Electronic Supplementary Material (ESI) for Soft Matter.

Supplementary information

The effect of headgroup methylation on polymorphic phase behaviour in hydrated N-methylated phosphoethanolamine: palmitic acid membranes

*Matthew Allen, Yuval Elani, Nicholas J. Brooks, and John M. Seddon**

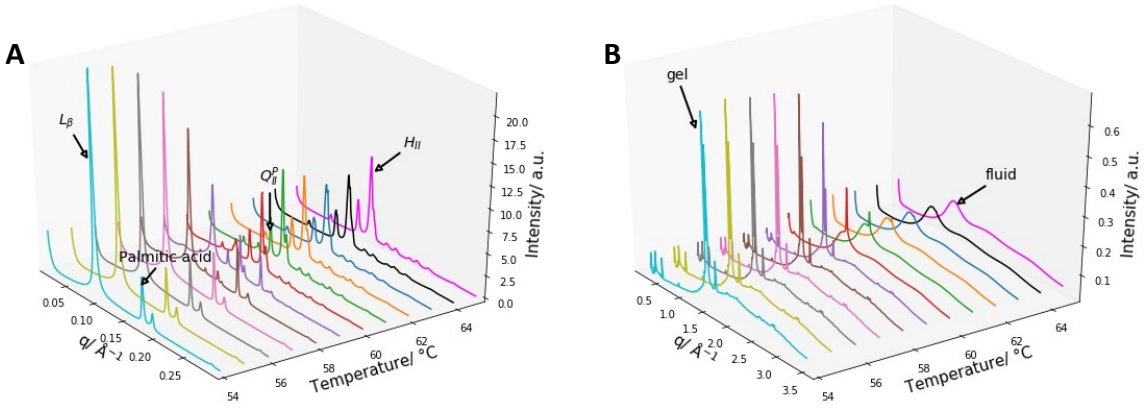

Figure S1: X-ray diffraction data of 3:1 PA: DPPE-me mixtures **A**: SAXS patterns from 54 to 65°C with identification of the main liquid-crystalline phase peaks and excess palmitic acid precipitate. **B**: WAXS patterns from 54 to 65°C with indication of the gel and fluid phases.

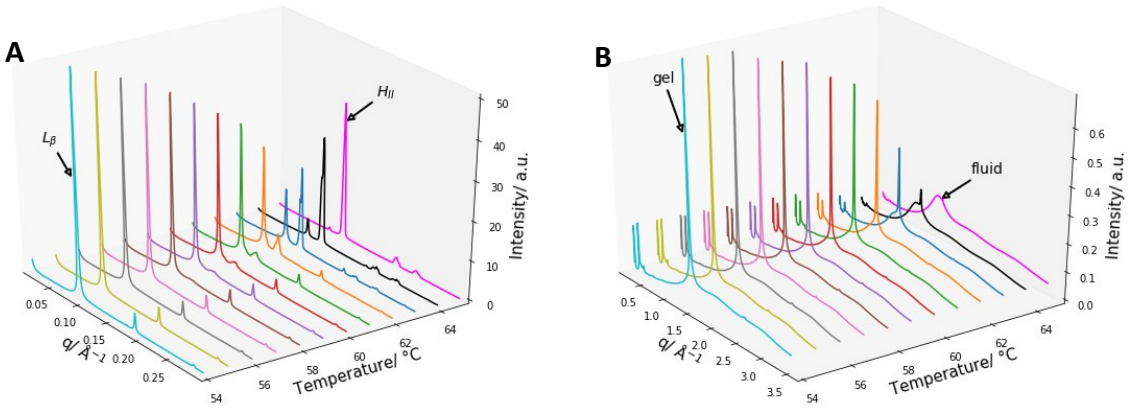

Figure S2: X-ray diffraction data of 1:1 PA: DPPE-me mixtures **A**: SAXS patterns from 54 to 65°C with identification of the main liquid-crystalline phase peaks. **B**: WAXS patterns from 54 to 65°C with indication of the gel and fluid phases.

