Phytantriol Phase Behaviour in Choline Chloride Urea and Water Mixtures – Supplementary Information

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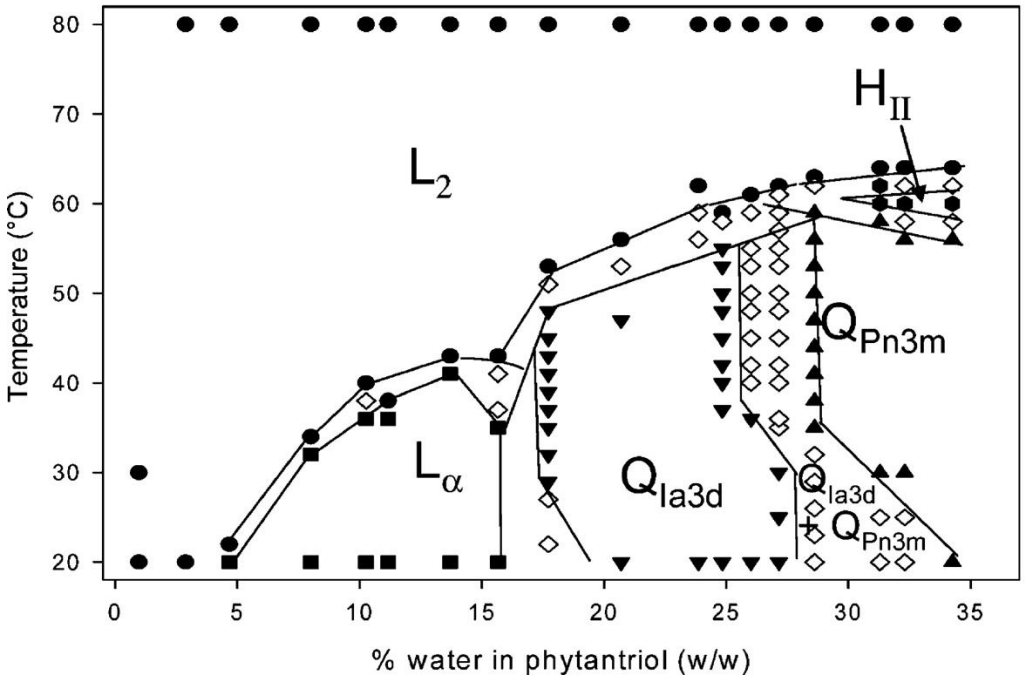


Figure S1. Phase diagram of phytantriol in water based on synchrotron SAXS.. Symbols demonstrate different phases including reverse micellar phase (L2, circles), lamellar phase (Lα, squares), gyroid bicontinuous cubic phase (QII Ia3d, downward triangles), diamond bicontinuous cubic phase (QII Pn3m, upward triangles), and reverse hexagonal phase (HII, hexagons), open diamonds denote multiphase transition regions. Reprinted with permission from [16], Copyright 2008 American Chemical Society.

Equations

Phase assignments are based on indexing the Bragg peaks in accordance with standard procedures.[65]

The inverse hexagonal phase is a two-dimensional phase with reflections indexing as:

$$d_{hk} = \frac{\sqrt{3}}{2} \frac{a}{\sqrt{(h^2 + hk + k^2)}} \quad (1)$$

Where a is the length of the unit cell and d_{hk} is the distance between adjacent reflection planes with miller indices h, k. The allowed reflections are hk = 10, 11, 20, 21, 30, 22…

For the Pn3m cubic phase, the reflections index according to:

$$d_{hkl} = \frac{a}{\sqrt{(h^2 + k^2 + l^2)}} \quad (2)$$

Different cubic phases are indexed based on restrictions to the allowed reflections. Pn3m phases must satisfy the condition $k + l = 2n$ where n is a positive integer.[65]

The lattice parameters were calculated using the python software to determine the values of a for each phase.[64]

