

## Supporting Information

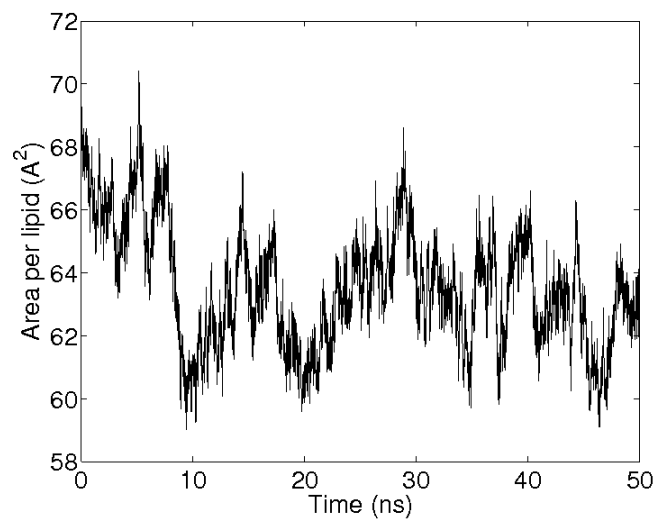


Figure S1: Area per lipid in a 50-ns NPT simulation of POPC. The  $x/y$  aspect ratio was allowed to change freely in the first 500 ps of simulation. The average area per lipid is  $62.6 \pm 1.3 \text{ \AA}^2$  calculated using the last 10 ns of the trajectory.

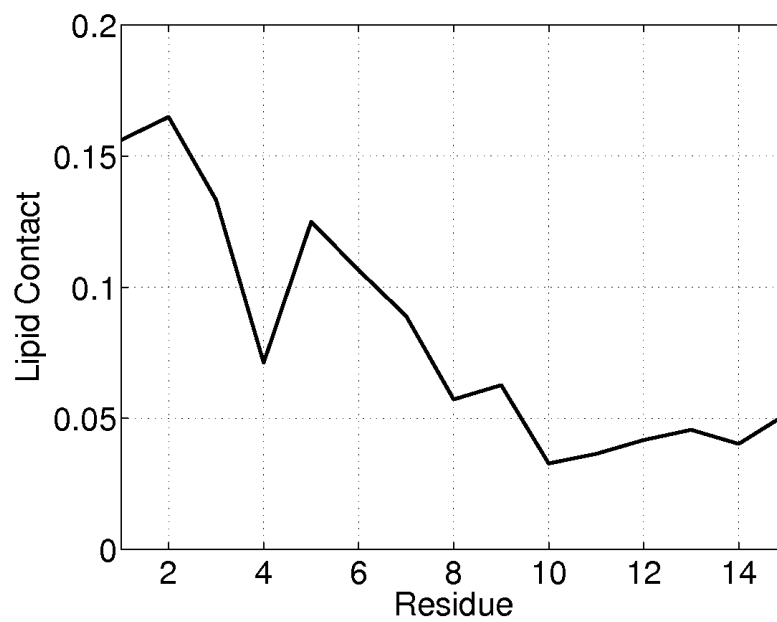


Figure S2: The number of peptide atoms in contact with lipid molecules in the CM15r-POPG:POPC simulation. See the Methods section and Fig 5 for calculation details.

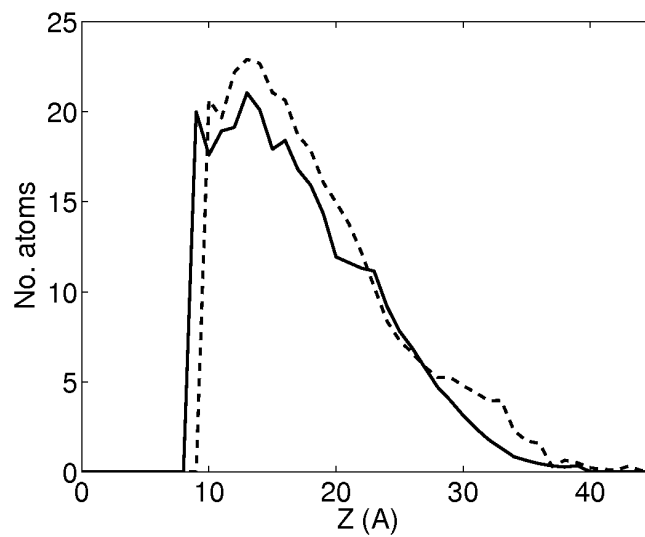


Figure S3: Total number of peptide atoms in contact with lipid molecules in the CM15r-POPC (solid) and CM15r-POPG:POPC (dashed) simulations.

