

Supplementary Information for:

**Lipid Bilayer Membranes with Asymmetrically
Distributed LPC and DAG**

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Supplementary Table

Table S1: List of the simulation surface area.

	Upper Leaflet : Lower Leaflet	Surface Area (nm ²)
Symmetric Bilayer Composition	POPC : POPC	40.70 ± 0.92
	POPC/LPC12 : POPC/LPC12	48.14 ± 0.10
	POPC/LPC14 : POPC/LPC14	47.91 ± 0.95
	POPC/LPC16 : POPC/LPC16	47.78 ± 0.33
	POPC/PIP ₂ : POPC/PIP ₂ (n=1)	39.35 ± 0.80
	POPC/DAG : POPC/DAG (n=1)	37.01 ± 0.92
	POPC/PIP ₂ : POPC/PIP ₂ (n=2)	39.60 ± 1.11
	POPC/DAG : POPC/DAG (n=2)	37.21 ± 0.93
Asymmetric Bilayer Composition	POPC : POPC/LPC12	44.67 ± 1.07
	POPC : POPC/LPC14	44.37 ± 0.93
	POPC : POPC/LPC16	44.23 ± 0.92
	POPC/PIP ₂ : POPC/DAG (n=1)	38.24 ± 0.94
	POPC/PIP ₂ : POPC/DAG (n=2)	38.79 ± 1.04

Supplementary Figures

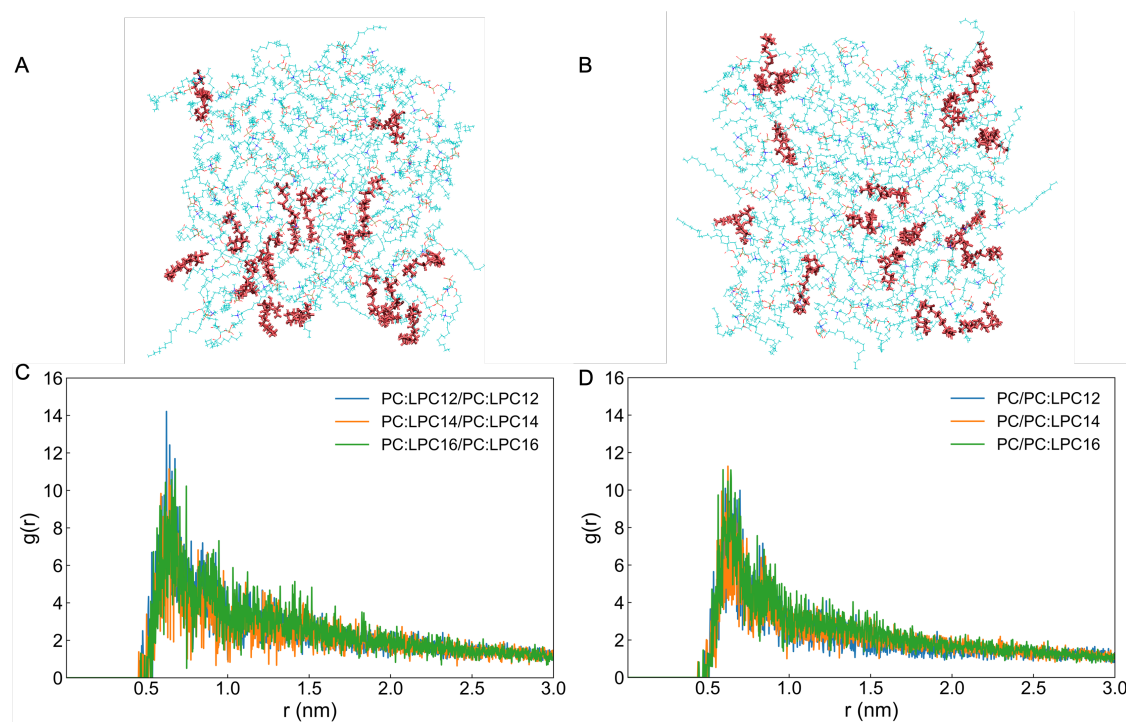


Figure S1: Snapshots of the LPC12 insertion system showing (A) transient local clustering and (B) dispersed distribution. Radial distribution functions for bilayers with symmetric (C) and asymmetric (D) LPC insertion, obtained by concatenating the final 200 ns from each of five independent replicate trajectories.

