Supporting Information: Molecular simulation of rapid translocation of cholesterol, diacylglycerol and ceramide in model raft and non-raft membranes.

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Figures

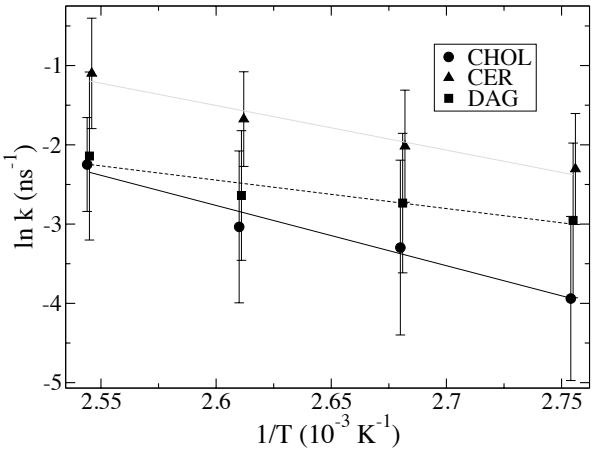

Figure S1: Arrhenius plots for the rate of the lipid moving from the bilayer center to its equilibrium position in the Raft bilayer. Least squares fits to the cholesterol (black), ceramide (grey) and diacylglycerol (dashed) data are shown. Error bars are the standard error of the mean from 41 independent simulations.

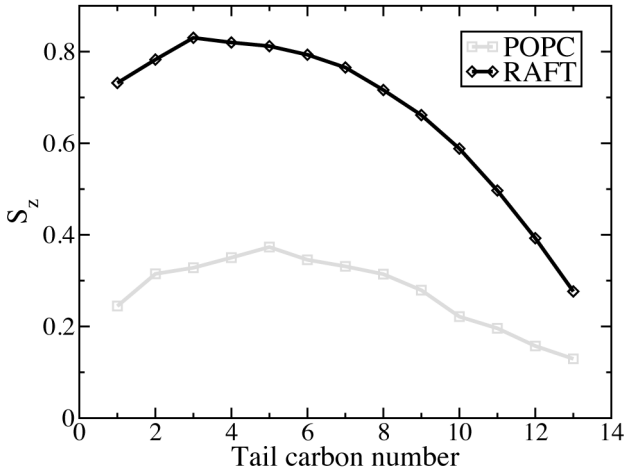

Figure S2: Chain order parameters for the palmitoyl chain of diacylglycerol in the POPC and Raft bilayers during an equilibrium simulation averaged over 50 ns. A value of 1 indicates perfect alignment of the chain with the bilayer normal, while 0 indicates a random orientation.

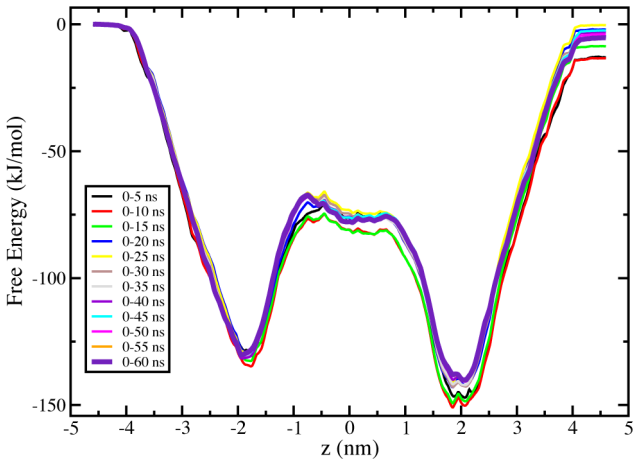

Figure S3: Free energy profiles for cholesterol moving from water to the bilayer center using different simulation lengths. Profiles for both bilayer leaflets are shown, and should be symmetric given infinite sampling. The PMFs were arbitrarily set to 0 kJ/mol at -4.6 nm from the bilayer center.