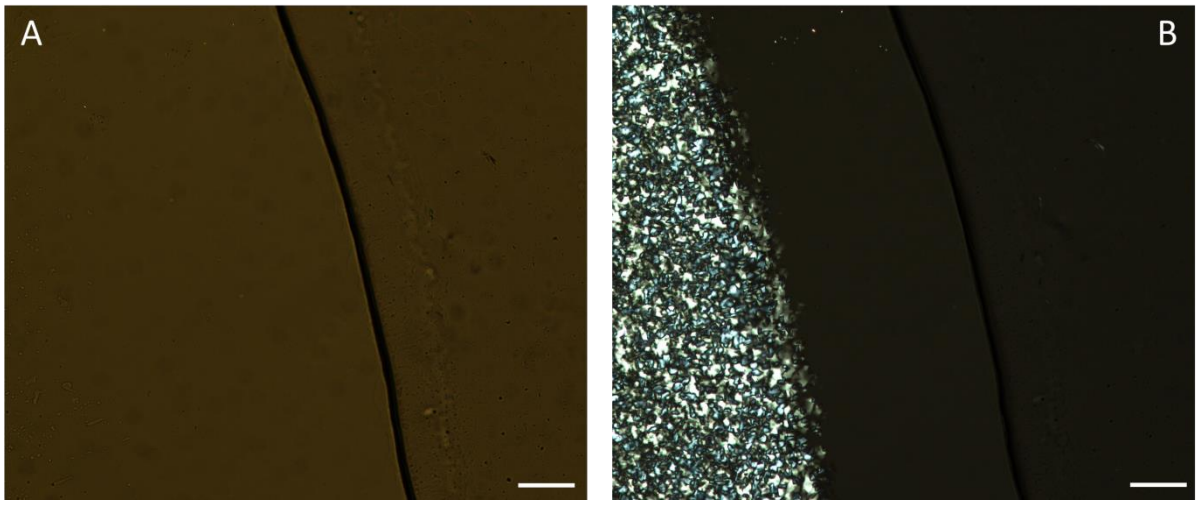


Figure S2. Cross polarised optical microscopy images of 10 wt% phytantriol in solvent composed of 40 wt% ChCl:U and 60 wt% water at 25 °C (A) and 30 °C (B). Scale bars are 100 μm.