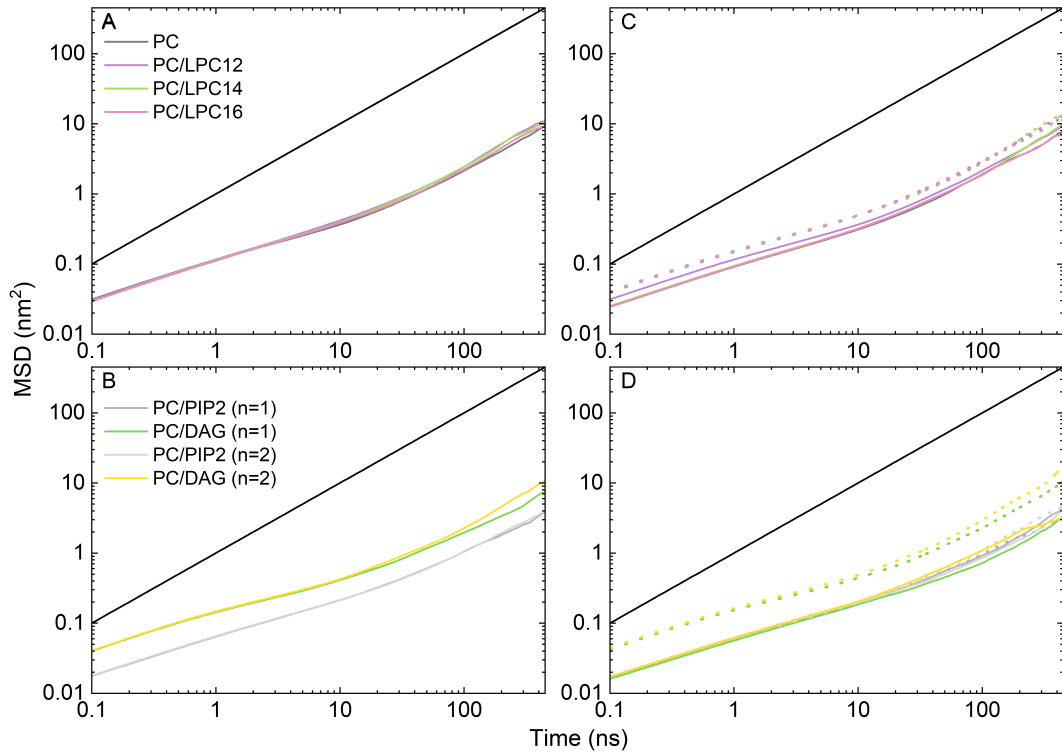


Figure S2: Two-dimensional mean square displacement (MSD) of lipid molecules in bilayer systems with symmetric LPC insertion and PIP₂-DAG conversion (A, B), or with asymmetric LPC insertion and PIP₂-DAG conversion (C, D). The solid and dotted lines in panels (C) and (D) represent the MSD of lipid molecules in the upper and lower leaflets, respectively.

