Supporting Information for:

How do Ethanolamine Plasmalogens Contribute to Order and Structure of Neurological Membranes?

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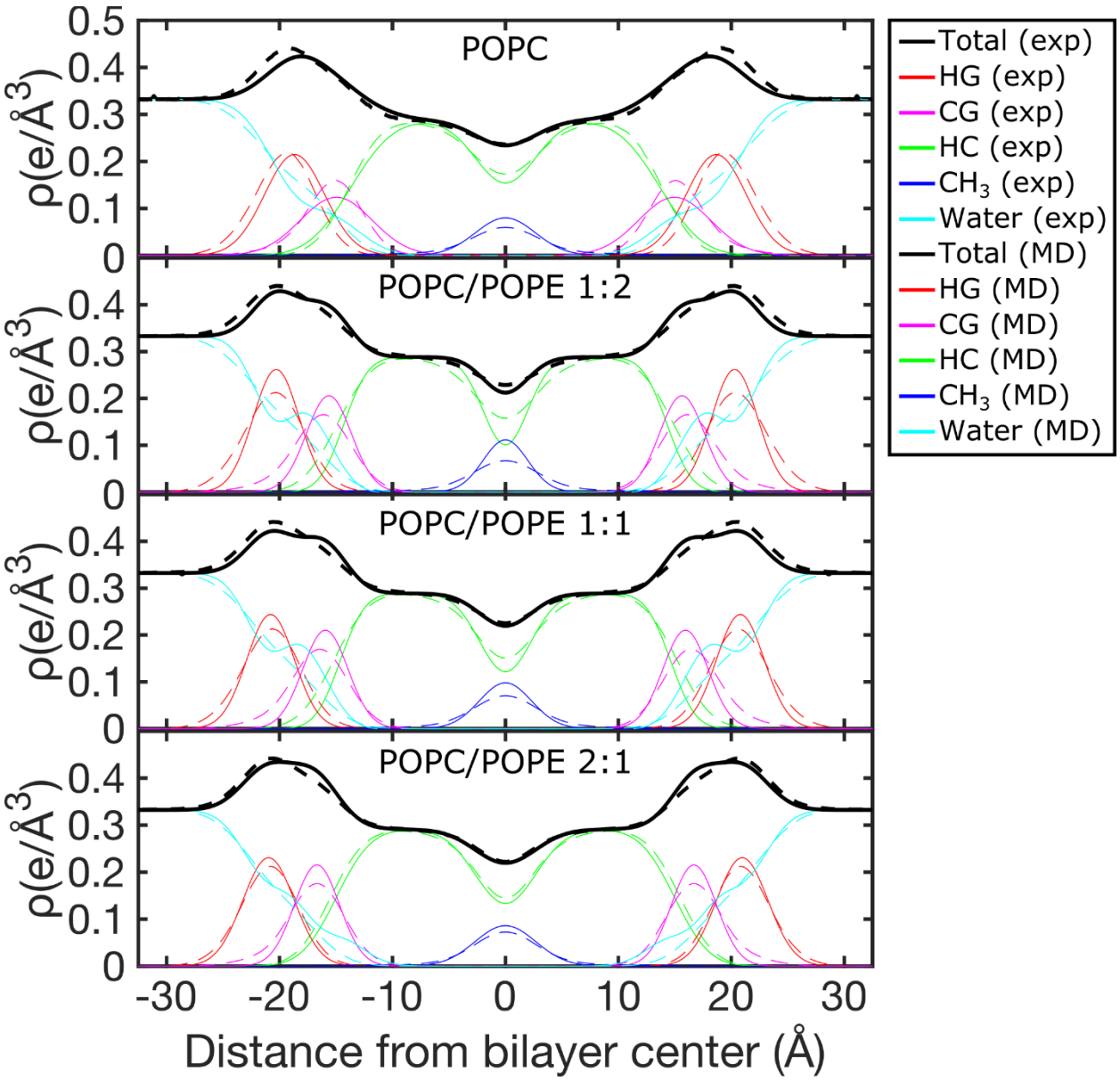

Figure S1. Electron density profiles based on the SDP model fit to $F(q_z)$ for the phosphate (Phos), carbonyl-glycerol (CG), hydrocarbon (HC) without the methyl and methyl (CH_3) groups. The water fills in the remaining volume. MD simulations are in dashed lines with POPC taken from a previous publication at 40°C.[1]

