Supplemental Information for Lipid-GPCR interactions in an asymmetric plasma membrane

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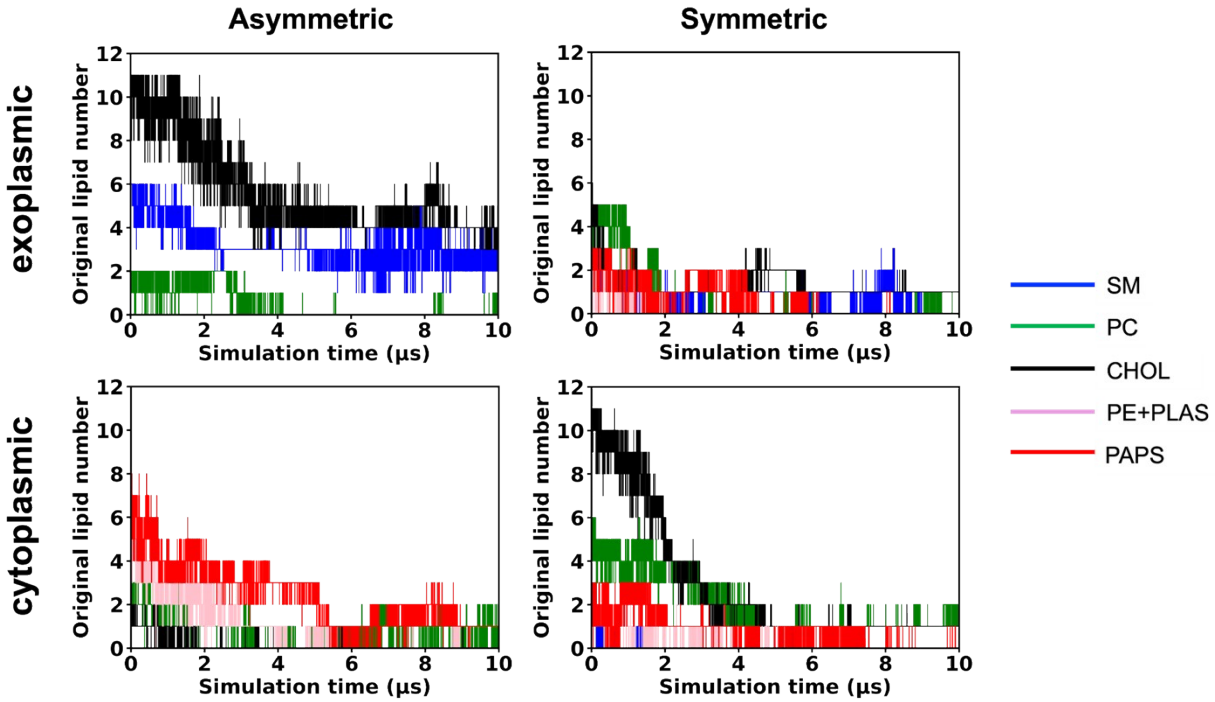
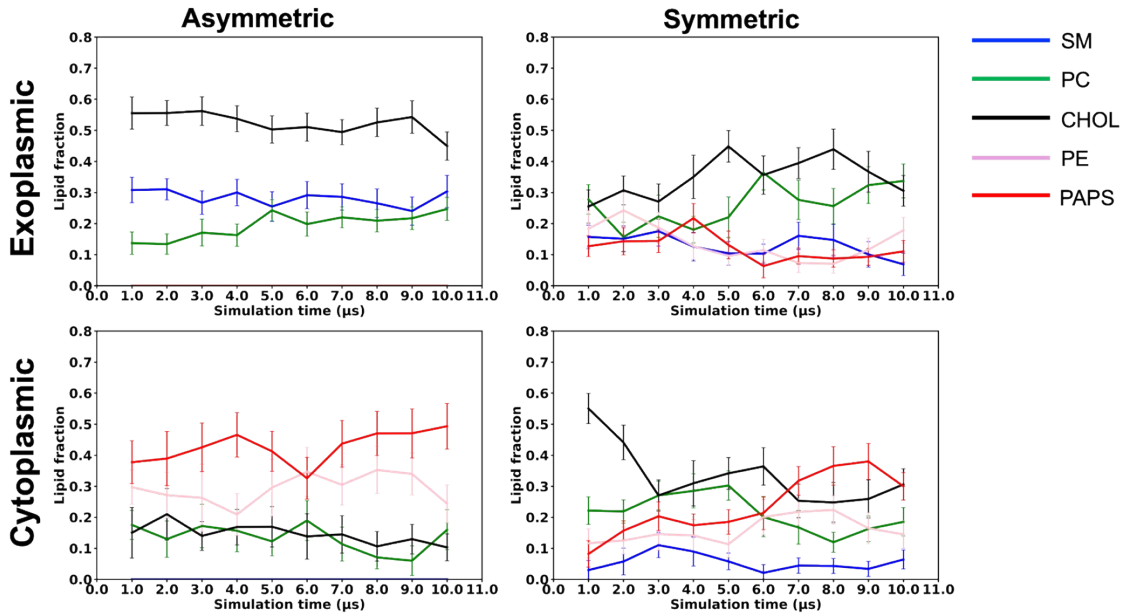
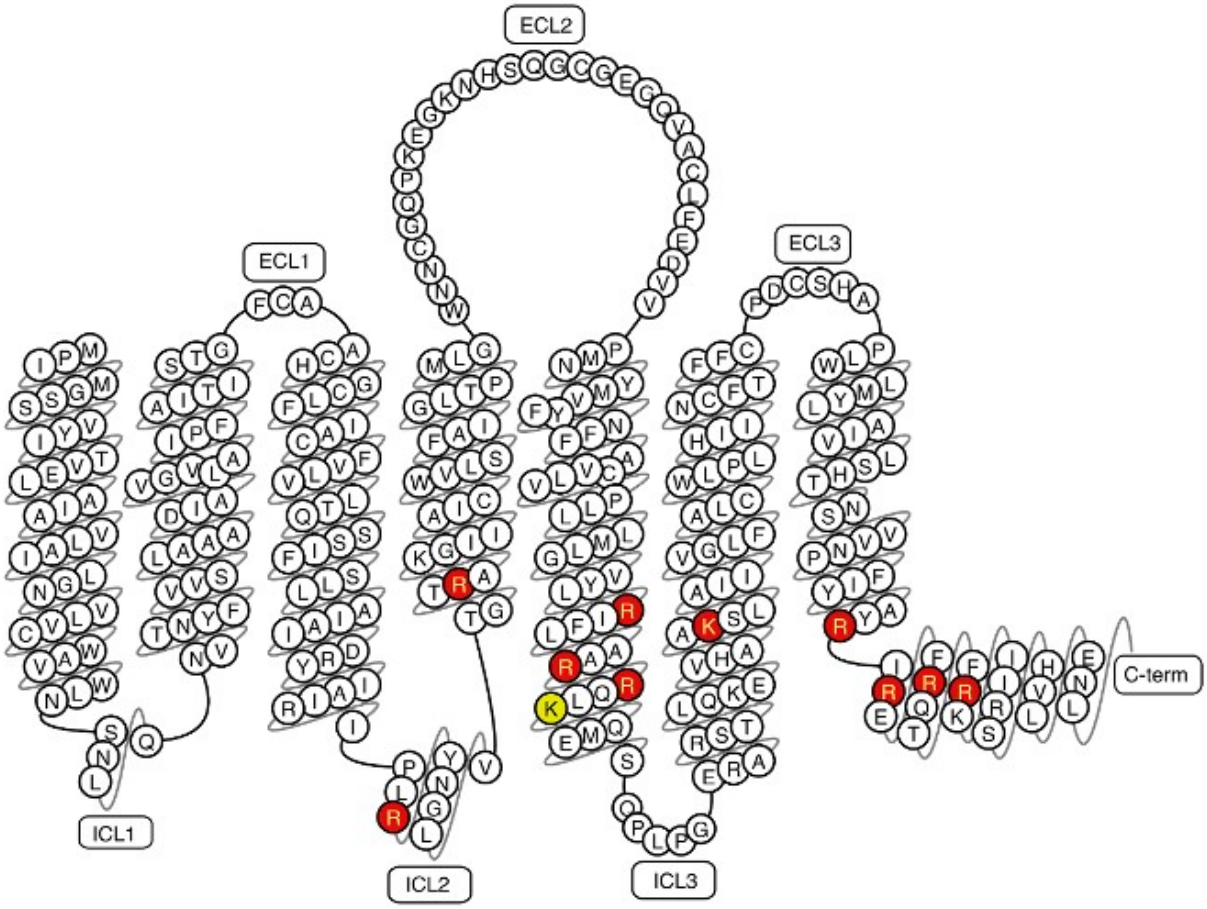