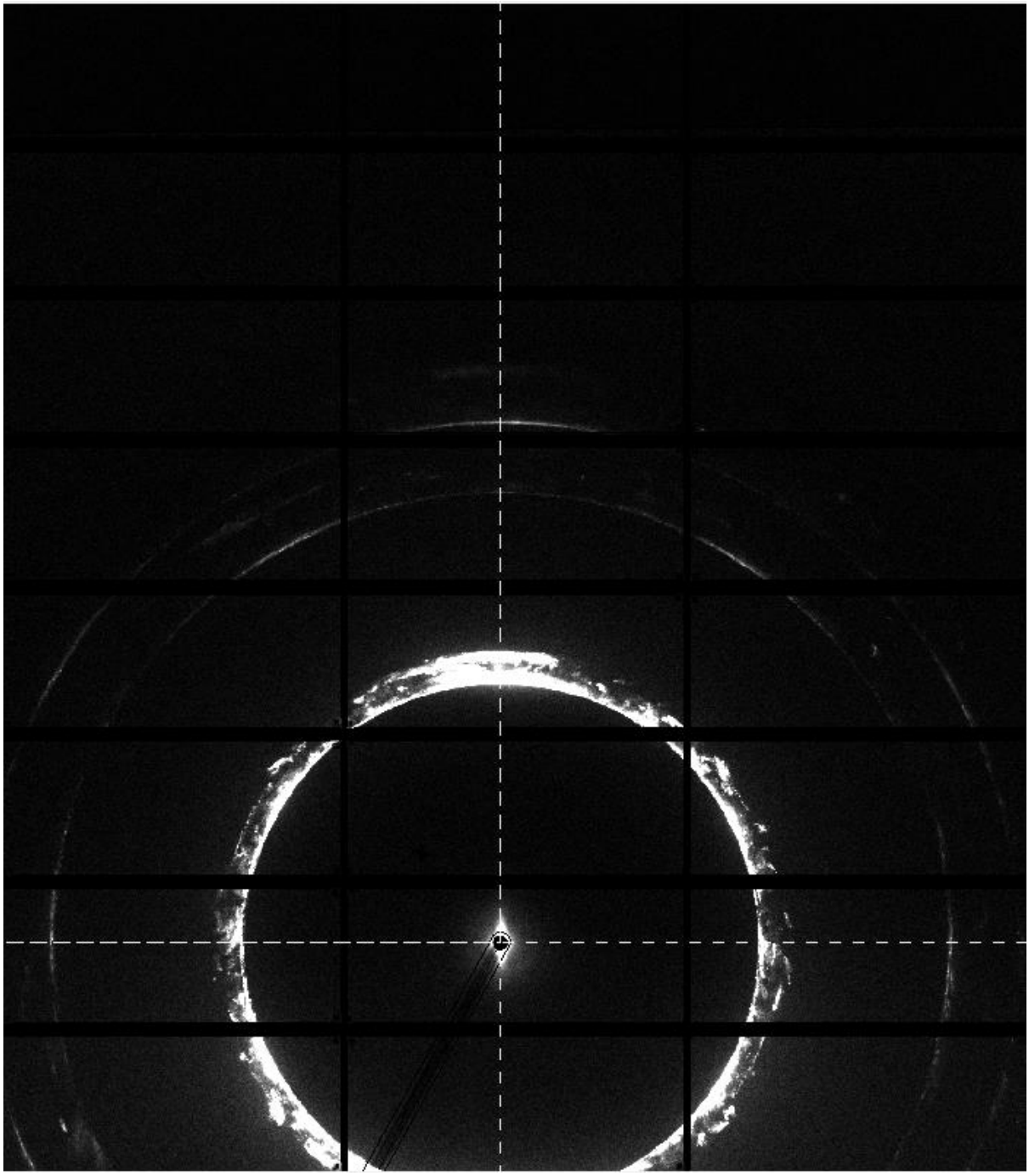
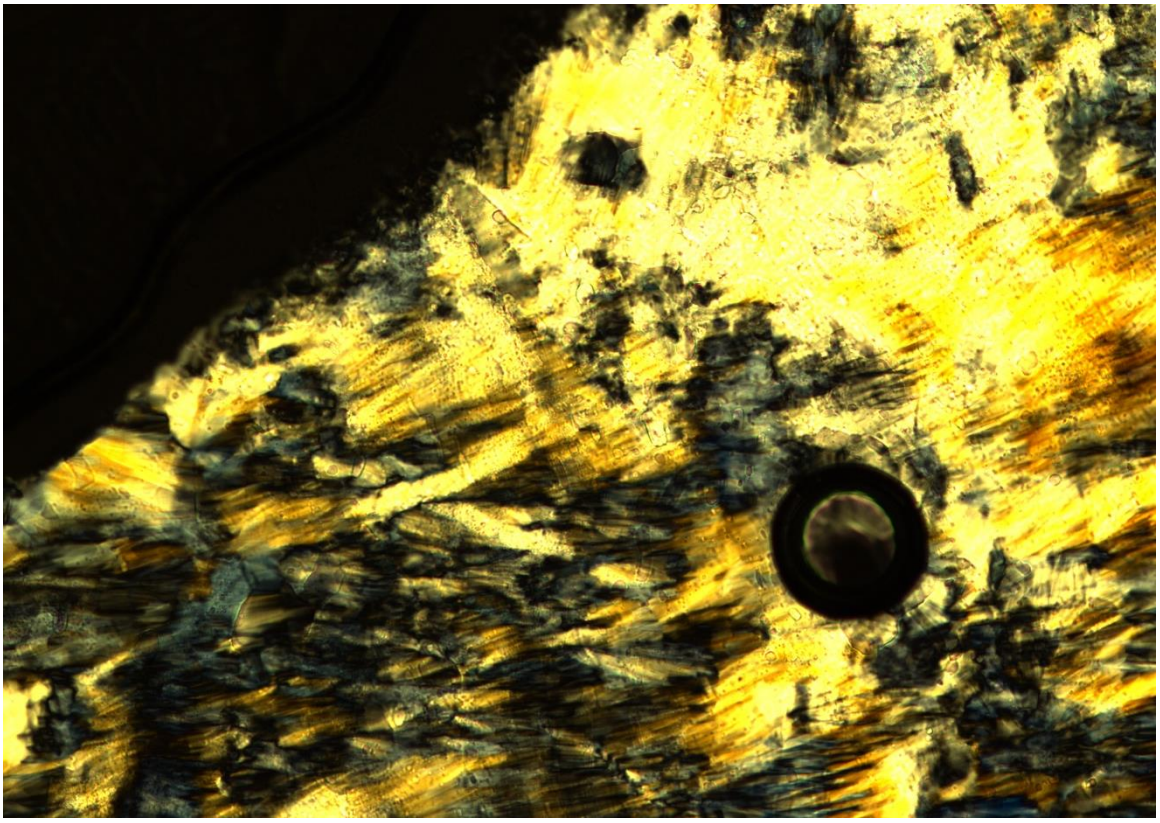