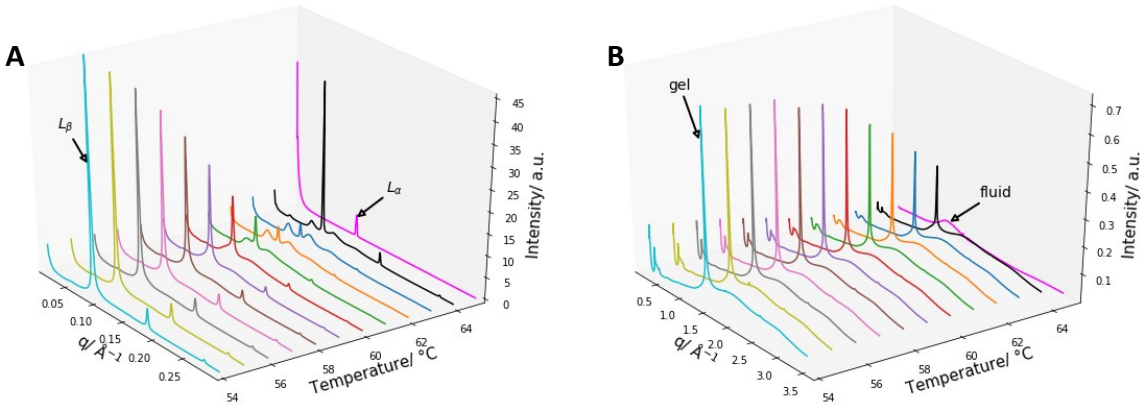

Figure S3: X-ray diffraction data of 0.5:1 PA: DPPE-me mixtures **A**: SAXS patterns from 54 to 65°C with identification of the main liquid-crystalline phase peaks. Higher order L_α peaks are present, however due to their low intensities are not visible on this scale. **B**: WAXS patterns from 54 to 65°C with indication of the gel and fluid phases.

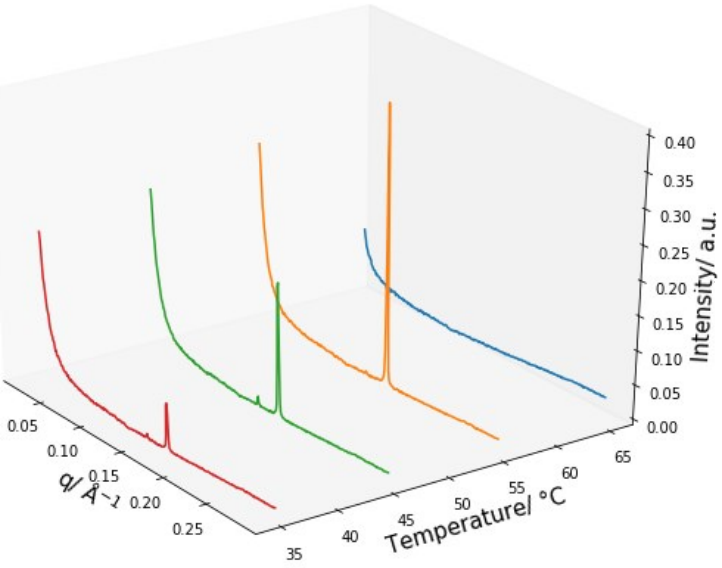

Figure S4: Pure hydrated palmitic acid SAXS patterns from 35 to 65°C. The palmitic acid peaks disappear at temperatures above the melting point due to palmitic acid melting into an isotropic liquid.

