Differential Effects of Cholesterol, Ergosterol and Lanosterol on a Dipalmitoyl Phosphatidylcholine (DPPC) membrane: A Molecular Dynamics Simulation Study

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Supporting Information

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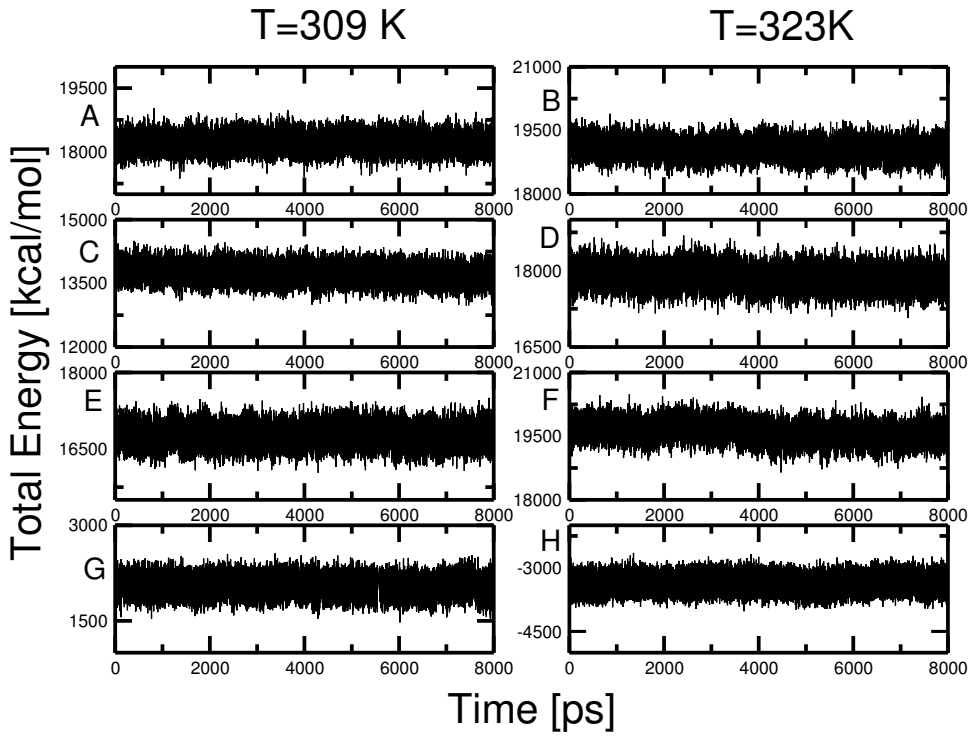

Figure S 1: Time evolution of the total energy for the production run of the simulated systems. (A) and (B) chol-DPPC, (C) and (D) erg-DPPC, (E) and (F) lan-DPPC, (G) 64-DPPC in the gel phase and (H) 72-DPPC in the liquid phase.

