Electronic Supplementary Material for:

Effect of Monoglycerides and Fatty Acids on Ceramide Bilayer

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Tilt angle distribution

In order to distinguish between isotropic distribution of the molecular tilt and the molecular tilt being close to the magic angle, we calculated the probability distribution of the tilt angle θ_z for different atoms. Figure S1 shows the tilt angle distribution for OA, LA, MA and ME in the CER2 bilayer (the mole fraction of monoglycerides or fatty acids were 0.2 for each of these systems). The distributions are shown for the atoms n = 7 – 12 (to cover and compare the angles near the double bonds). The distributions clearly illustrate that for the saturated and *trans*-unsaturated oils (i.e. MS and ME) the tilt angle is sampled mostly at 10-15° (and 165-170°), while near the *cis*-double bonds (ex. in OA and LA) the distributions become somewhat broader and shift towards the magic angle. For LA, the widths of the angle distributions for atoms 10 and 12 are very similar. However, the distribution is peaked around 50° for atom 10 and about 15° for atom 12. Thus the reduction in S_z from 0.65 (for atom 12) to 0.3 (for atom 10) is entirely due to the tilt angle being close to the magic angle.

The distributions for the tilt angle for the long tail of CER2 at X_{MO} = 0.3 and 0.5 are given in the Figure S2. At X_{MO} = 0.3 (when the mixed bilayer is stable and well-ordered) the angles are mostly peaked at 10°, while at X_{MO} = 0.5, the concentration at which the bilayer disintegrates, the angles are distributed practically uniformly. This indicates an almost complete loss of the order in the system.

The distributions for the tilt angle for the terminal tail atoms (n = 2 – 6) are shown in Figure S3 for monostearin at X_{MS} = 0.2. The distributions show the broadening of the angle distributions towards the end of the tail, indicating increasing disorder of the tails near the bilayer midplane.

