C₆₀ fullerene promotes lung monolayer collapse

SUPPORTING INFORMATION

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Figure S1. Fullerene-DOPC contact fraction vs simulation time, in simulations at different surface tension.





Figure S2. Bond order parameter for each bond in the lipid chains, calculated in all simulations (with and without fullerene) in which no collapse was observed.



Figure S3. Distributions of DPPC tilt angles in simulations with high concentration of cholesterol (left) and low concentration of cholesterol (right). The tilt angle was calculated as the angle between the lipid vector and the z axis. The lipid vector was defined as the vector between the mid point of the glycerol backbone and the mid point of the terminal particle of the lipid chains.