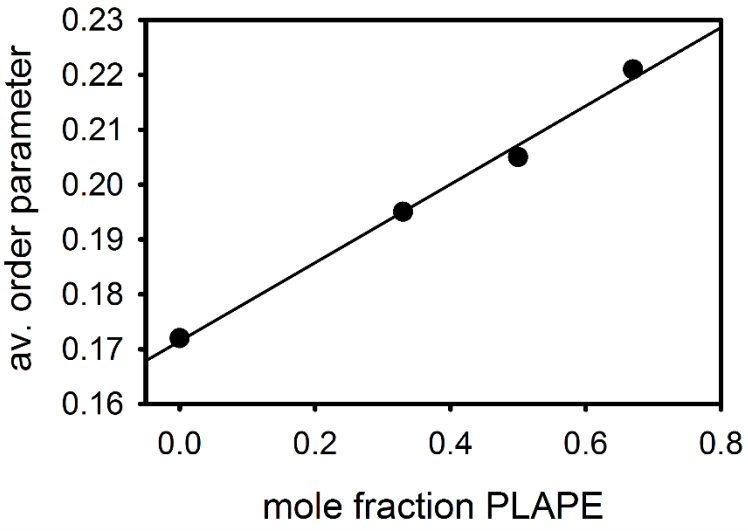

Figure S2. Average order parameters of the palmitoyl chain of POPC-d_{31} in POPC-d_{31}/PLAPE mixtures as a function of the mole fraction of PLAPE.

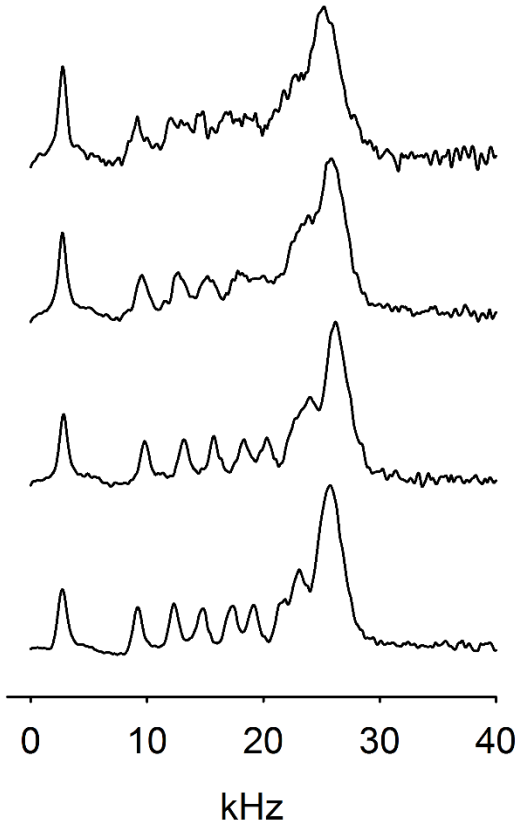

Figure S3. DePaked ^{2}H-NMR spectra of POPC-d_{31}/PLAPE mixtures at 30^{o}C recorded 24 h after sample samples preparation when the plasmalogen bond is entirely oxidized. From bottom to top: POPC-d_{31}, POPC-d_{31}/PLAPE 2/1, 1/1, 1/2. A fraction of the POPC-d_{31}/PLAPE, 2/1 had converted to a gel phase.

S4. Partial atomic charges of linear vinyl ethers from QM calculations. QM results for partial atomic charges of model vinyl ethers are shown in Fig. S3. While carbons bonded to ether oxygens carry substantially positive partial charges if no vinyl group is present, the presence of a vinyl group reduces the positive charge of the bonded carbon. As with saturated linear ethers,[2] partial charges on carbons then alternate positive/negative moving outward from the ether oxygen on both ends of 1-ethoxypropene.