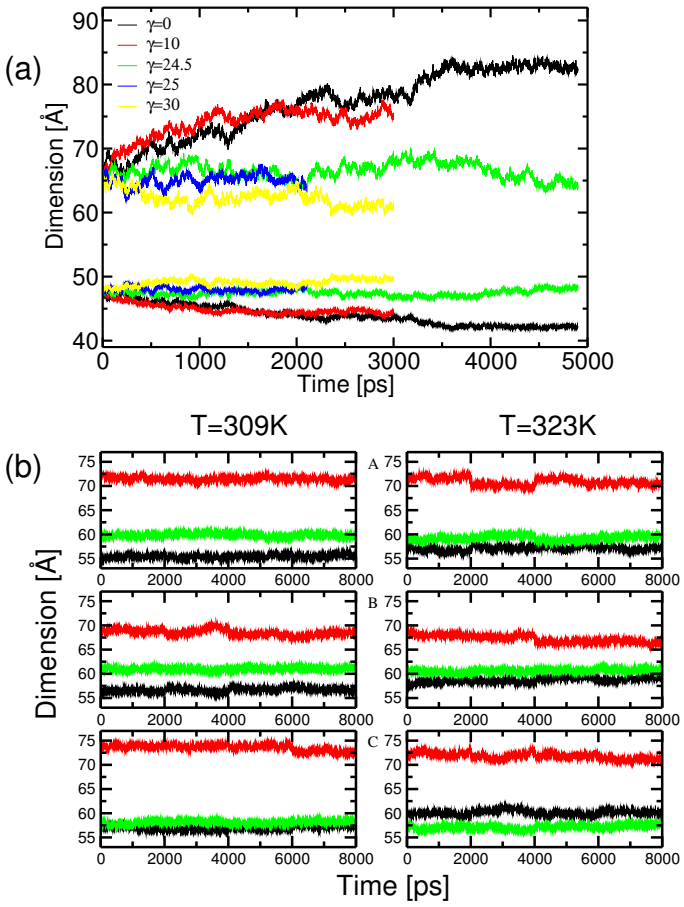

Figure S 2: Time evolution of the unit cell dimensions for (a) the liquid 72-DPPC system (T=323K), simulated with different values of γ. The upper curves correspond to the z-coordinate and the lower curves to the x-coordinate (b) (A) cholesterol-DPPC, (B) ergosterol-DPPC, (C) lanosterol-DPPC at T=309K and at T=323K. The black line represents the x coordinate, the red line the y coordinate and the green line represents the z coordinate.

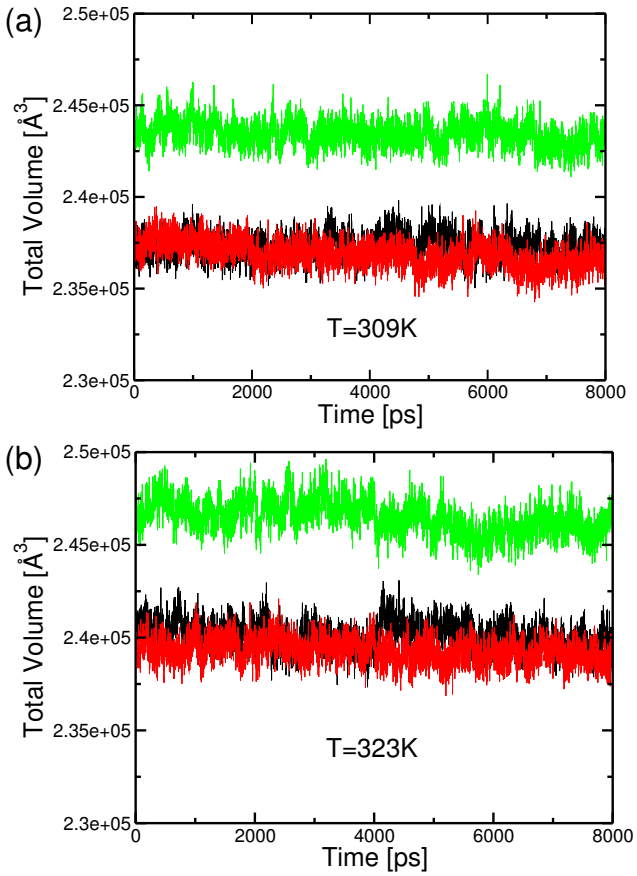

Figure S 3: Total volume of the unit cell. Cholesterol-DPPC: black, ergosterol-DPPC: red and lanosterol-DPPC: green for (a) 309K and (b) 323K.

