Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Modeling Lipid Raft Domains Containing a Mono-Unsaturated Phosphatidylethanolamine Species

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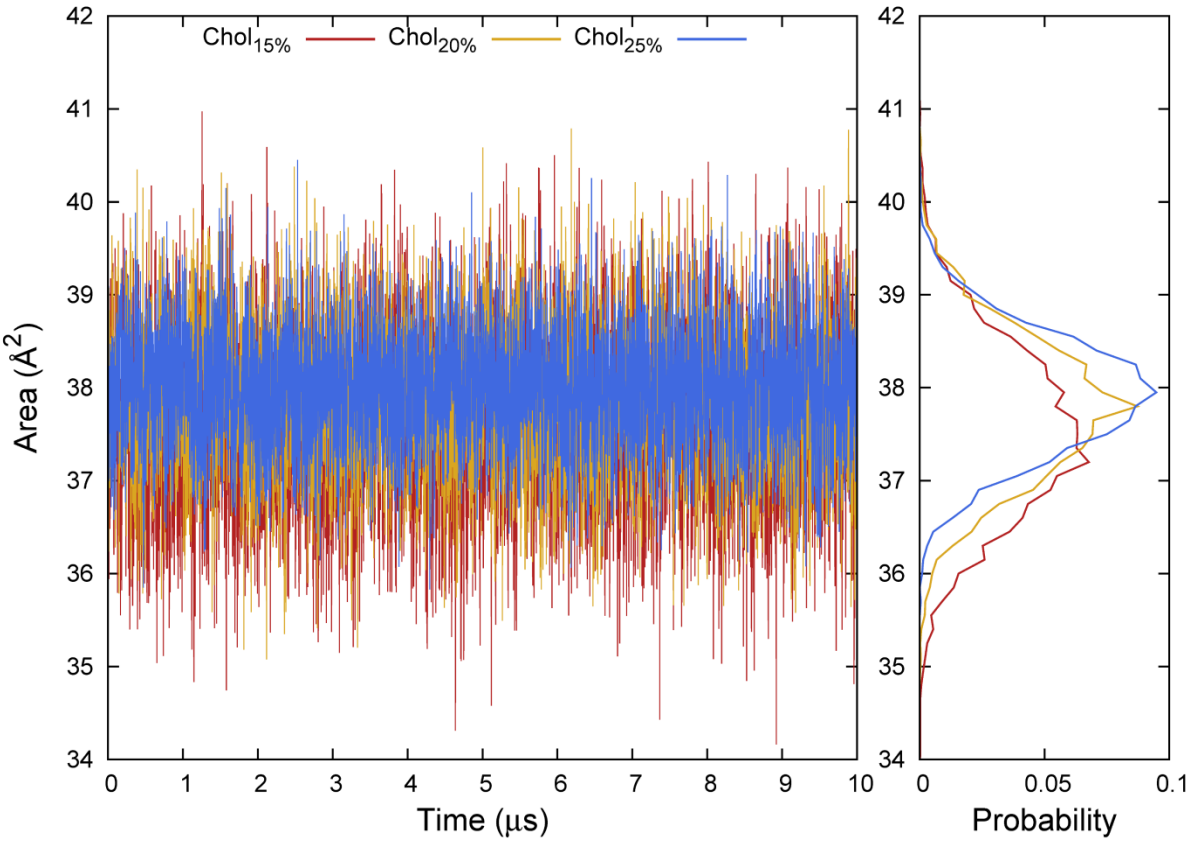

Fig. S1 Individual area per lipid calculated for Chol in the three simulated systems plotted as time series (left) and as a probability distribution (right).