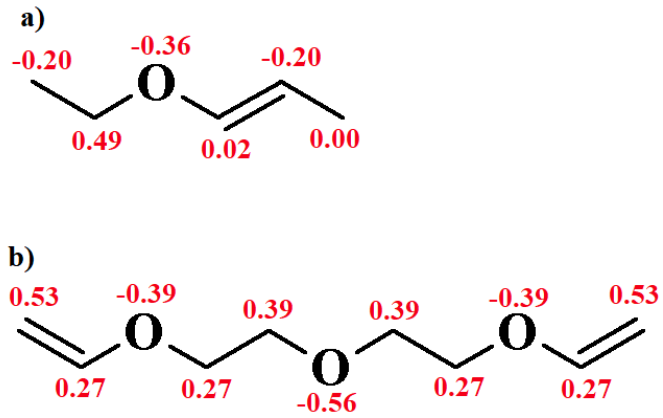

Figure S4. Partial atomic charges for model vinyl ethers. QM results for (a) 1-ethoxypropene and (b) diethylene glycol divinyl ether. Units of elementary charge, $+e$, averaged for symmetry where applicable.

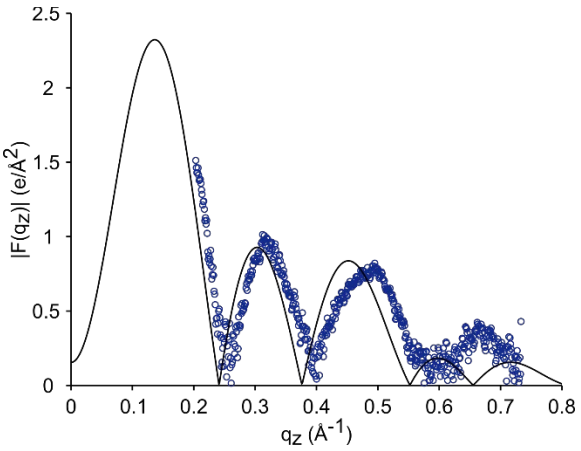

Figure S5. X-ray form factors ($|F(q_z)|$) as function of the total scattering (q_z) obtained from simulations at 310K (black line) of the system POPC/PLAPE 1:2 with the discarded charge set. The data are compared with experimental results (blue dots). The results from the simulations are not in agreement with the experimental ones: the calculated goodness of fit between form factors obtained from simulations and from experiment is 0.053. The calculated SA/lipid for the system was 61.5±0.04 $Å^2$.

Table S1. Overall SA/lip from simulation for POPC/POPE and POPC/PLAPE mixtures with standard errors. Values for pure POPC (1:0) are taken from past work at 313K.[1]

SA/lip ($Å^2$)	*POPC/PLAPE*		
	2:1	*1:1*	*1:2*
303 K	61.3±0.5	60.2±0.2	59.5±0.3
310 K	65.4±0.1	64.5±0.1	63.5±0.1

SA/lip ($Å^2$)	*POPC/POPE*			
	1:0	*2:1*	*1:1*	*1:2*
310 K (exp)	67.9±1	65.0±1	63.6±1	62.1±1
310 K (MD)	66.7±0.3	62.3±0.1	60.9±0.1	59.7±0.1

