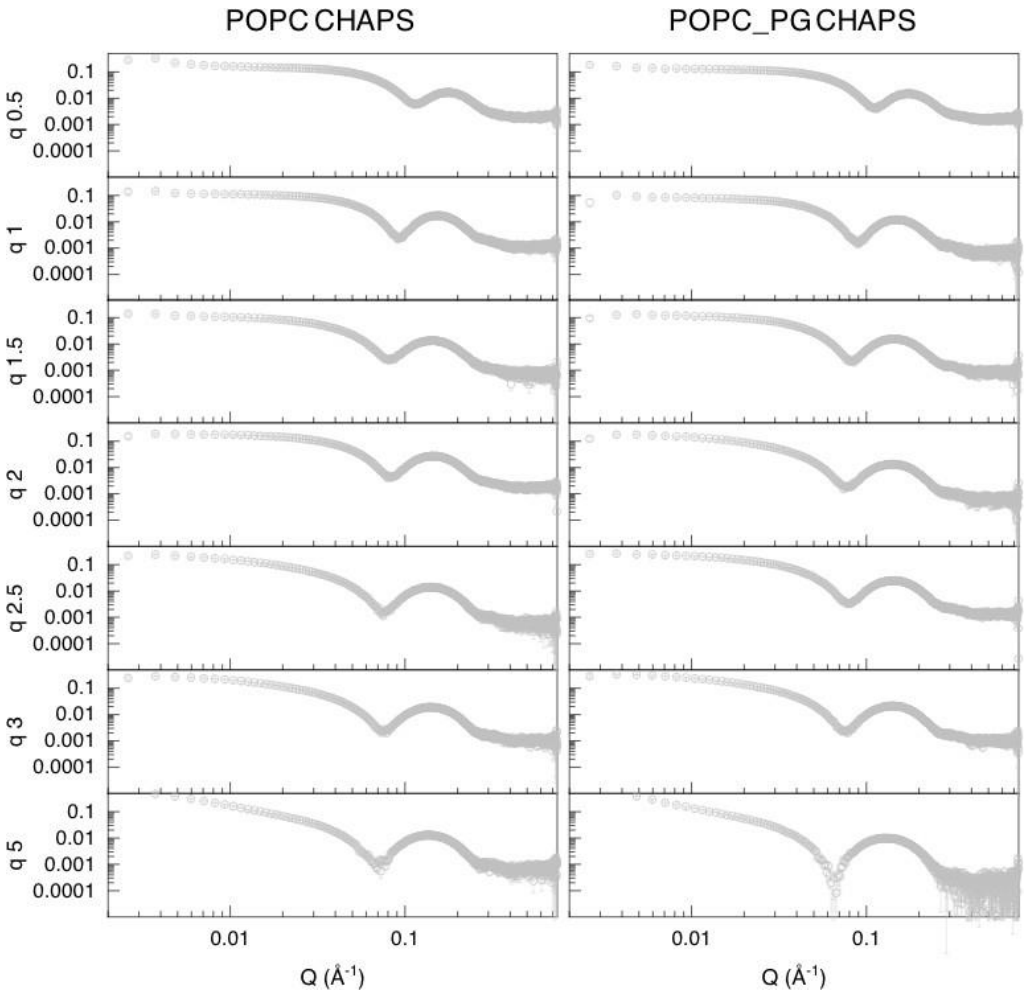


**Figure S6.** SAXS curves for the POPC and POPC-POPG (80:20) samples mixed with CHAPS.

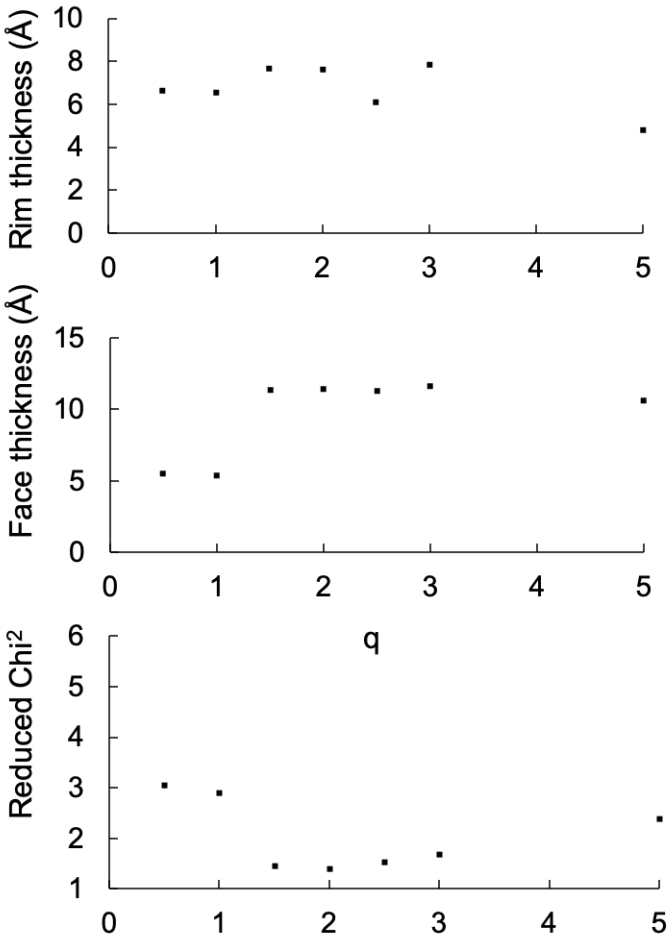


**Figure S7.** Remaining fit parameters for the POPC-DHPC fits.

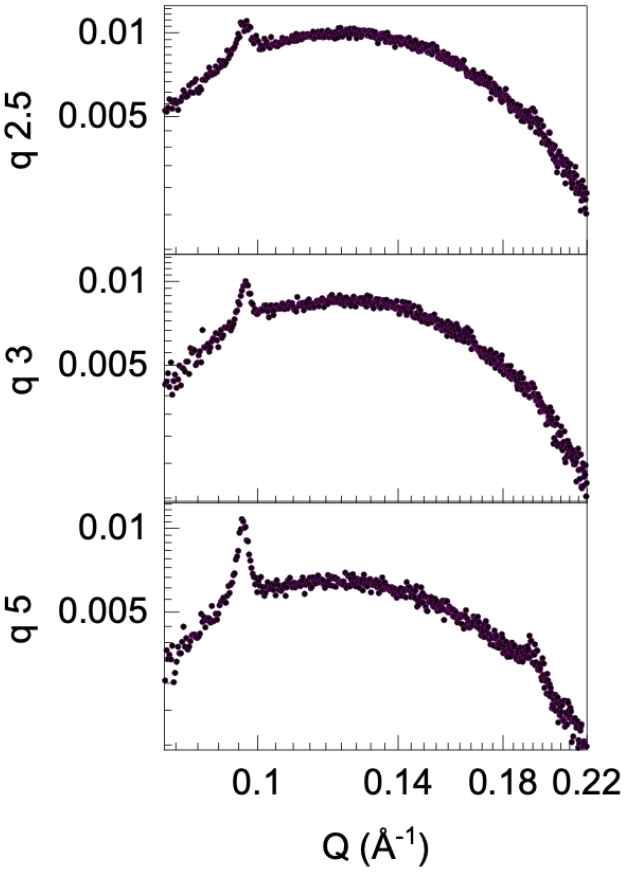


**Figure S8.** Evolution of the Bragg peaks in the POPC-DHPC sample at q = 2.5, q = 3 and q=5.