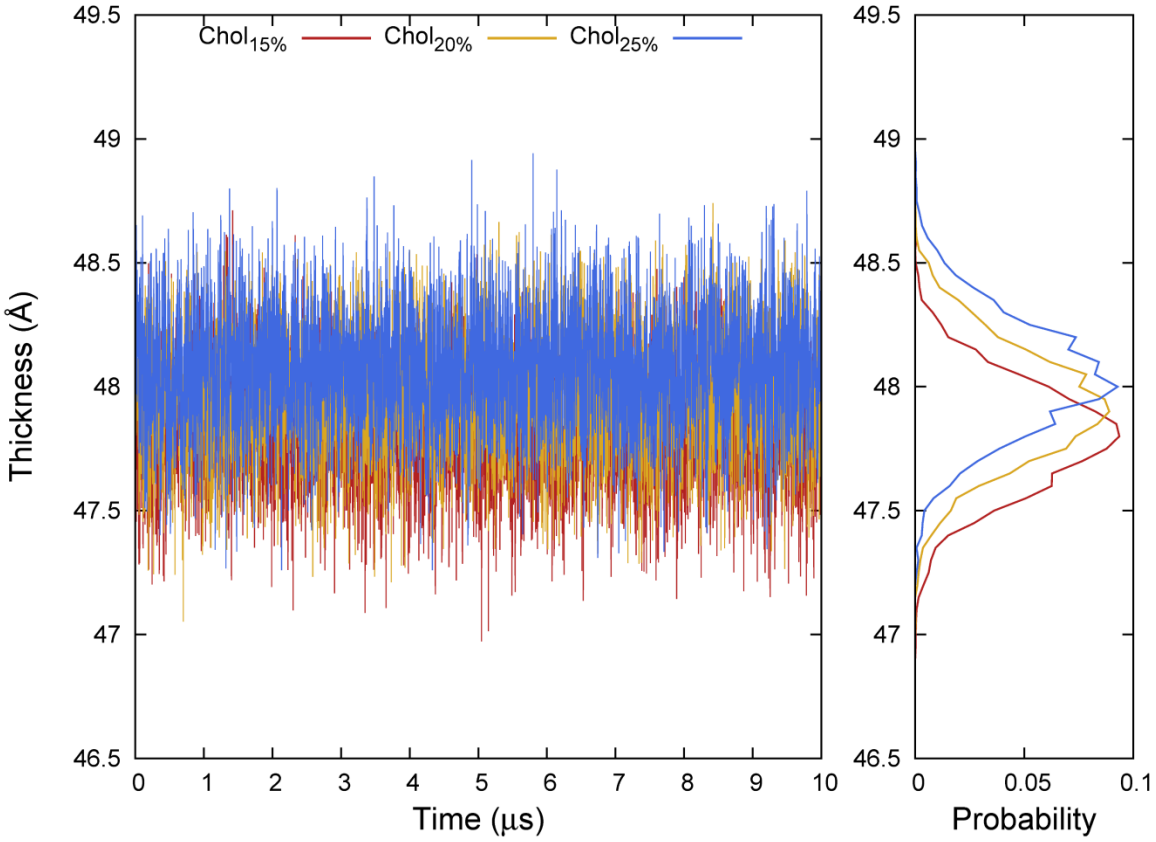

Fig. S2 Membrane thickness plotted as time series (left) and as a probability distribution (right).