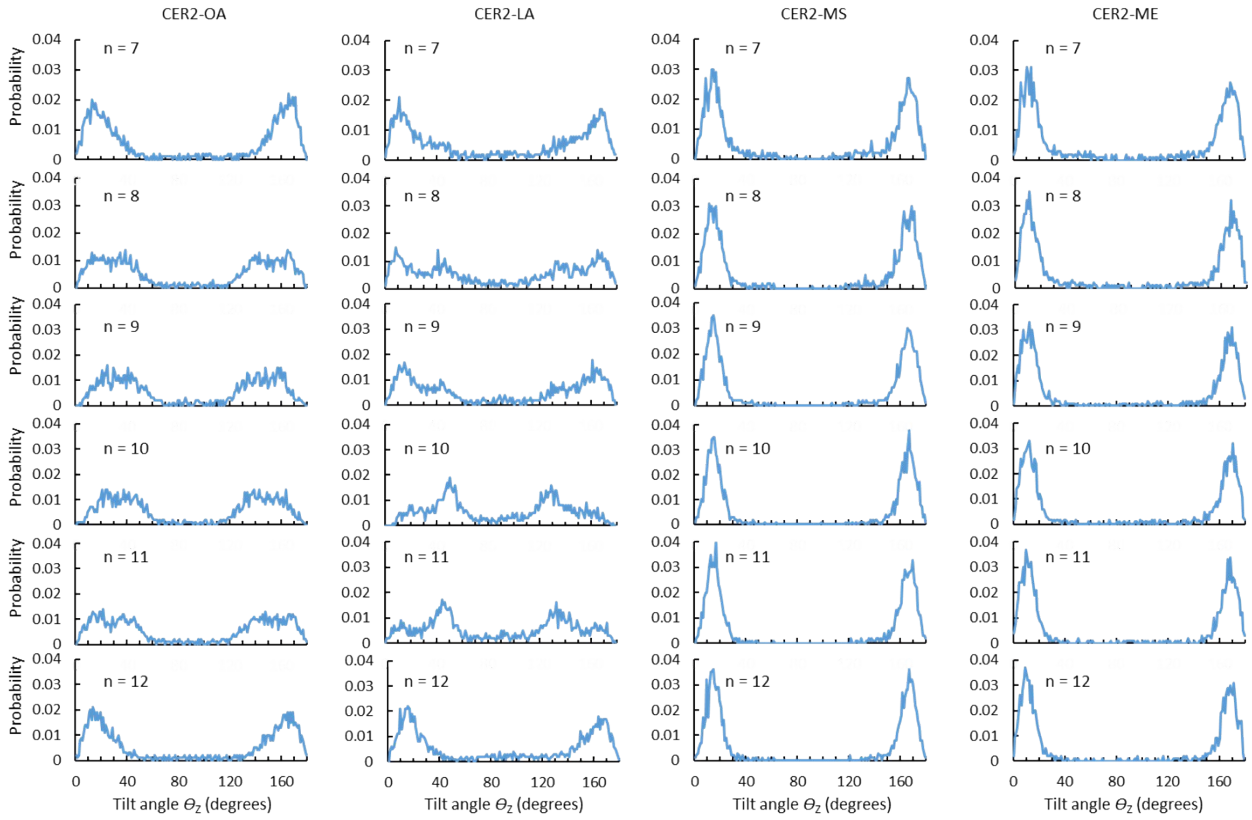

Figure S1. The tilt angle distribution for atoms n = 7 – 12 in the tail of monoglycerides and fatty acids indicated on the graph. The data are obtained at the mole fraction of oils X_{OIL} = 0.2.

