

Supporting Information for “Incorporation of the Dopamine D2L receptor and bacteriorhodopsin within bicontinuous cubic lipid phases. 2. Relevance to *in meso* crystallization of integral membrane proteins in novel lipid systems”

(1) Representative 1-D diffraction plots

In all images the {hkl} reflections corresponding to the particular lipid mesophase adopted are highlighted. Peaks corresponding to a Q_{II}^D cubic phase are indicated in normal type, peaks corresponding to a Q_{II}^G cubic phase in bold type and peaks corresponding to a H_{II} phase in italic type. For some plots the intensity has been plotted on a logarithmic scale to visualize less intense peaks.

Incorporation of dopamine D2L receptor within FE

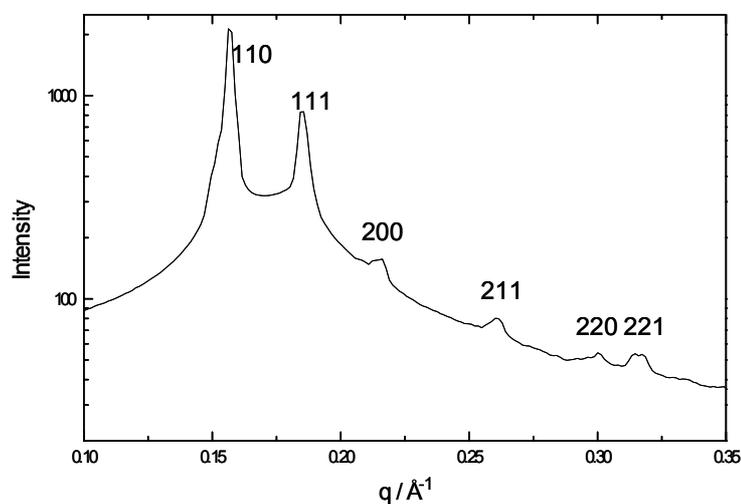


Figure S1. 1D diffraction pattern for FE 40wt% D2L receptor buffer. T=20°C. Peaks corresponding to a Q_{II}^D phase are observed.

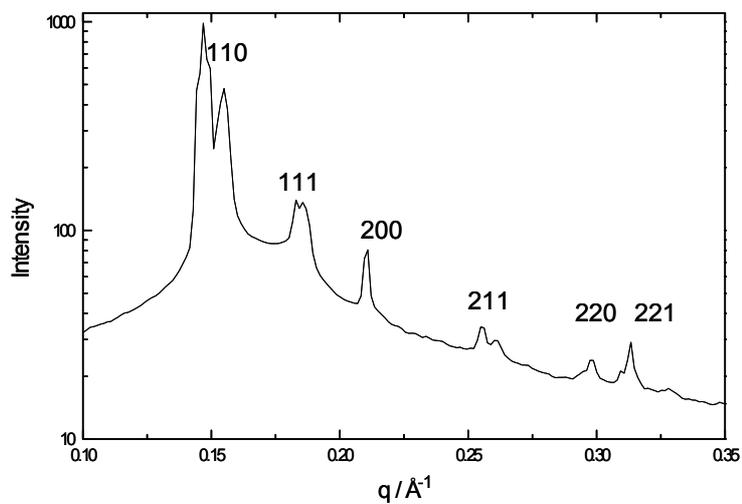


Figure S2. 1D diffraction pattern for FE 40wt% D2L receptor at 0.55 mg/ml. $T=20^{\circ}\text{C}$. Peaks corresponding to a Q_{II}^D phase are observed. The 2-D diffraction pattern is spotty resulting in split peaks.