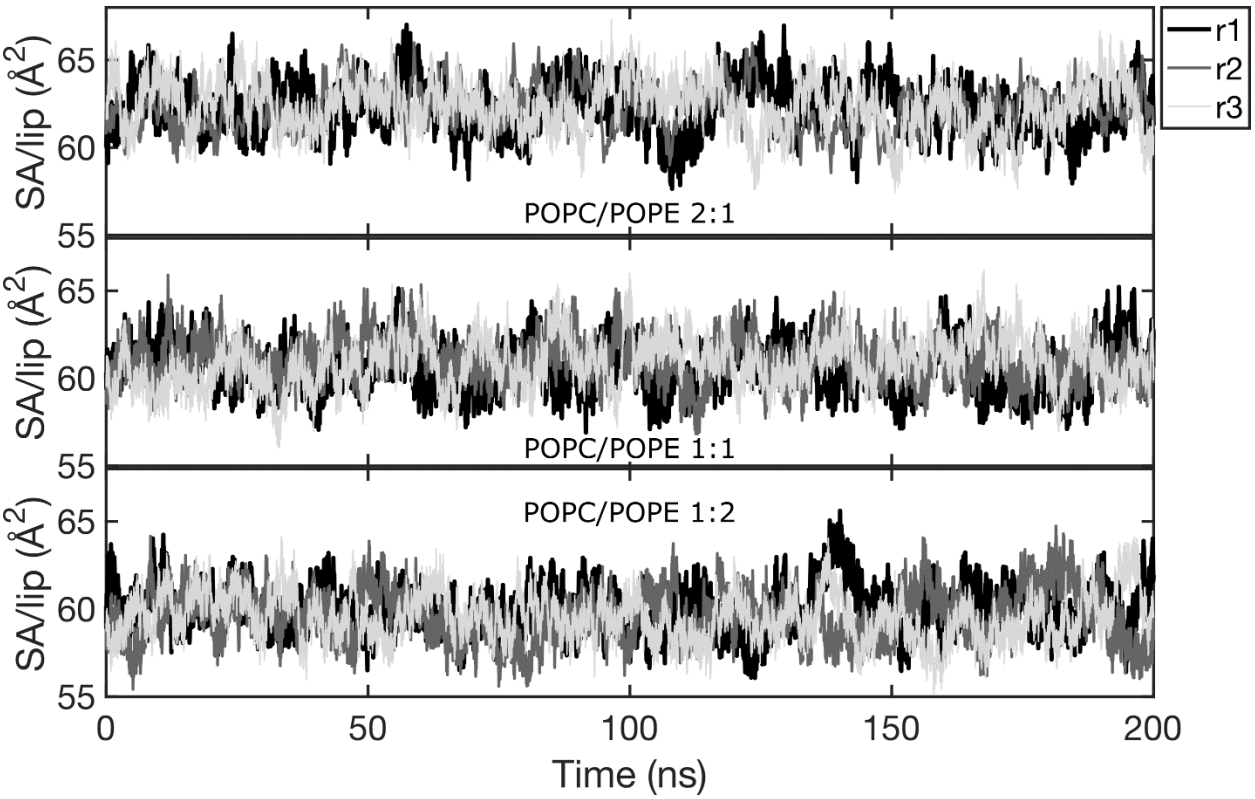

Figure S6. SA/lip vs. time for POPC/POPE

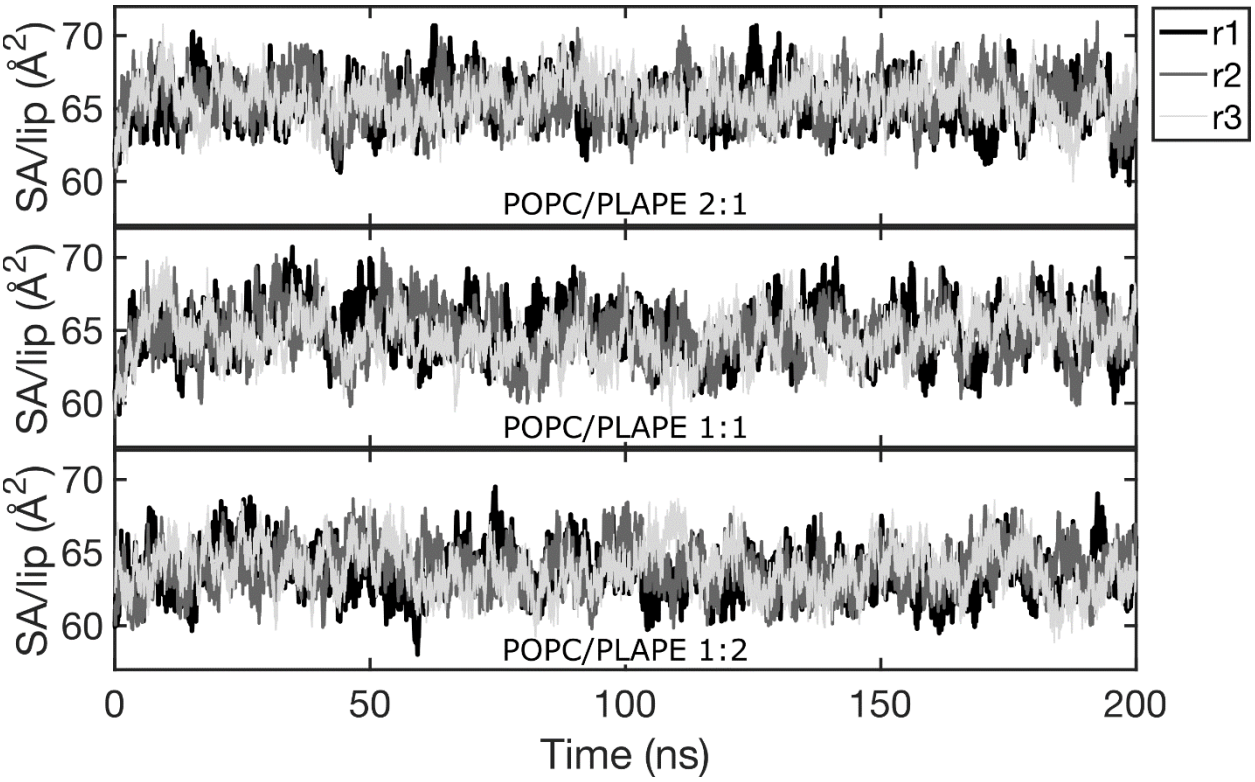

Figure S7. SA/lip vs. time for POPC/PLAPE.

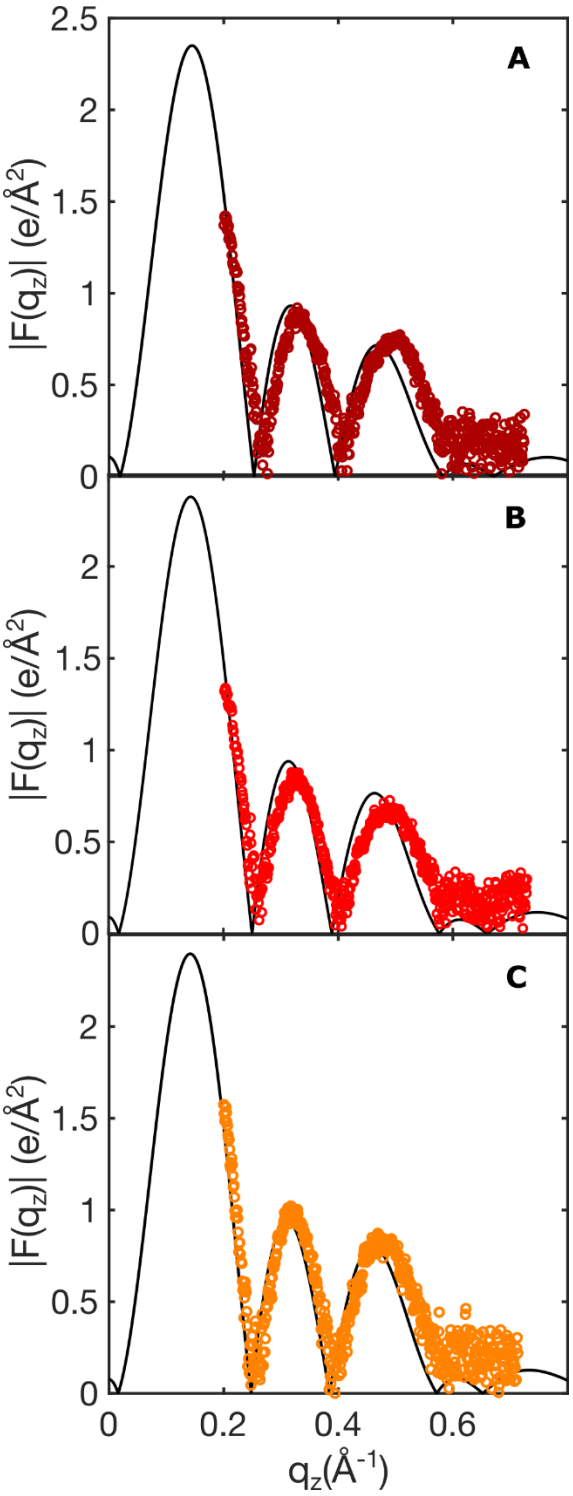

Figure S8. X-ray form factors ($|F(q_z)|$) as function of scattering angle (q_z) obtained from simulations at 310K (black line) of three POPC/POPE molar ratios, (A) 2:1, (B) 1:1 and (C) 1:2. The simulation results (solid line) are compared to experimental results (dots).