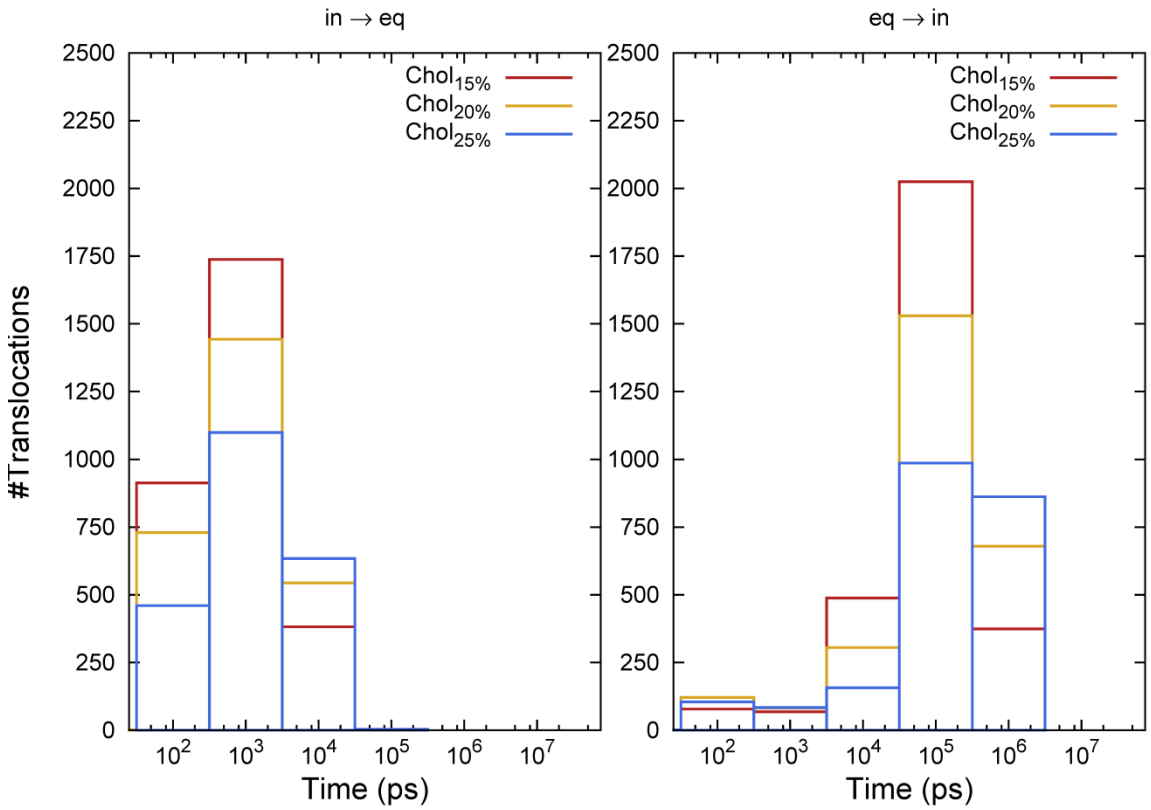

Fig. S3 Logarithmically binned histogram of the time spent by Chol molecules in the inter-leaflet region (left panel) and in the average equilibrium position (right) between successive translocations calculated for the three simulated systems.