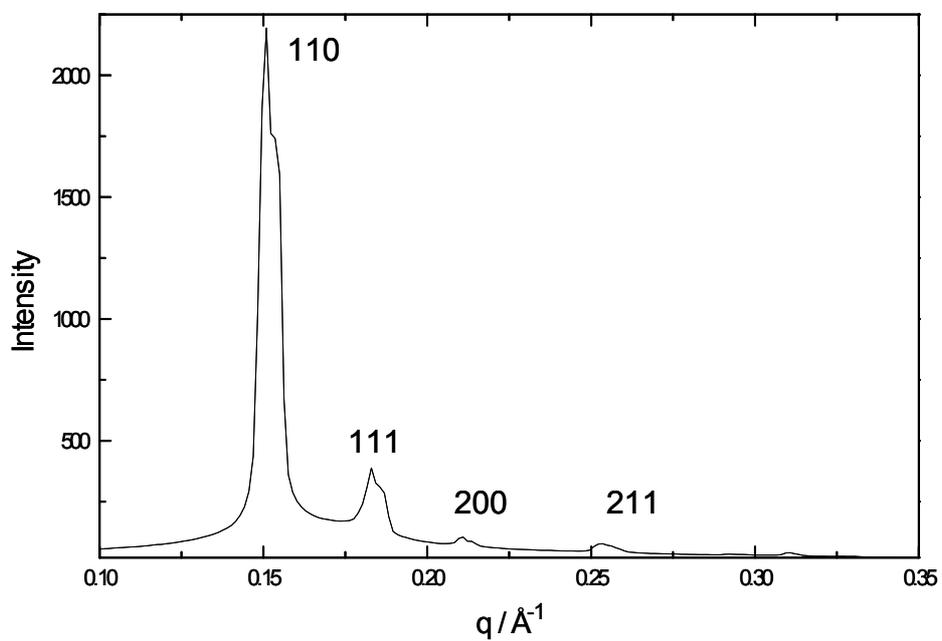


Figure S3. 1D diffraction pattern for FE 40wt% D2L receptor at 1.1 mgs/ml. $T=20^{\circ}\text{C}$. Peaks corresponding to a Q_{II}^D phase are observed. This corresponds to Fig. 4(A) but with intensity plotted on a linear axis.

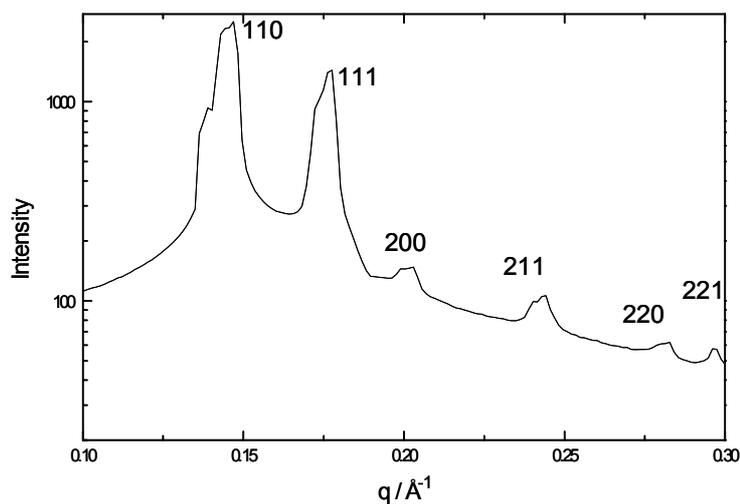


Figure S4. 1D diffraction pattern for AE 50wt% D2L receptor buffer. $T=15^{\circ}\text{C}$. Peaks corresponding to a Q_{II}^D phase are observed.