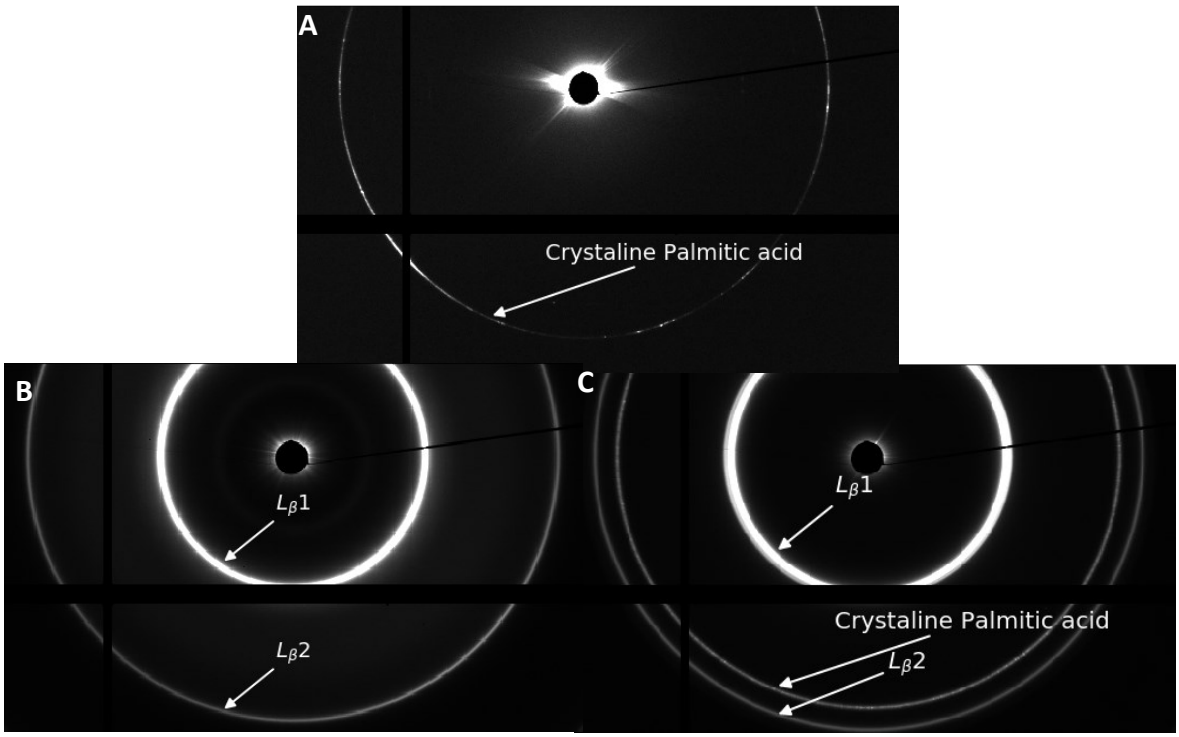

Figure S5: 2D diffraction patterns of (A) pure Palmitic acid, (B) 0.5:1 PA:DPPE-me, and (C) 2:1 PA:DPPE-me at 55°C. The extra diffraction ring within the 2:1 PA:DPPE-me pattern when compared to the 0.5:1 PA:DPPE-me sample has the same characteristic bright spots as the diffraction ring for the pure palmitic acid sample.

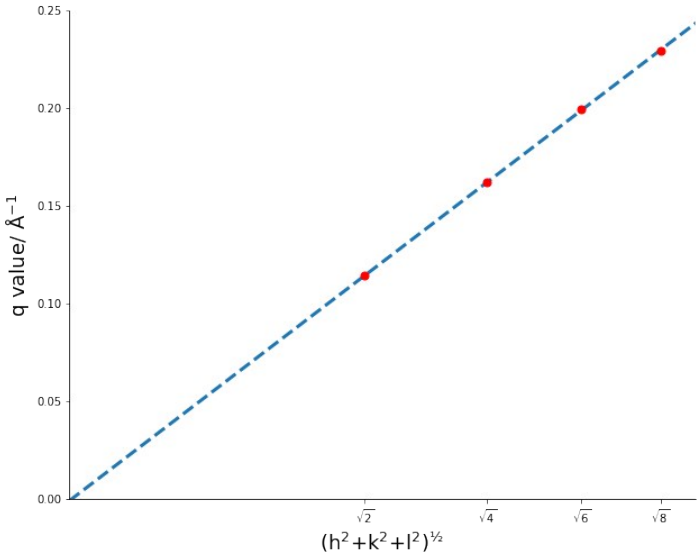

Figure S6: Plot of lattice reflection q values against the Bragg ratios for an Im3m inverse bicontinuous cubic phase in 2:1 PA: DPPE-me. The high quality of the linear fit passing through (0,0) indicates that this is a correct phase assignment. The lattice parameter for this phase was obtained by $a = \frac{2\pi}{m}$ where m is the value of the gradient. N.B the same type of plots and fitting process was used to obtain d spacing values for the L_β and H_{II} phases.