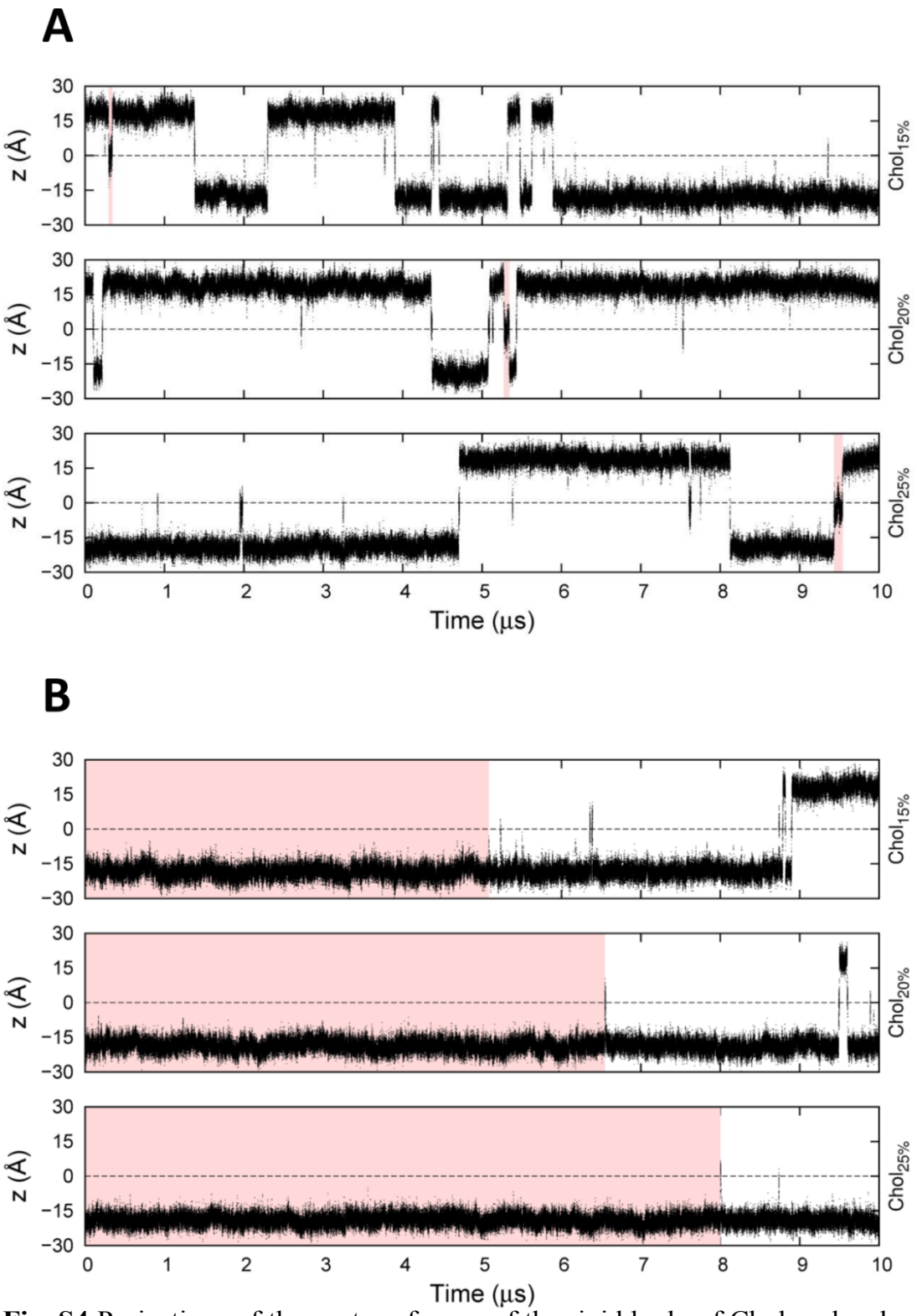

Fig. S4 Projections of the centre-of-mass of the rigid body of Chol molecules along the *z* axis for the slowest *in→eq* and *eq→in* translocations (panel A and B, respectively) detected in the three simulated systems. The survival times for the reported events (shaded areas) are 47.15, 69.60, and 110.10 ns (panel A), and 5084.10, 6546.15, 8001,85 ns (panel B) for Chol15%, Chol20%, and Chol25%, respectively