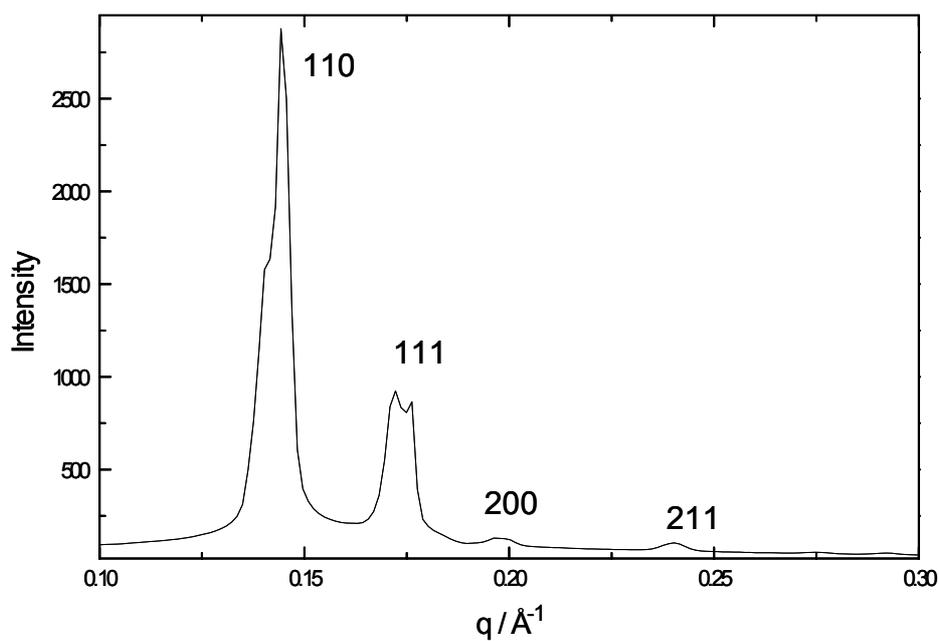


Figure S5. 1D diffraction pattern for AE 50wt% D2L receptor at 0.55 mgs/ml. $T=15^{\circ}\text{C}$. Peaks corresponding to a Q_{II}^D phase are observed. This corresponds to Fig. 4(B) but with intensity plotted on a linear axis.

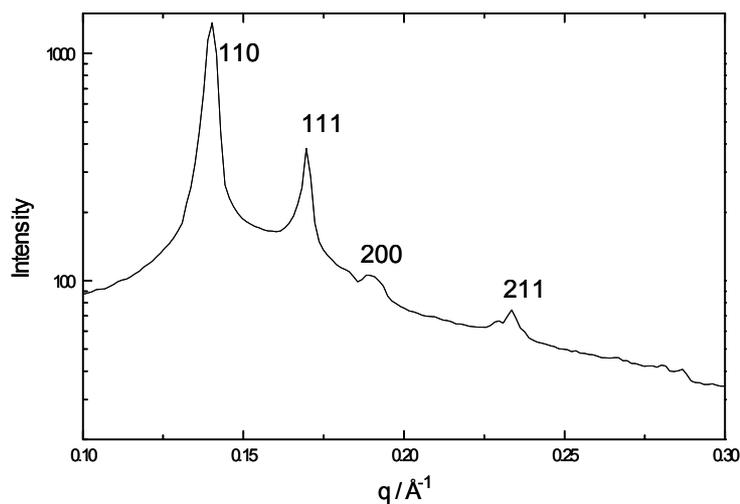


Figure S6. 1D diffraction pattern for AE 50wt% D2L receptor at 1.1 mgs/ml. $T=15^{\circ}\text{C}$. Peaks corresponding to a Q_{II}^D phase are observed.

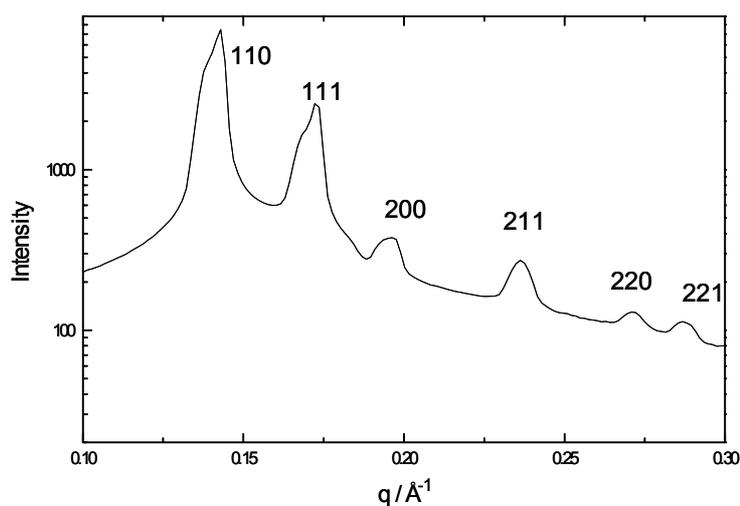


Figure S7. 1D diffraction pattern for AE 50wt% D2L receptor at 2.2 mgs/ml. $T=15^{\circ}\text{C}$. Peaks corresponding to a Q_{II}^D phase are observed.