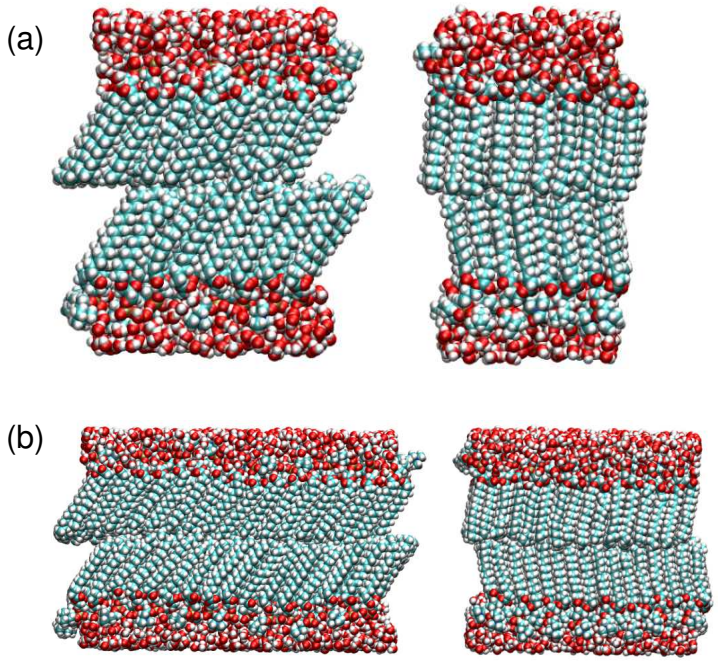

Figure S 4: The final frames of the gel DPPC membrane (309K) (a) of 64 lipids taken at t=8ns and (b) of 256lipids at t=4ns. Oxygens are shown in red, hydrogens in white, carbons in turquoise, nitrogens in blue and phosphorus in yellow. The views are shown in the (x, z) plane (left) and in the (y, z) plane (right).

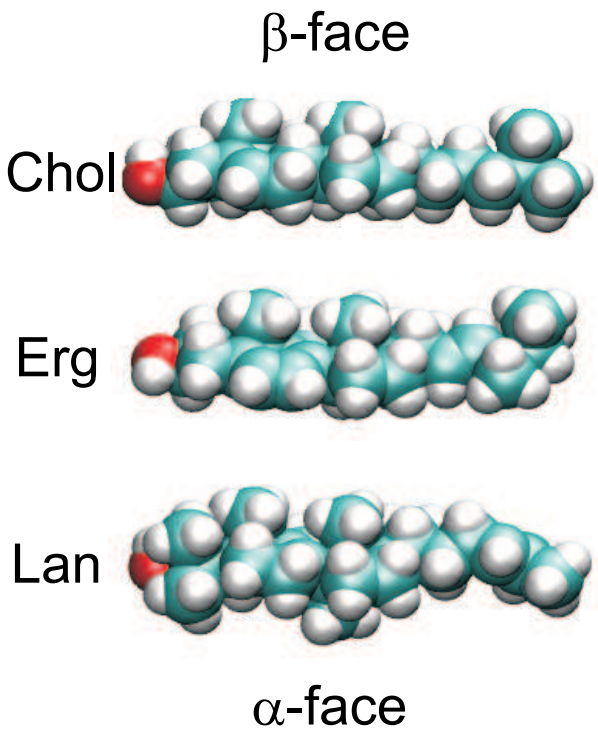

Figure S 5: A space filling representation of cholesterol, ergosterol and lanosterol.