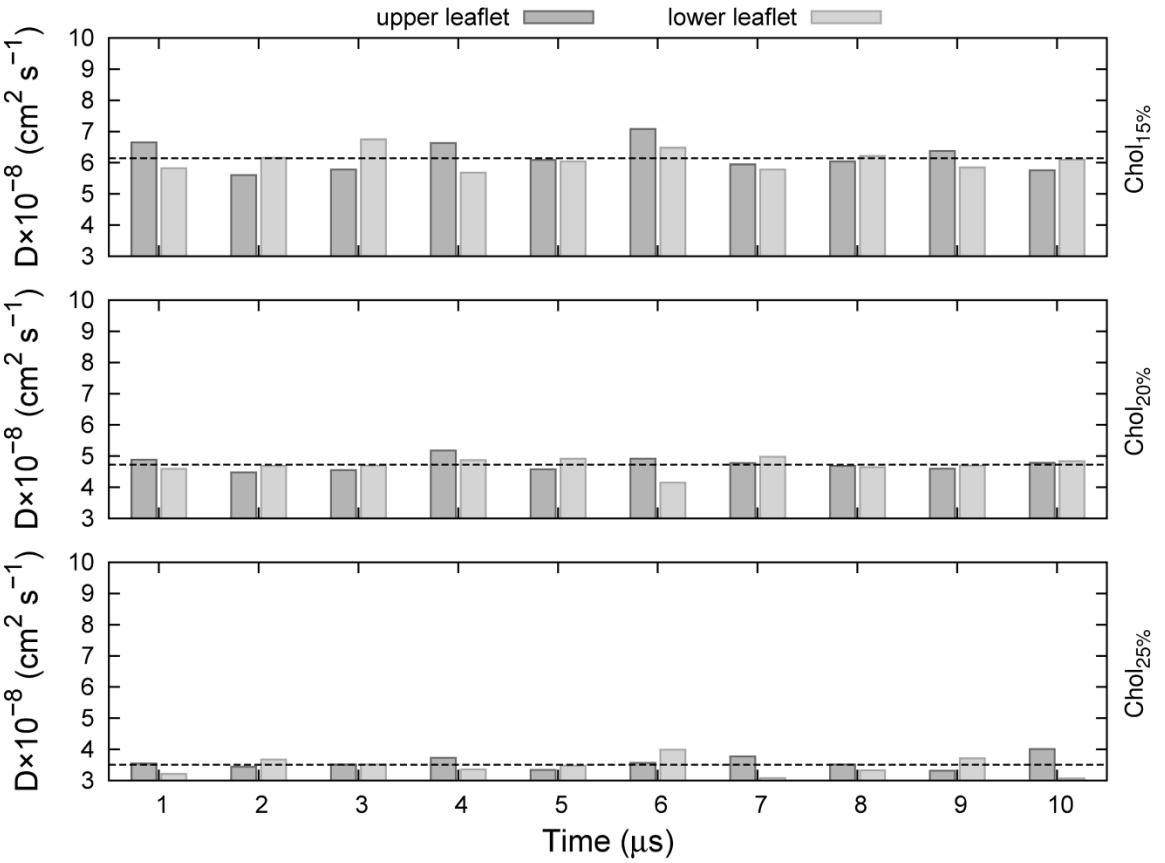

Fig. S5 Diffusion coefficient calculated for DSPC lipid species in the three simulated systems plotted as a function of time. The diffusion coefficient is separately reported for the two bilayer leaflets, and the black broken line shows the average over the whole trajectory.