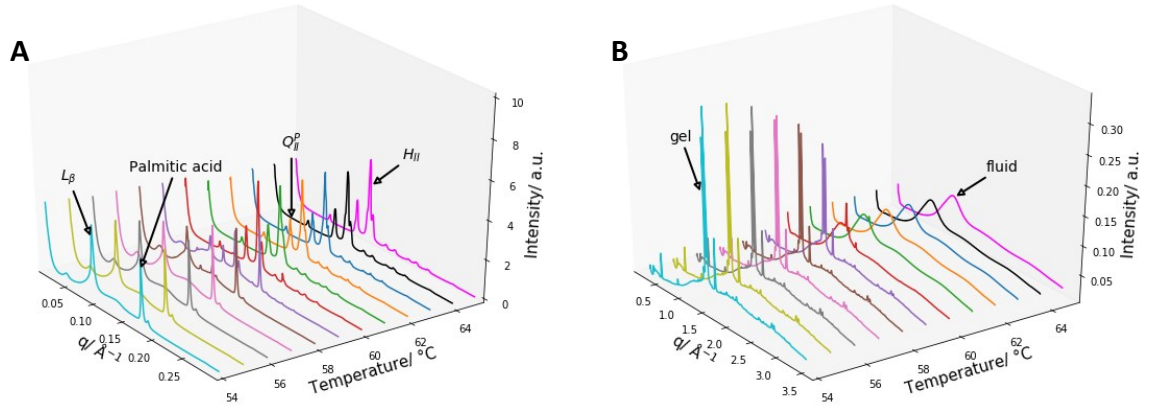

Figure S7: X-ray diffraction data of 3:1 PA: DPPE-me$_2$ mixtures **A**: SAXS patterns from 54 to 65°C with identification of the main liquid-crystalline phase peaks and the palmitic acid precipitate. **B**: WAXS patterns from 54 to 65°C with indication of the gel and fluid phases.

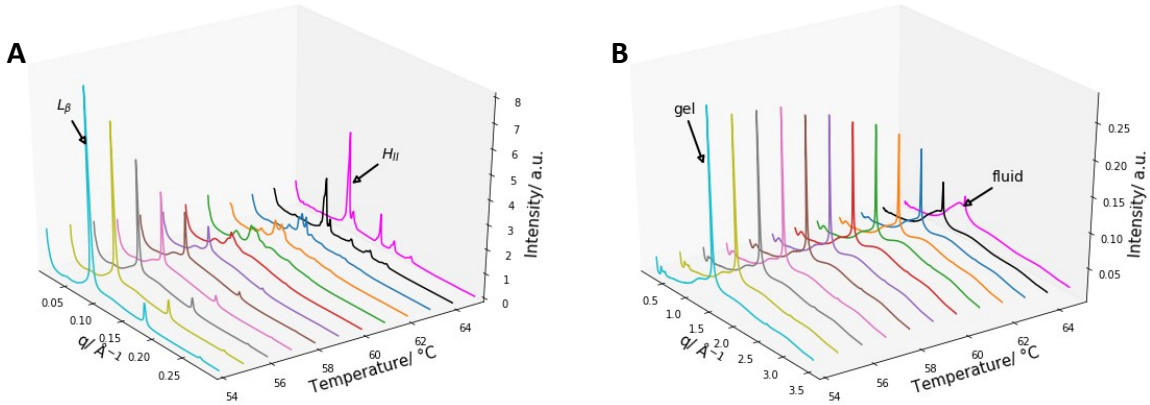

Figure S8: X-ray diffraction data of 1:1 PA: DPPE-me$_2$ mixtures. **A**: SAXS patterns from 54 to 65°C with identification of the main liquid-crystalline phase peaks. At 65°C there is a suggestion of an Im3m phase with peaks at 0.108 ($\sqrt{2}$) and 0.153 ($\sqrt{4}$); however there is too little evidence to reliably assign this phase. **B**: WAXS patterns from 54 to 65°C with characteristic indications of the gel and fluid phases.