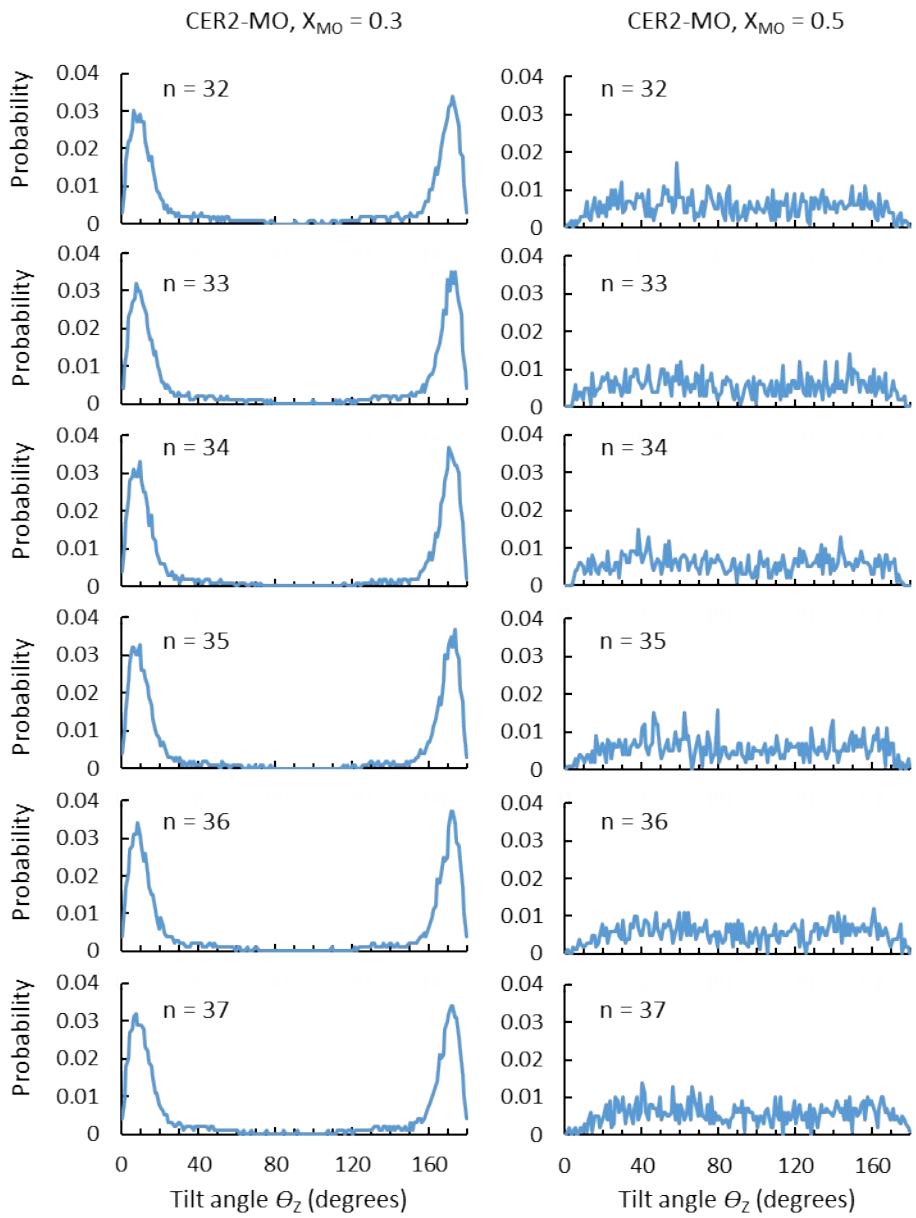

Figure S2. The tilt angle distribution for the middle tail atoms n = 32 – 37 in the long tail of CER2 for MO mole fractions X_{MO} = 0.3 and 0.5.

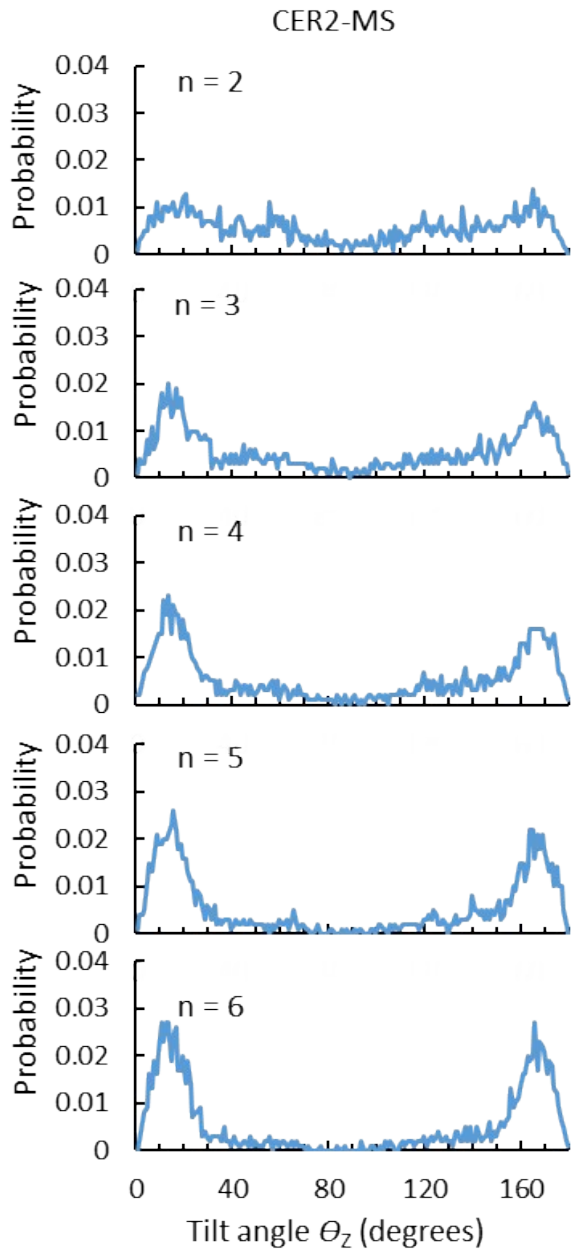

Figure S3. The tilt angle distribution for end tail atoms n = 2 – 6 of monostearin at the mole fraction of MS X_{MS} = 0.2.