Figure S3. 2-Dimensional SAXS image from 80 wt% ChCl:U with 10 % phytantriol, demonstrated smeared primary band. (P1, A3, 55C)



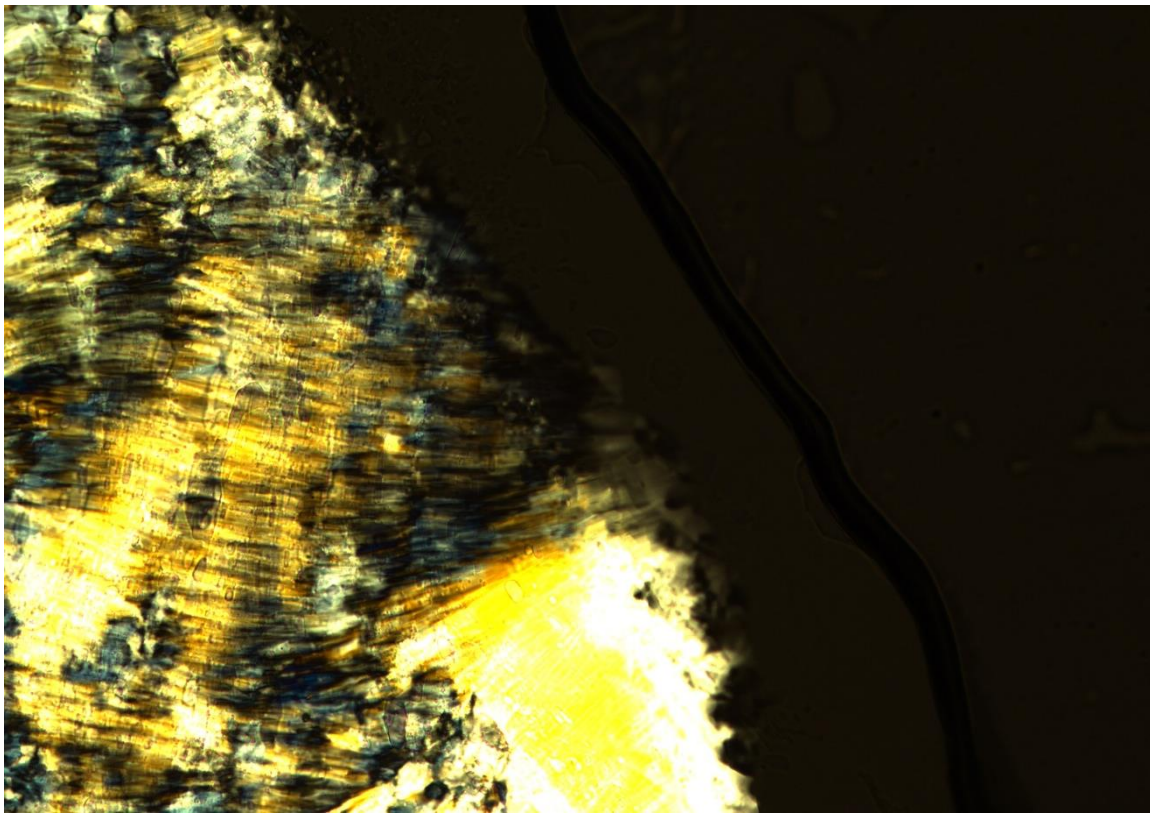


Figure S4. Cross polarised optical microscopy images of 10 wt% phytantriol in a ChCl:U/water mix with either 70 wt% ChCl:U (top) or 80% ChCl:U (bottom). Berifringent textures are indicative of a hexagonal phase.

