Monte Carlo simulation of protein-induced lipid demixing in a membrane with interactions derived from experiment

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SUPPORTING MATERIAL

Monte Carlo simulations of larger lattices

Results of simulations in 200×200 lattices are shown below. Identical results were obtained in 300×300 lattices (not shown). In the presence of protein–protein interactions, the domain size in scales with the system size. In the 200×200 lattice the solution volume was 4×10^7 L/N$_A$ (Avogadro's number), and the total number of proteins in the system was 4×10^4, thus yielding a lipid and protein concentrations of 1 mM and 100 μM, the same as used in the 100×100 lattice simulations in the main paper. Similarly the volume and number of proteins were scaled by a factor of 9 in the 300×300 lattice simulations.

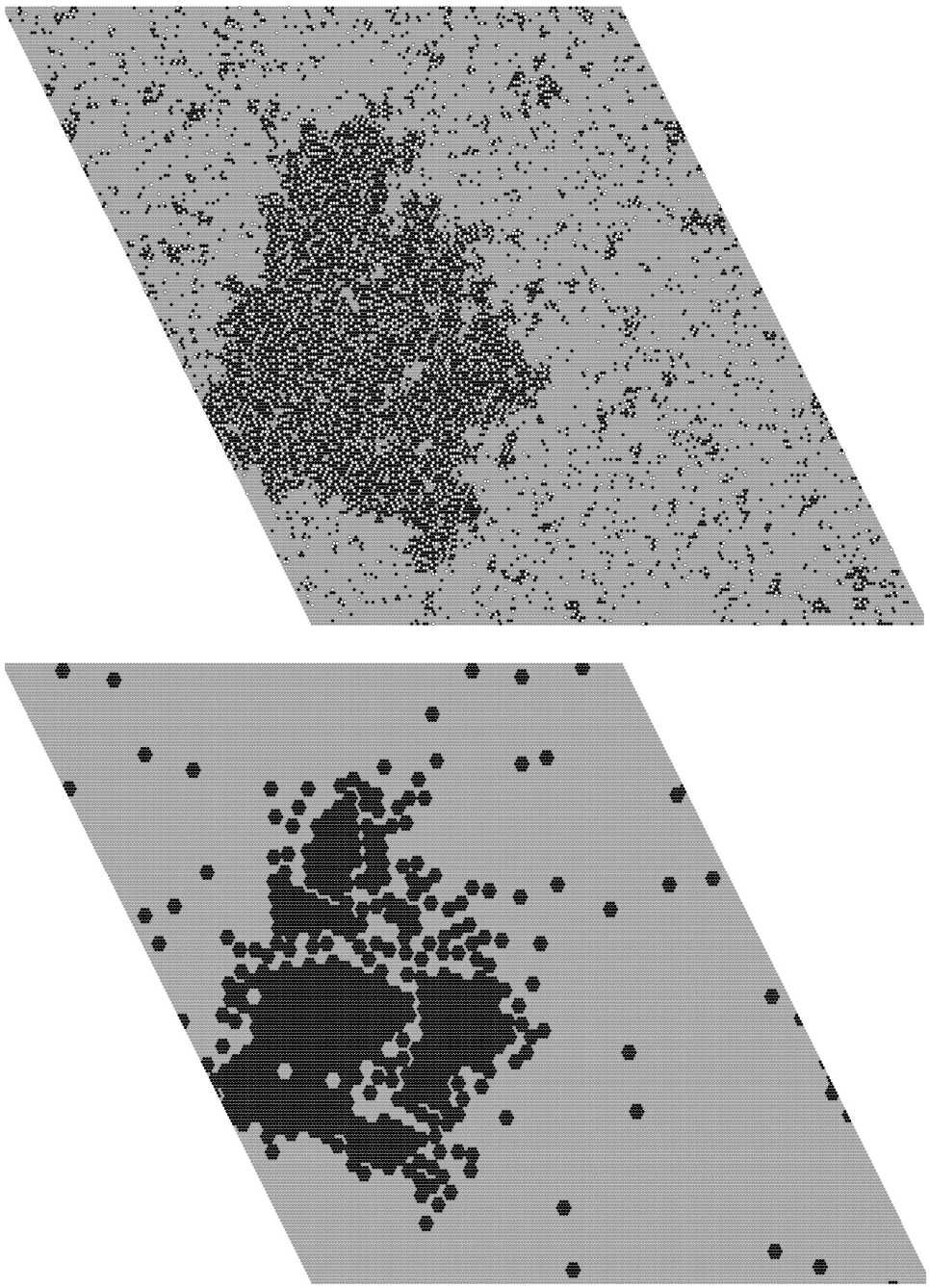

Figure S1 Snapshot of a 200×200 lattice simulation of PC/PS/Chol 70:20:10 in the presence of annexin. (top) Lipid and (bottom) protein, with a protein–protein interaction of $\epsilon_A = -0.68$ kcal/mol. Lipid: PS=black, PC=gray. Protein: black hexagons on lipid matrix (gray). (2×10^4 equilibration and 2×10^6 acquisition cycles.)