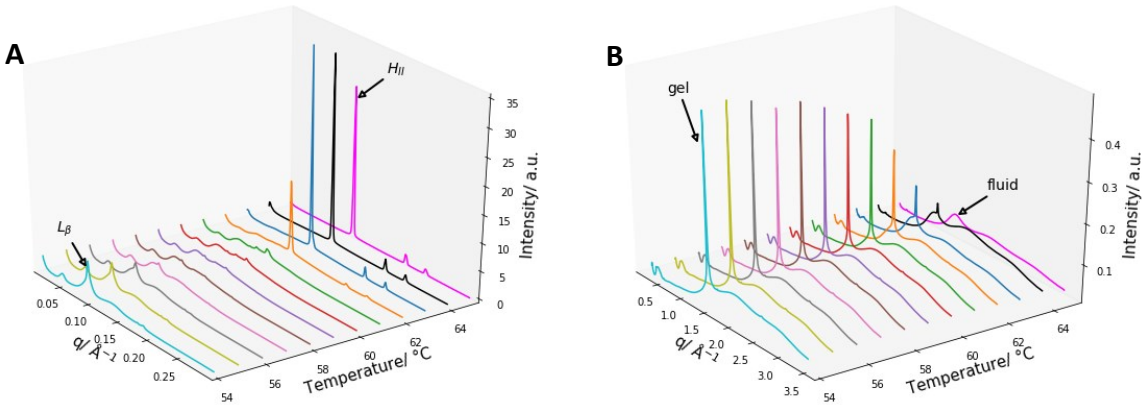

Figure S9: X-ray diffraction data of 0.5:1 PA: DPPE-me_2 mixtures. **A**: SAXS patterns from 54 to 65°C with identification of the main liquid-crystalline phase peaks. **B**: WAXS patterns from 54 to 65°C with indication of the gel and fluid phases.

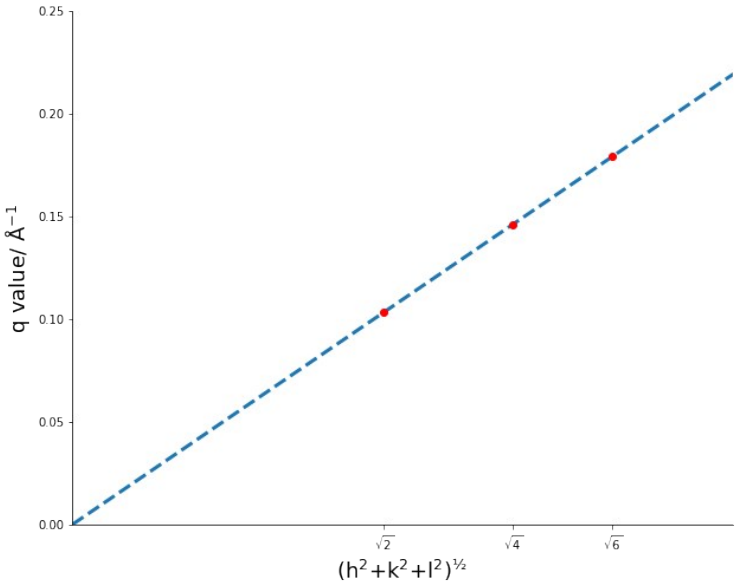

Figure S10: Plot of lattice reflection q-values against the Bragg ratios for an Im3m inverse bicontinuous cubic phase in 2:1 PA: DPPE-me_2. The high quality of the linear fit passing through the origin suggests that this is a correct phase assignment. The lattice parameter for this phase was obtained by $a = \frac{2\pi}{m}$ where m is the value of the gradient. N.B the same plots and fitting process was used to obtain d spacing values for the L_β and H_{II} phases.