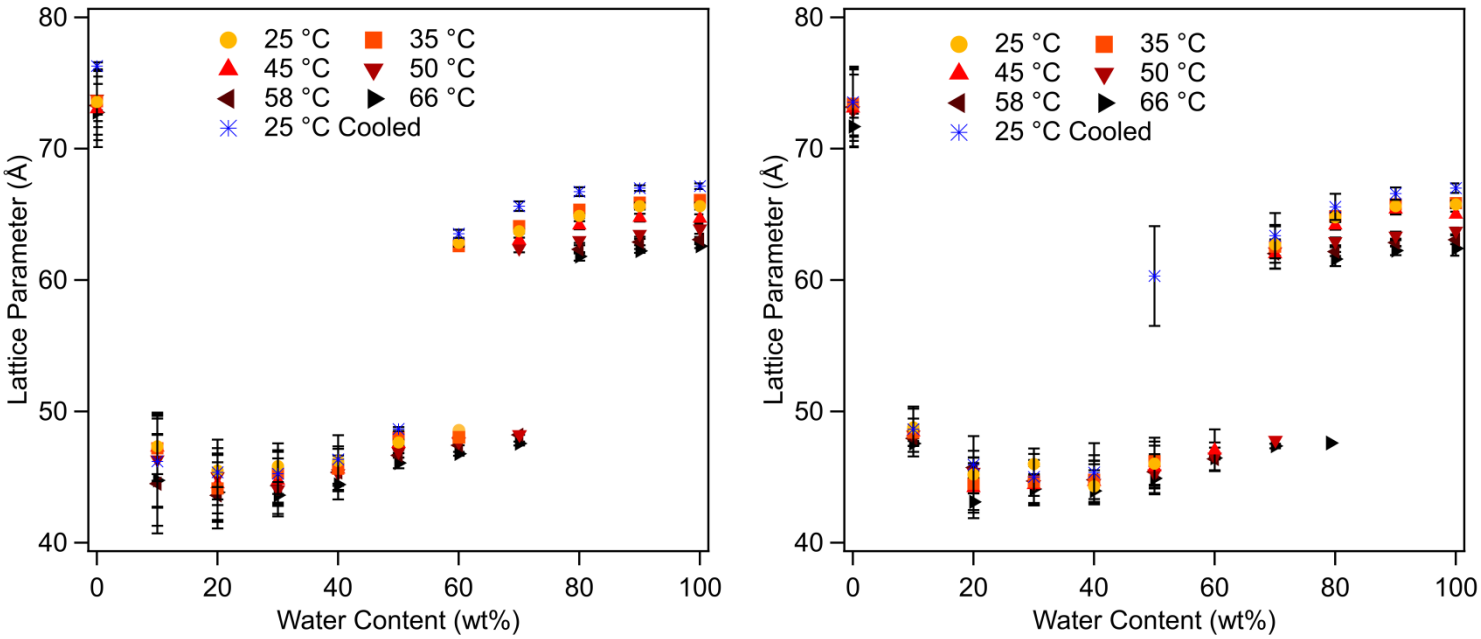


Figure S5. Lattice parameter of 10 wt% (left) and 30 wt% (right) phytantriol in ChCl:U/water mixtures at each temperature examined. Lattice parameters above 60 Å are associated with the Pn3m cubic phase while lattice parameters below 60 Å are associated with the inverse hexagonal phase. Error bars are based on the standard deviation of multiple measurements and in some cases are smaller than the symbols.