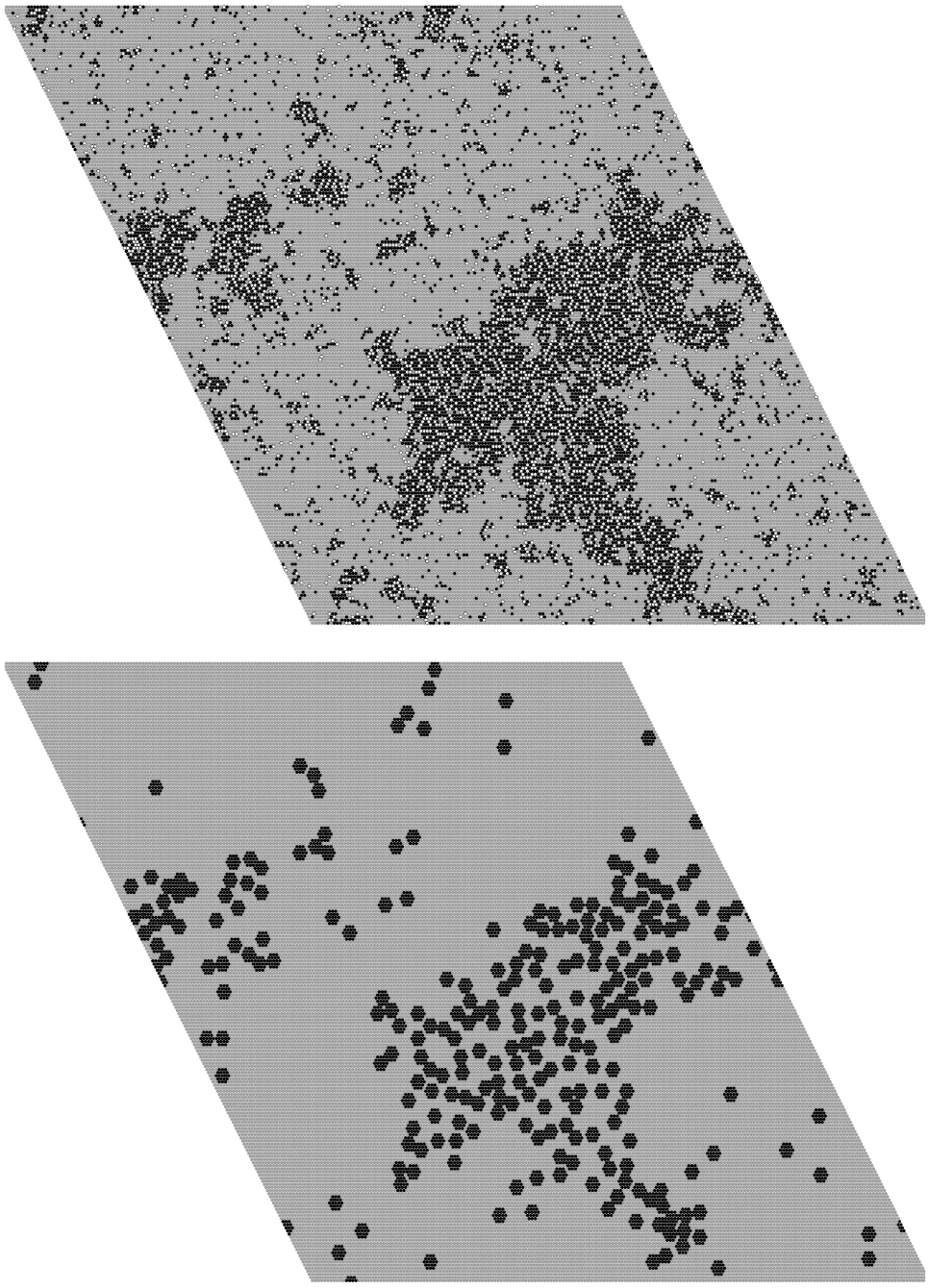

Figure S2 Snapshot of a 200×200 lattice simulation of PC/PS/Chol 70:20:10 in the presence of annexin. (top) Lipid and (bottom) protein, without protein–protein interactions ($\epsilon_A = 0$). Lipid: PS=black, PC=gray. Protein: black hexagons on lipid matrix (gray). (2×10^4 equilibration and 2×10^6 acquisition cycles.)

Effect of the Cholesterol–PS interaction on protein domain sizes

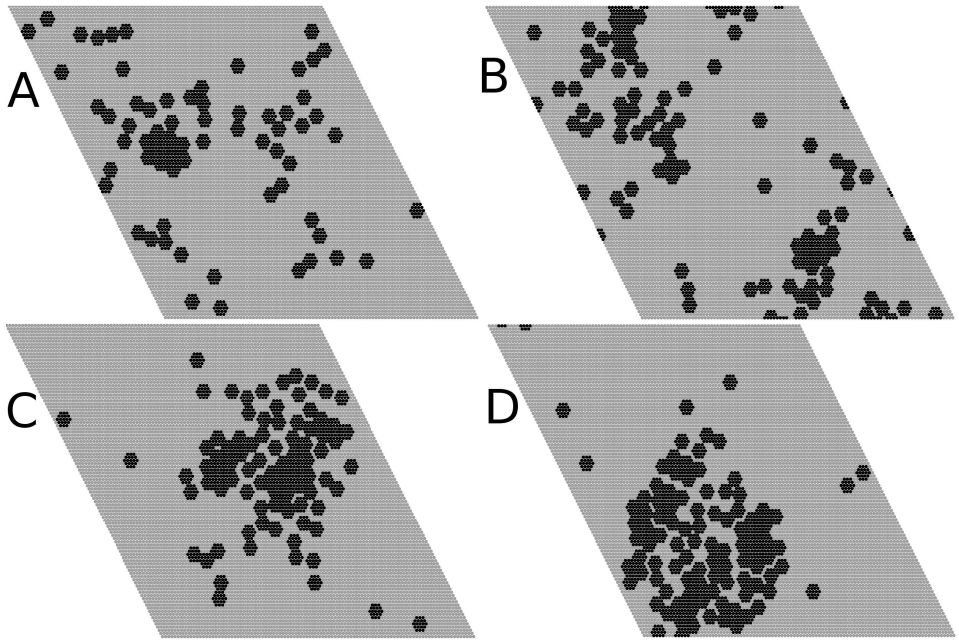

Figure S3 Effect of varying the PS-Chol interaction ($\omega_{PS-Chol}$) on protein domain size in PC/PS/Chol 70:20:10, in the presence of 100 μM annexin a5 (1000 proteins in the system). The four panels represent the same conditions as those in Fig. 6. (A) $\omega_{PS-Chol} = -250$ cal/mol, (B) -300 cal/mol, (C) -350 cal/mol, and (D) -400 cal/mol. Other parameters are the same as in Fig. 4. The proteins are the black hexagons on the lipid matrix (gray).