

SUPPLEMENTARY INFORMATION

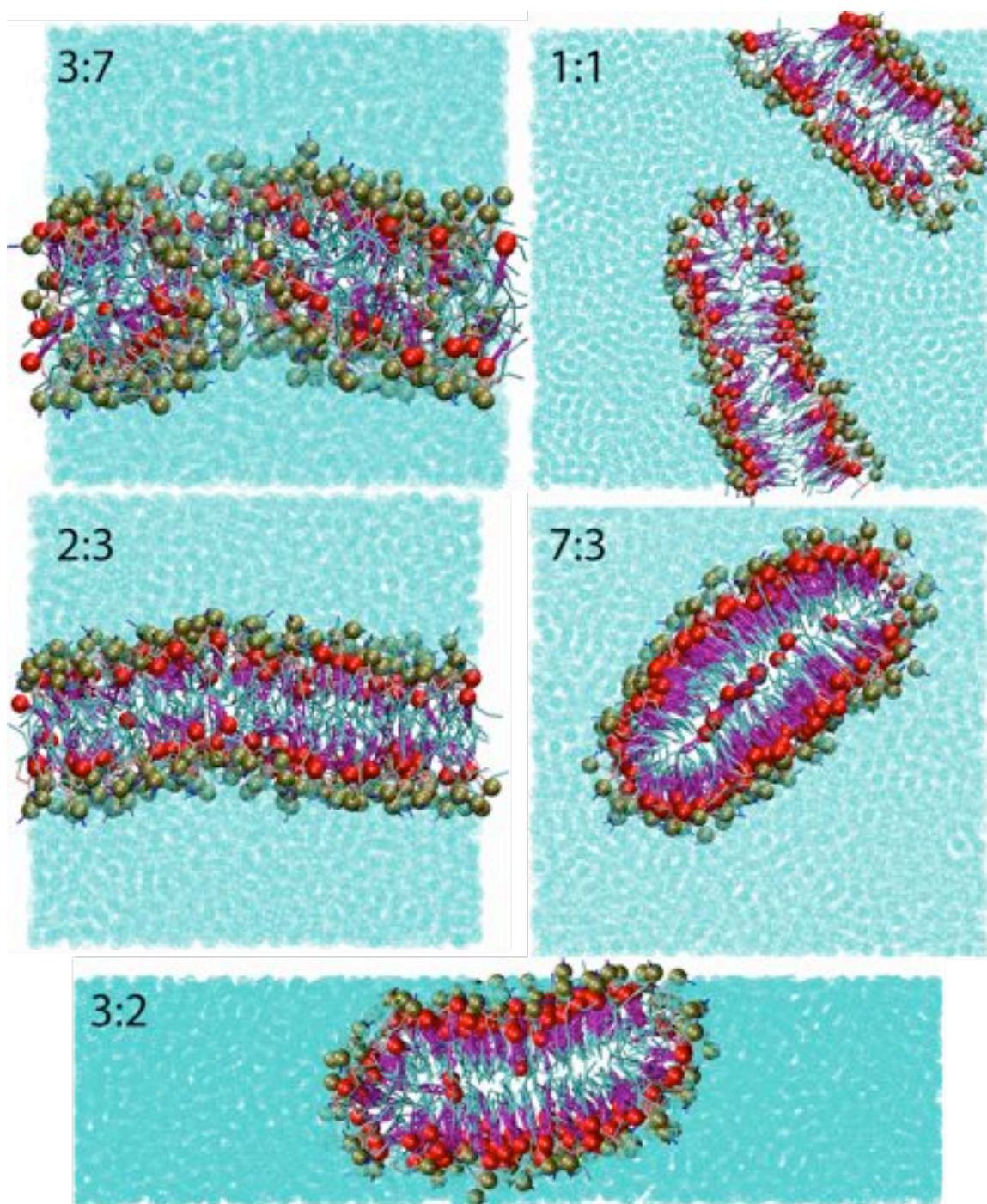


Figure S1: Final simulation snapshots from the CHOL:PGHC self-assembly simulation at the various CHOL:PGHC ratios.

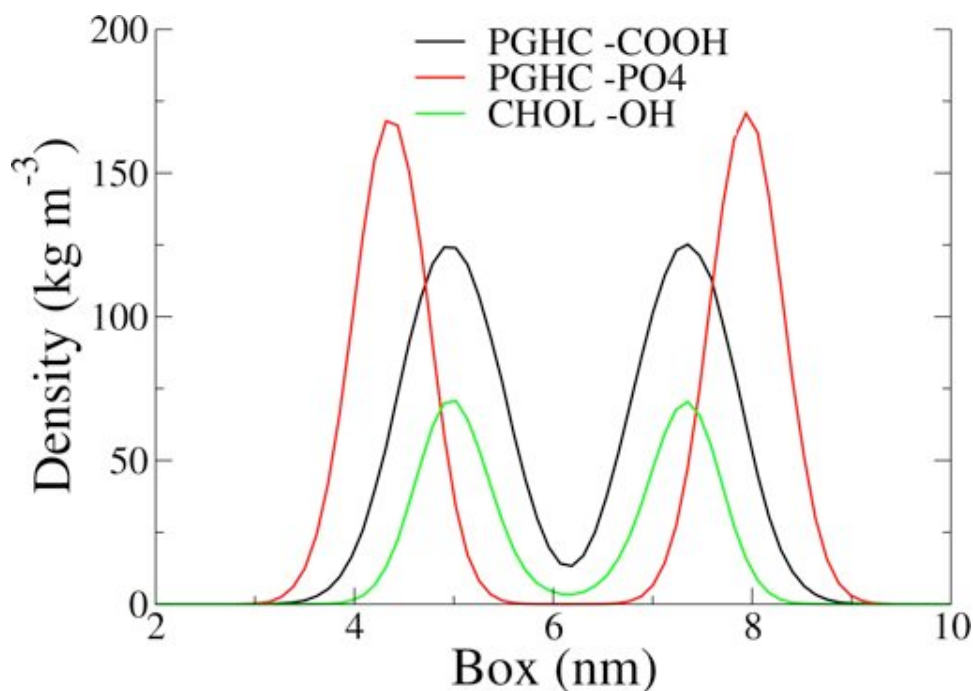


Figure S2: Density profiles along the bilayer normal for the CHOL+PGHC self-assembly simulation at CHOL:PGHC= 2:3. The cholesterol headgroup is at the same bilayer depth as the reoriented carboxyl group of PGHC. The non-zero density at the bilayer centre for the COOH group shows that not all the COOH reverse their orientation in the bilayer. The non-zero density of the cholesterol headgroup at the bilayer centre is a result of cholesterol flip-flop