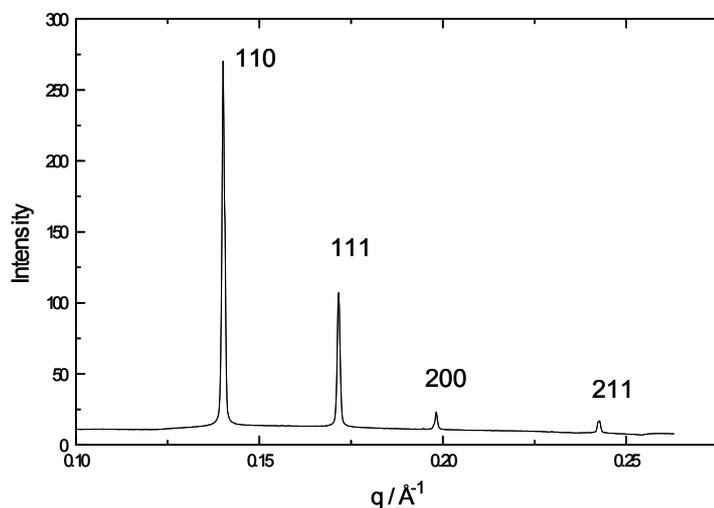


Figure S8. 1D diffraction pattern for FE 40wt% Na K phosphate buffer. $T=20^{\circ}\text{C}$.

Peaks corresponding to a Q_{II}^D phase are observed

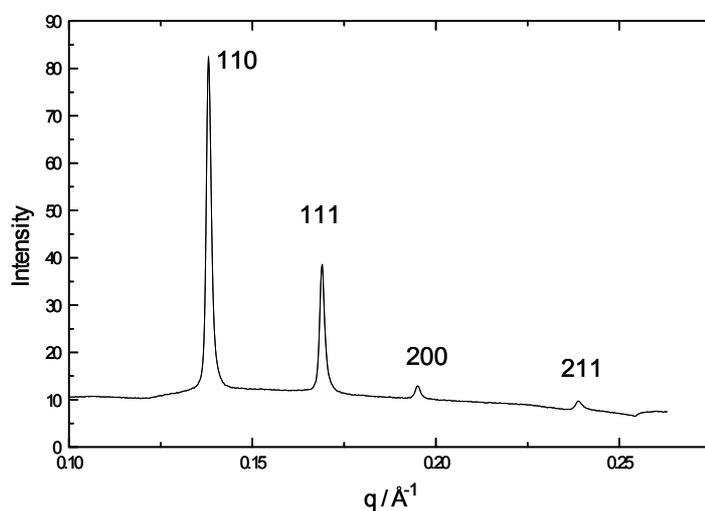


Figure S9. 1D diffraction pattern for FE 40wt% bR at 12 mgs/ml. $T=20^{\circ}\text{C}$. Peaks corresponding to a Q_{II}^D phase are observed.

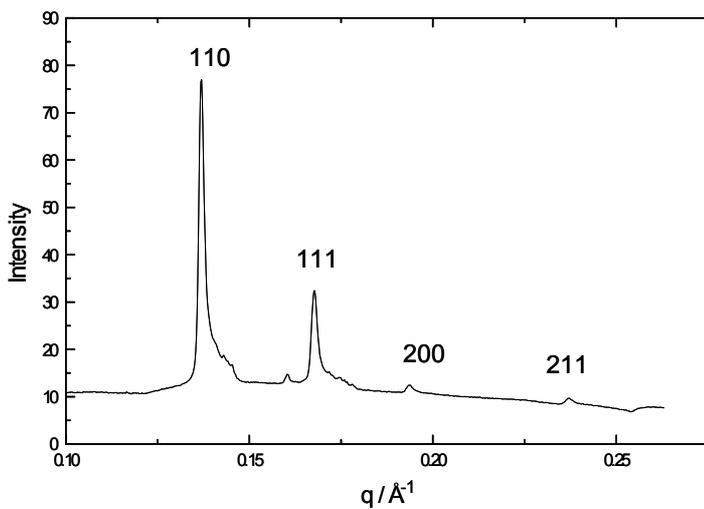


Figure S10. 1D diffraction pattern for FE 40wt% bR at 18 mg/ml. $T=20^{\circ}\text{C}$. Peaks corresponding to a Q_{II}^D phase are observed. Some additional peaks indicate an element of disorder within the sample at this protein concentration.