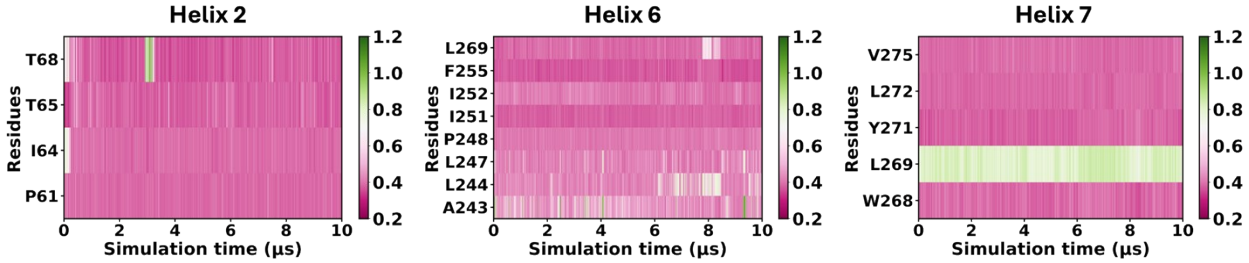
Supplemental Figure S1 Timeseries of first-shell lipid exchanges for both leaflets in both simulation models. Each time a lipid that is initially in the first shell exchanges with a lipid that is in the second shell the corresponding data series decreases by one. If all lipids of a particular type leave the first shell the corresponding data series is equal to zero