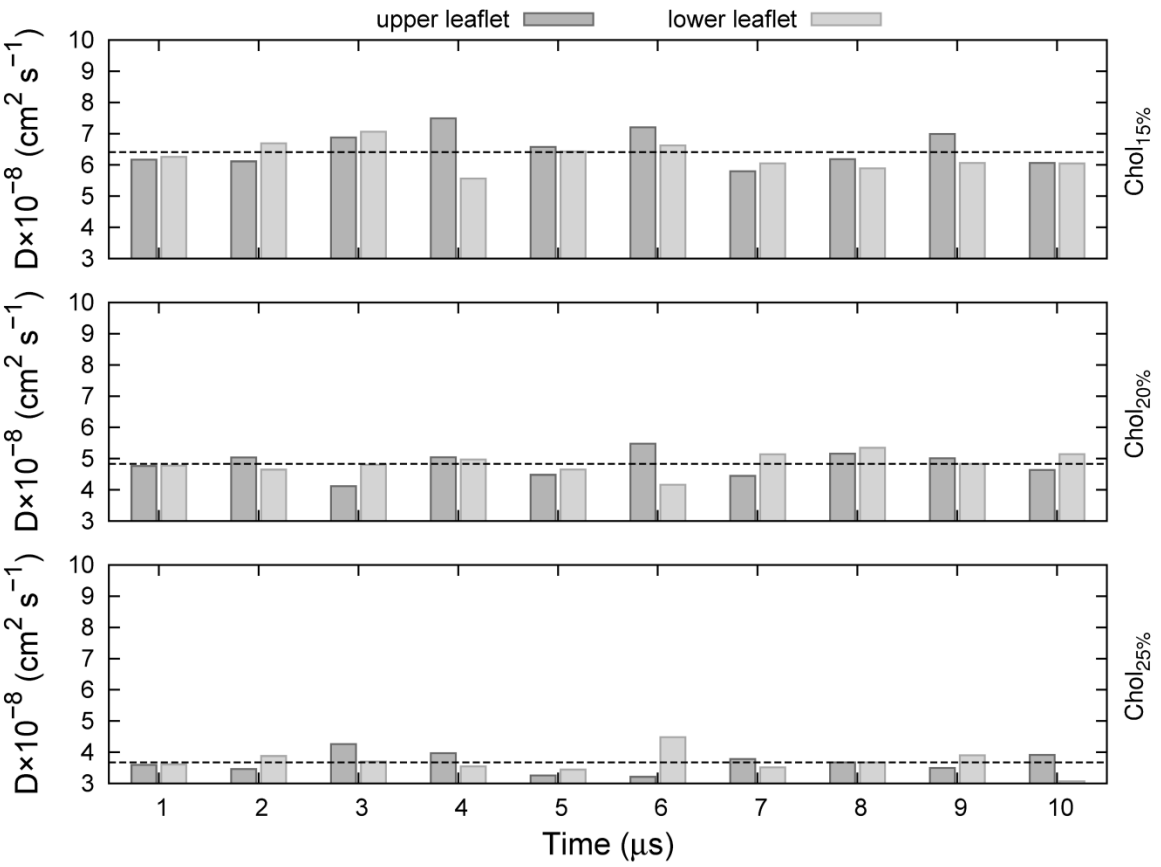

Fig. S6 Diffusion coefficient calculated for POPE lipid species in the three simulated systems plotted as a function of time. The diffusion coefficient is separately reported for the two bilayer leaflets, and the black broken line shows the average over the whole trajectory.

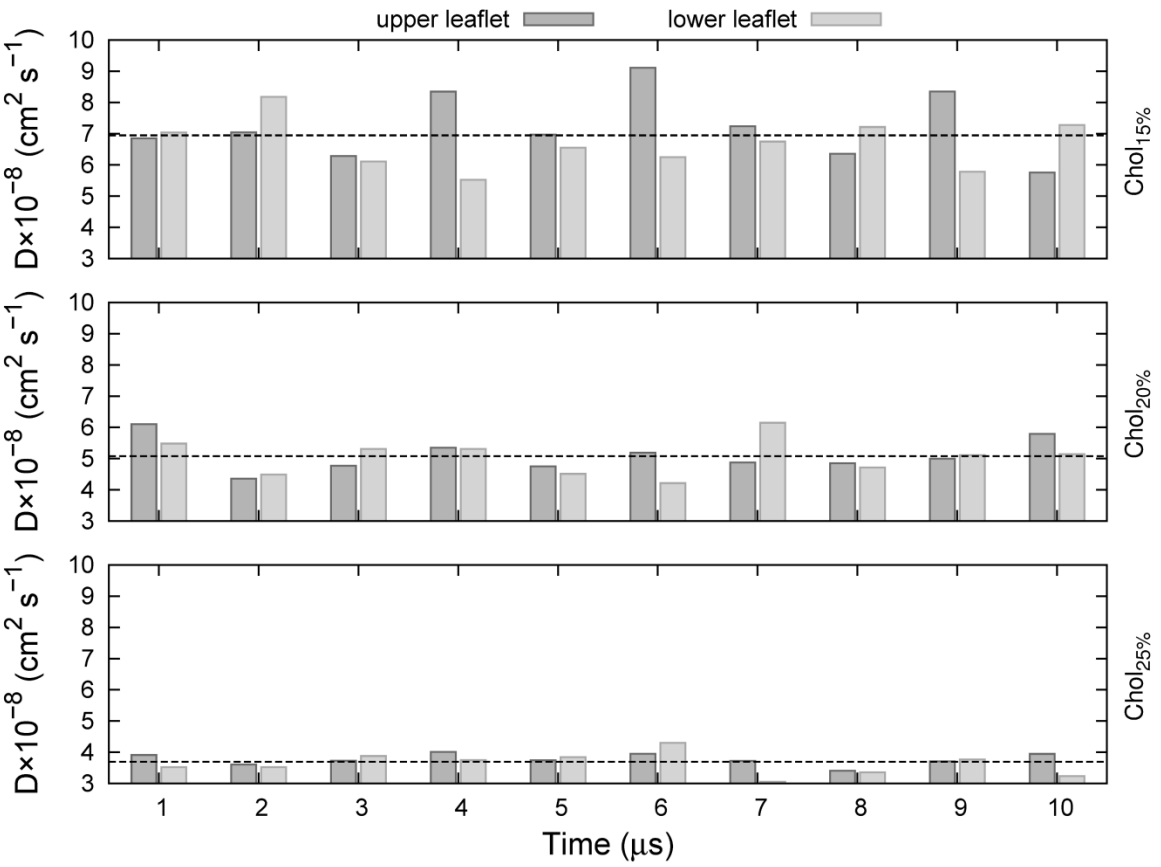

Fig. S7 Diffusion coefficient calculated for Chol lipid species in the three simulated systems plotted as a function of time. The diffusion coefficient is separately reported for the two bilayer leaflets, and the black broken line shows the average over the whole trajectory.