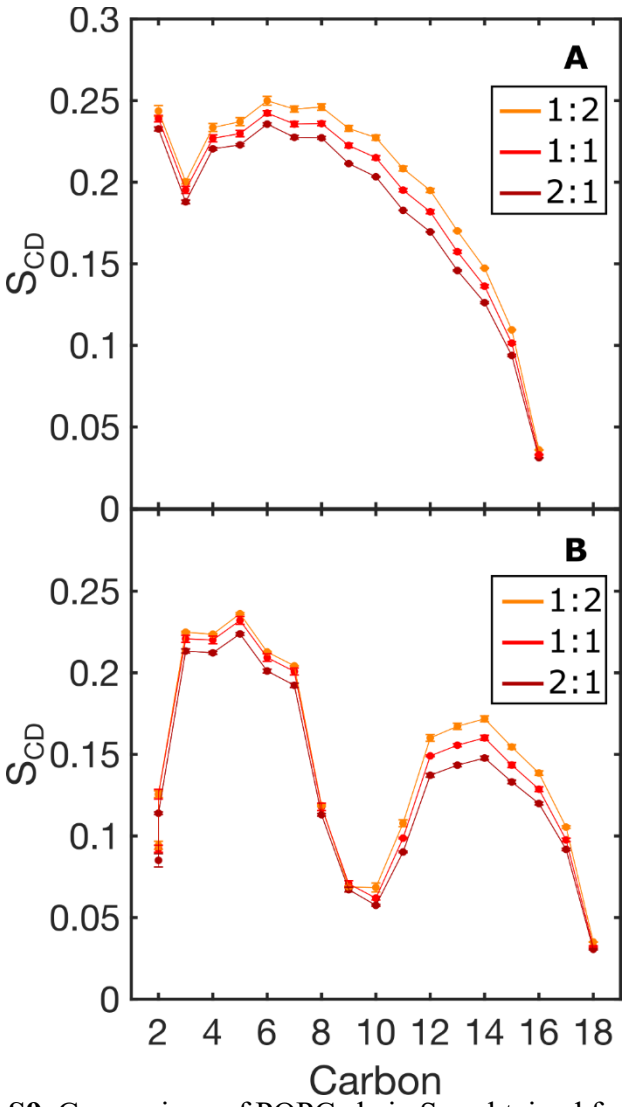

Figure S9. Comparison of POPC chain S_{CD} obtained from simulations with POPE at 310K for the *sn*-1 (**A**) and *sn*-2 (**B**) chains. The POPC/POPE molar ratios are listed in the legend.

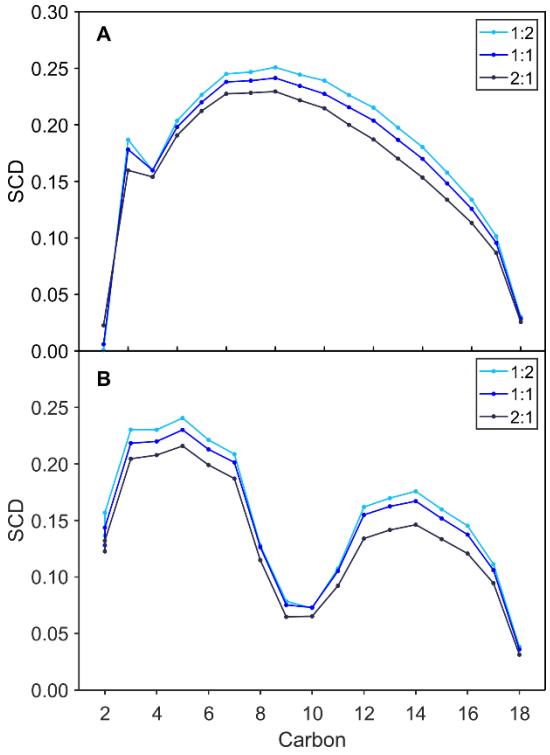

Figure S10. S_{CD} calculations of PLAPE *sn*-1 (A) and *sn*-2 (B) chains from MD simulations of POPC/PLAPE mixtures at 303K. For *sn*-2 chain, the hydrogens attached to carbon-2 have a different splitting, so the S_{CD} of 2R and 2S are shown separately instead of their average.