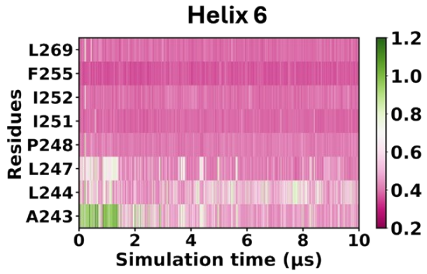
Supplemental Figure S2 The mole fraction of each lipid class in the first solvation shell, averaged over 1 μsec blocks of simulation time. The error bars are the standard deviation over the preceding 1 μsec block.



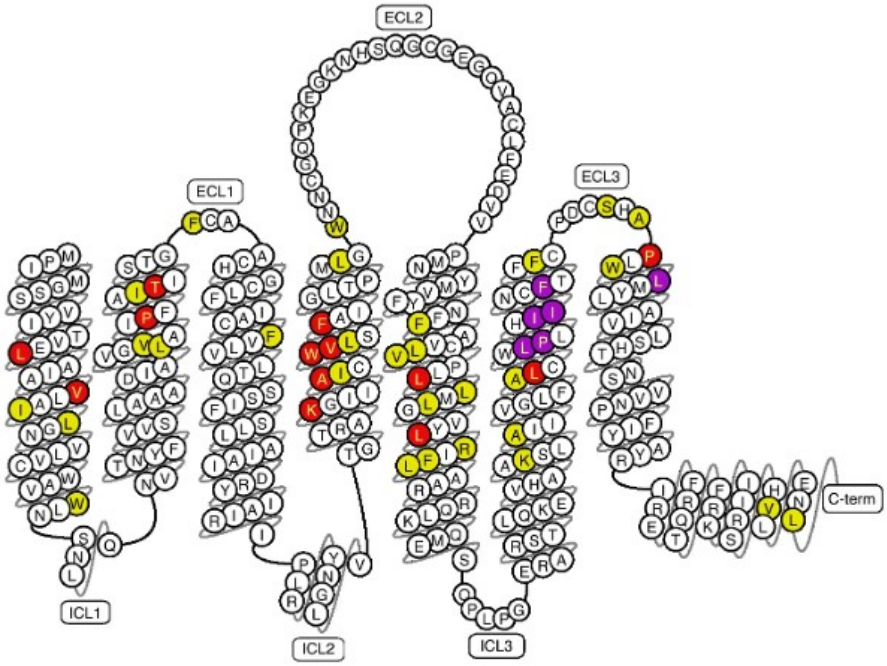
Supplemental Figure S3 Positively charged side chains that interact with a PS headgroup at least 80% of the time in the symmetric membrane simulation (red) or at least 50% of the time (yellow).



Supplemental Figure S4 Time series of side chain-cholesterol contacts for the three bound cholesterols shown in Figure 4 during the asymmetric membrane simulation. The color scale reports the shortest distance between any cholesterol and side chain heavy atom.



Supplemental Figure S5 Time series of side chain-cholesterol contacts for the cholesterol bound to helix 6 in the symmetric membrane simulation. The color scale reports the shortest distance between any cholesterol and side chain heavy atom.



Supplemental Figure S6 Cholesterol interactions with the receptor in the symmetric membrane simulation. Interactions are colored by residue, with purple indicating interaction with a single cholesterol for the entire duration of the simulation, red indicating interaction with any cholesterol for at least 80% of the simulation, and yellow any cholesterol for at least 50% of the simulation.