Molecular dynamics of anhydrous glycolipid self-assembly in lamellar and hexagonal phases.


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Supporting Information

Fig. S1. Structural properties from MD simulation of 2-decyl-tetradecyl-β-D-maltoside (C14-10G2) in the smectic (T=348K) and columnar (T=433 K) phases (a) The local density profiles of headgroup (turquoise), tail (magenta) and total (red) in the smectic phase and z is distance along the normal to the smectic layer (b) The local density profiles of headgroup (turquoise), tail (magenta) and total (red) in the columnar phase, and r is the radial distance measured from the center of a selected column; (c) The radial distribution functions of the center of mass of the glycolipid molecules in smectic (red) and columnar (green) phases.
Fig. S2. (a) The average mean square displacement ($\Delta r^2$) versus time in smectic phase (red) and columnar phase (green) of 2-decyl-tetradecyl-β-D-maltoside (C_{14-10}G_2) at 348 K and 433 K respectively. (b) The average mean square displacement ($\Delta r^2$) versus time in smectic phase (extended y-axis).

Fig. S3. The distribution of tilt angles $\alpha$ and $\beta$ versus time obtained during the REMD simulation of 2-decyl-tetradecyl-β-D-maltoside (C_{14-10}G_2) in the smectic phase at 348 K.
**Fig. S4.** The graphical representations of 2-decyl-tetradecyl-β-D-maltoside (C\textsubscript{14}10G\textsubscript{2}) in the sugar head region of smectic phase from the final REMD configurations at temperatures (a) 348 K, (b) 373 K, (c) 428 K and (d) 443 K.
Fig. S5. The fluctuation of the average tilt angle $\theta$ (which is the angle made by the sugar head vector with the column axis) over time of 2-decyl-tetradecyl-$\beta$-D-maltoside (C$_{14-10}$G$_2$).