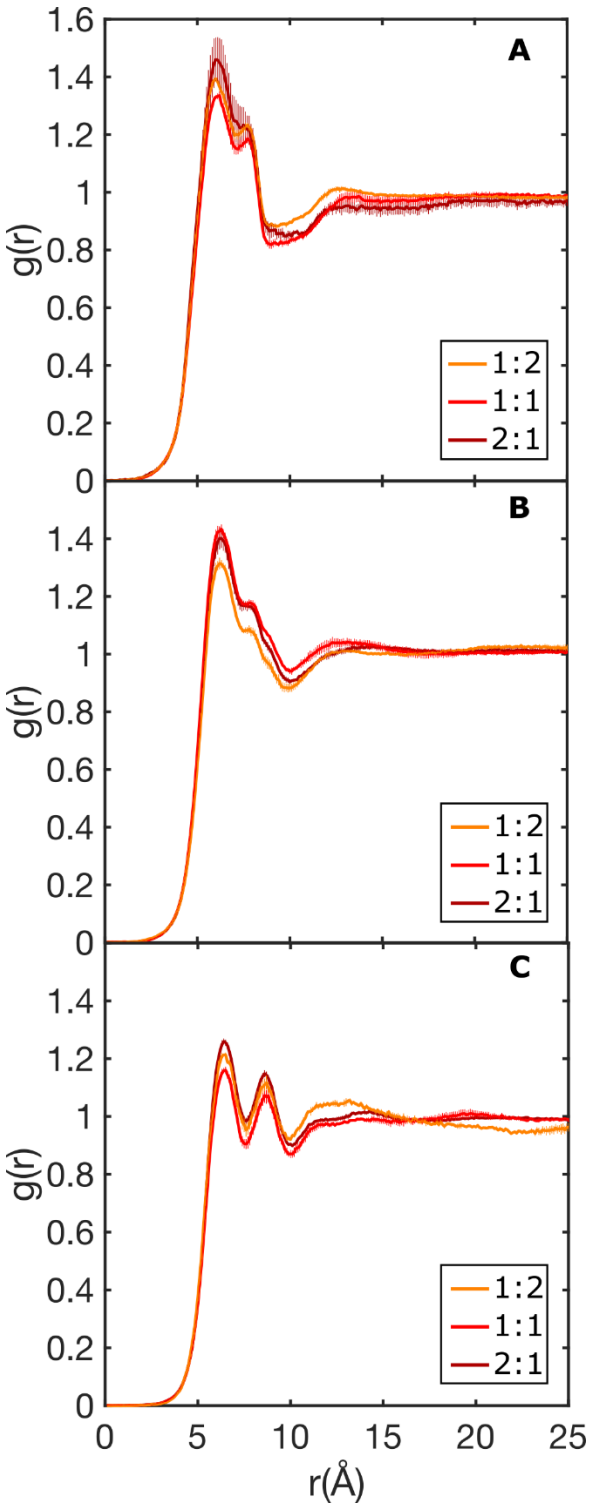

Figure S11. Comparison of two-dimensional radial distribution functions (RDFs) of POPE-POPE (**A**), POPE-POPC (**B**), and POPC-POPC (**C**) in POPC/POPE mixtures. The results are from simulations carried out at 310 K with POPC/POPE molar ratios listed in the legend.

Table S2. The fraction of hydrogen bonds per lipid (H-acceptor distance of less than 2.4 Å and the donor-hydrogen-acceptor angle of greater than 150º) is provided below. These were calculated from simulation at 310K for POPC/POPE and 303K at POPC/PLAPE. The weighted average of hydrogen bonds per lipid for PE and PC is denoted as: $\langle PE, PC \rangle$.

	POPC/PLAPE		
	2:1	*1:1*	*1:2*
PE	0.795±0.026	0.762±0.001	0.746±0.012
PC	0.237±0.002	0.339±0.011	0.417±0.005
$\langle PE, PC \rangle$	0.423±0.014	0.551±0.006	0.636±0.009

	POPC/POPE		
	2:1	*1:1*	*1:2*
PE	0.780±0.001	0.759±0.008	0.755±0.010
PC	0.226±0.005	0.338±0.010	0.422±0.006
$\langle PE, PC \rangle$	0.411±0.003	0.548±0.009	0.643±0.008

References

1. Zhuang, X.; Makover, J.; Im, W.; Klauda, J. B., A systematic molecular dynamics simulation study of temperature dependent bilayer structural properties. *Biochim. Biophys. Acta, Biomembr.* **2014,** *1838* (10), 2520-2529.
2. Leonard, A. N.; Pastor, R. W.; Klauda, J. B., Parameterization of the CHARMM All-Atom Force Field for Ether Lipids and Model Linear Ethers. *The journal of physical chemistry. B* **2018,** *122* (26), 6744-6754.