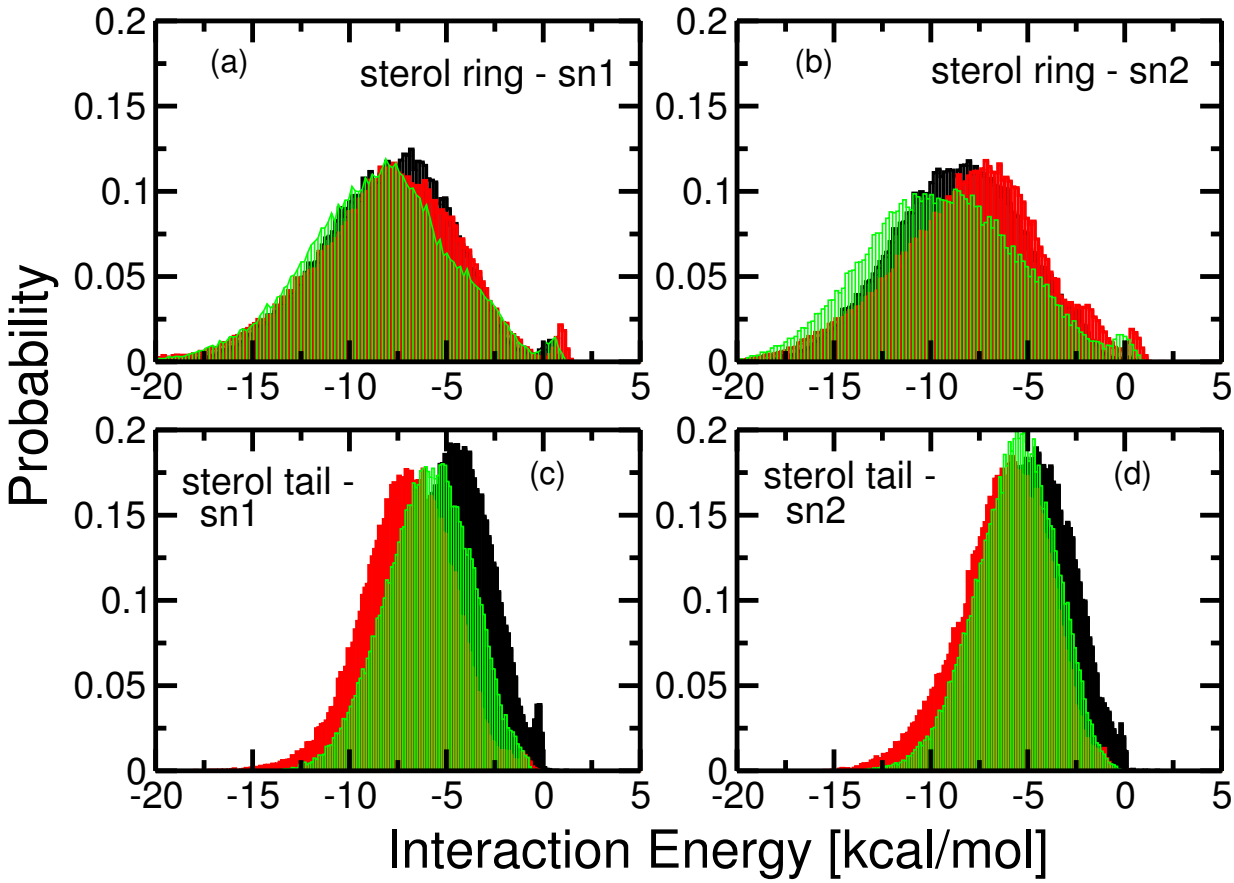

Figure S 6: Distribution of interaction energies for T=323K and (a) sterol ring system and DPPC chain sn1, (b)sterol ring system and DPPC chain sn2, (c)sterol side chain and DPPC chain sn1, (b)sterol side chain and DPPC chain sn2. Cholesterol in black, ergosterol in red and lanosterol in green.

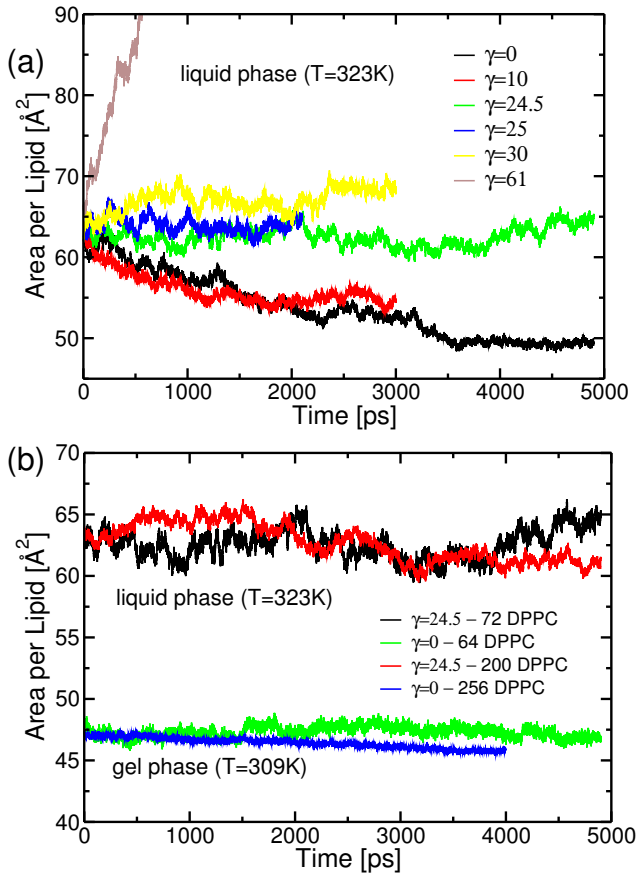

Figure S 7: Areas per DPPC (a) for T=323K and for the 72-DPPC system, simulated with different values of γ. With γ=0 or γ=10 dyn/cm, the area per lipid did not converge after 5ns and is severely underestimated. γ=61 results in an over-stretching of the membrane (see also Figure 2 of the main text) and an extreme overestimation of the area per lipid. The surface tension values γ=24.5 and γ=25 seem to reasonably reproduce the experimental area per lipid. The mean values observed in these simulations are 62.6$\pm$1.2 and 63.7$\pm$0.8. (b) Time series of the area per lipid for T=323K and γ=24.5 for the 72- and 200-DPPC system and for T=309K for the 64- and 256-DPPC system. A system size dependence is found for the area per lipid of the liquid DPPC (T=323K, upper curves), while no system size dependence is observed for the gel phase (T=309K). The area per DPPC molecule was calculated from the NP$_N\gamma$T trajectories of DPPC by diving the surface area of the bilayer ($x \times y$) by the number of lipids in one leaflet. All values of γ are in dyn/cm.