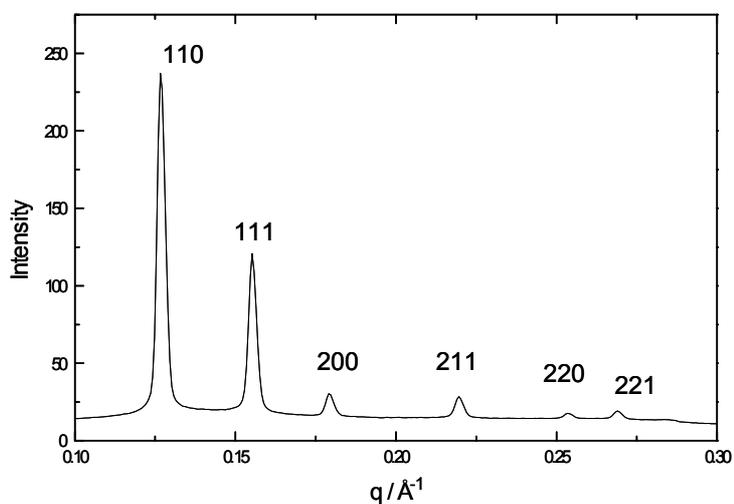


Figure S11. 1D diffraction pattern for AE 50wt% bR at 9 mg/ml. $T=9^{\circ}\text{C}$. Peaks corresponding to a Q_{II}^D phase are observed.

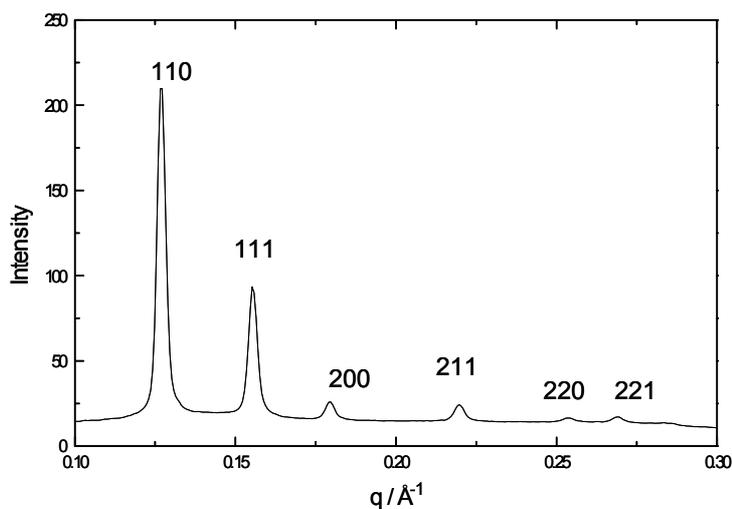


Figure S12. 1D diffraction pattern for AE 50wt% bR at 18 mgs/ml. $T=9^{\circ}\text{C}$. Peaks corresponding to a Q_{II}^D phase are observed.

(2) Analysis of bilayer thickness and water channel radius

For a sample of known sample composition, lipid length, l , was calculated from the lattice parameter, a , by using Eq. 1¹⁸

$$\Phi_l = 2A_0 \left(\frac{l}{a} \right) + \frac{4\pi\chi}{3} \left(\frac{l}{a} \right)^3 \quad (1)$$

Where Φ_l is the percentage of lipid by volume within the sample, and A_0 and χ are the dimensionless surface area and the Euler characteristic of the specific cubic phase [$A_0 = 3.091$ (Q_{II}^G); 1.919 (Q_{II}^D) and $\chi = -8$ (Q_{II}^G) and -2 (Q_{II}^D)].

Φ_l , the percentage of lipid by volume within the sample, is calculated from the known sample composition, c , using Eq. 2¹⁹ where $\Phi_l = 1 - \Phi_w$, the water density $\rho_w = 1\text{g/cm}^3$ and the density of the lipid sample ρ_L . $\rho_{AE} = 0.92\text{g/cm}^3$. ρ_{FE} is not known but is assumed to be the same as phytantriol (Phy) which has a similar branched structure $\rho(\text{Phy}) = 0.94\text{g/cm}^3$.

$$\Phi_w = \frac{c}{c + (1-c) \frac{\rho_w}{\rho_L}} \quad (2)$$

The water channel radius, r_w , may then be calculated using Eq. 3.¹⁸

$$r_w = \sqrt{\frac{-A_0 a^2}{2\pi\chi}} - l \quad (3)$$