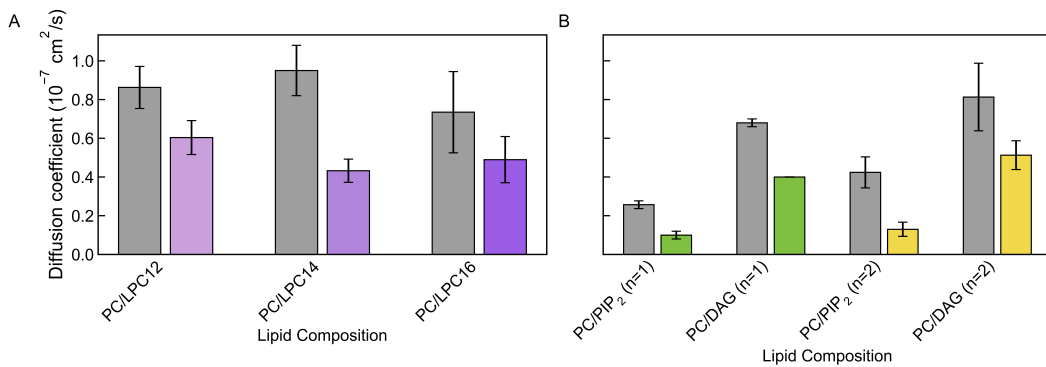


Figure S3: Lateral diffusion coefficients of LPC (A) and PIP₂/DAG (B) in symmetric and asymmetric bilayer systems. In each set of histograms, the left (gray) and right (colored) histograms correspond to symmetric and asymmetric systems, respectively. *n* denotes the degree of unsaturation.

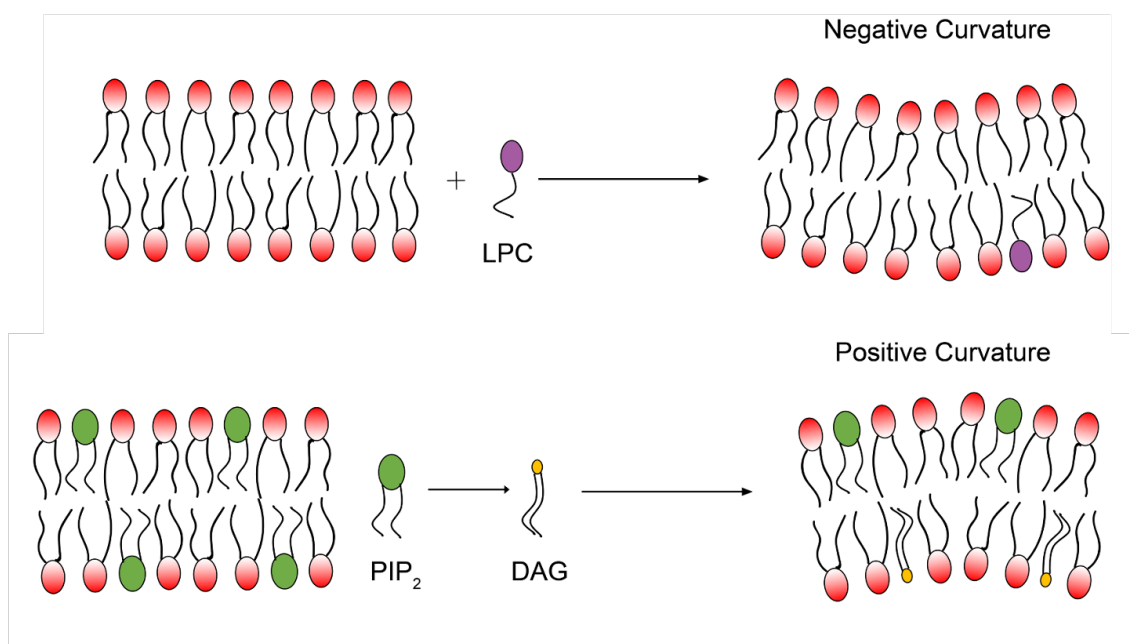


Figure S4: The curvature trends with different lipid compositions. The direction of membrane curvature was defined from the perspective of an observer located below the lower leaflet of the bilayer, looking towards the upper leaflet. A concave curvature of the membrane (bending away from the lower leaflet) was defined as positive, while a convex curvature (bending toward the lower leaflet) was defined as negative.