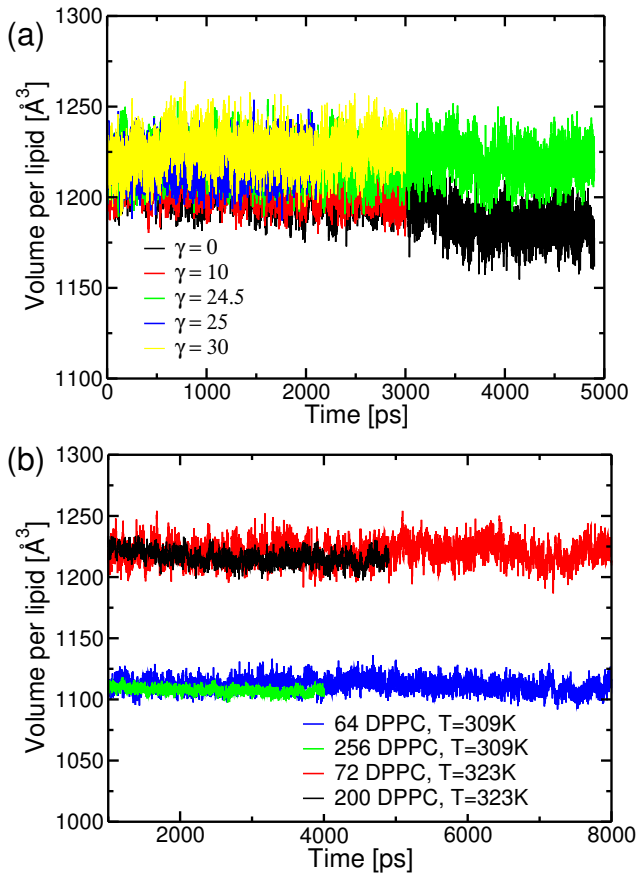

Figure S 8: Volumes per DPPC (a) for T=323K and for the 72-DPPC system at different surface tensions and (b) for T=323K and γ=24.5 dyn/cm for the 72-DPPC (red) and 200-DPPC (black) systems and for T=309K for the 64-DPPC (blue) and 256-DPPC (green) systems (γ=0 dyn/cm). The volume per lipid does not exhibit any system size dependence and has considerably smaller fluctuation than the area per lipid.

Torsion Angle	DPPC:Chol		DPPC:Erg		DPPC:Lan	
	309K	323K	309K	323K	309K	323K
C_4-C_5-C_{10}-C_1	-45.9±5.5	-45.9±5.6	-44.8±5.4	-44.7±5.5	-47.3±4.8	-47.3±4.9
C_7-C_8-C_9-C_{10}	59.6±4.8	59.5±4.9	36.2±5.8	36.1±5.7	5.4±4.0	5.4±4.1
C_{17}-C_{13}-C_{14}-C_{15}	41.1±4.0	41.3±4.1	44.0±3.8	44.1±3.9	44.4±3.4	44.3±3.5
C_{10}-C_5-C_6-C_7	-2.1±3.7	-2.1±3.8	-10.3±5.9	-10.3±6.0	-56.2±6.5	-56.2±6.6
C_5-C_6-C_7-C_8	13.4±6.2	13.4±6.4	-0.5±5.0	-0.5±5.2	27.7±9.2	27.7±9.5
C_6-C_7-C_8-C_9	-41.2±6.7	-41.1±6.9	-13.5±5.4	-13.4±5.5	-2.4±8.0	-2.4±8.2
C_8-C_{14}-C_{13}-C_{12}		-60.2±4.5		-59.7±4.5		-61.8±3.8
C_{14}-C_{15}-C_{16}-C_{17}		5.4±7.4		8.5±7.1		12.0±6.5
C_{15}-C_{16}-C_{17}-C_{13}		20.0±7.1		18.1±7.1		15.3±6.3

Table S 1: Selected torsional angles (in degrees) from the steroid rings, averaged over all sterol molecules.