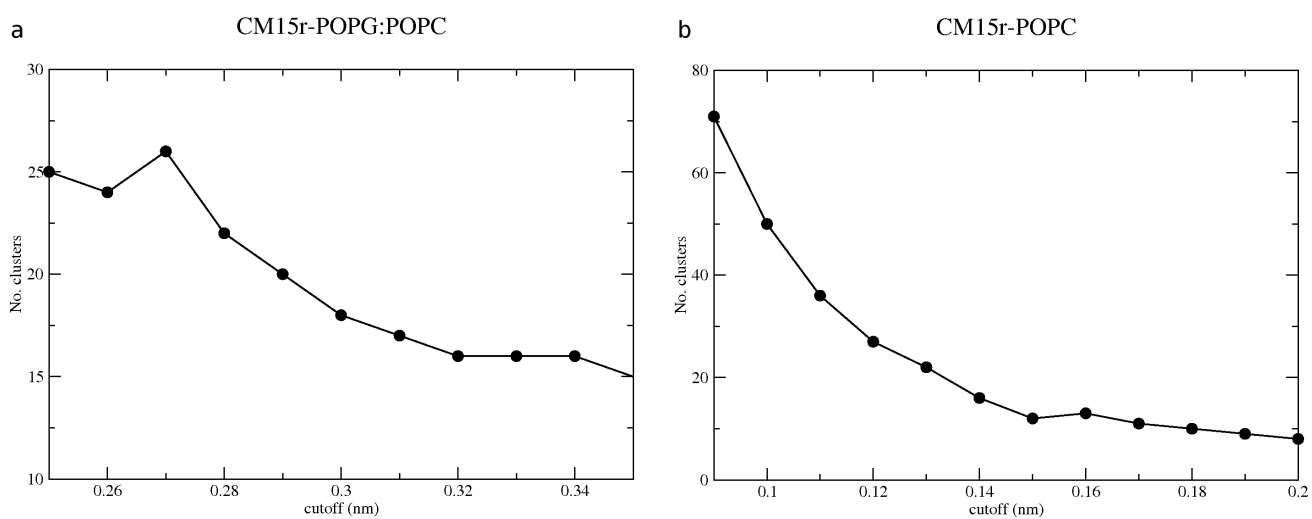


Figure S4: Parameter scan for the clustering analysis. The number of total clusters are plotted as a function of the cutoff used in the calculations. Cutoffs (0.32 nm for CM15r-POPG:POPC and 0.15 nm for CM15r-POPC) were chosen such that further increase in their values will not result in significant change in the number of clusters.

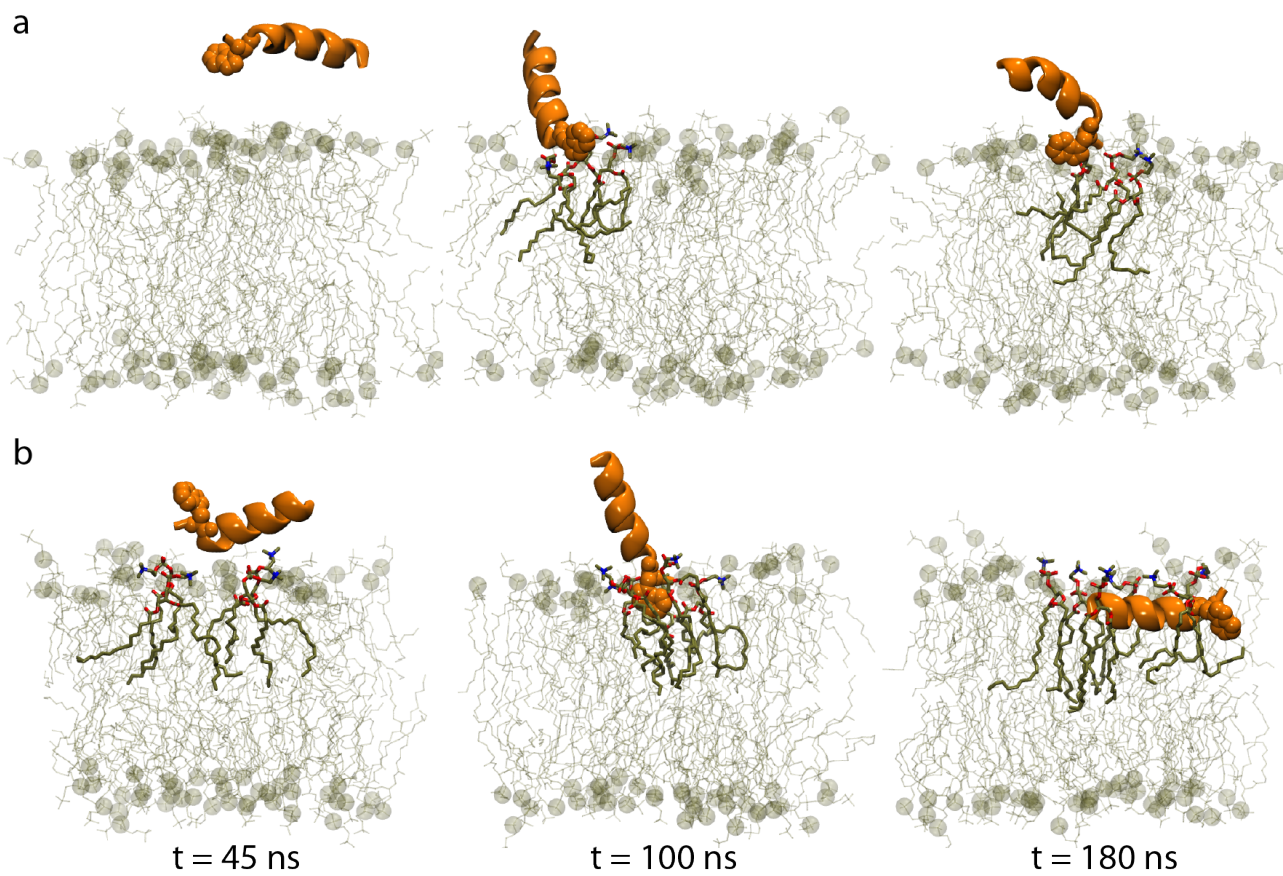


Figure S5: Snapshots of two 180-ns simulations of CM15H-POPC. Color scheme as Fig 3.

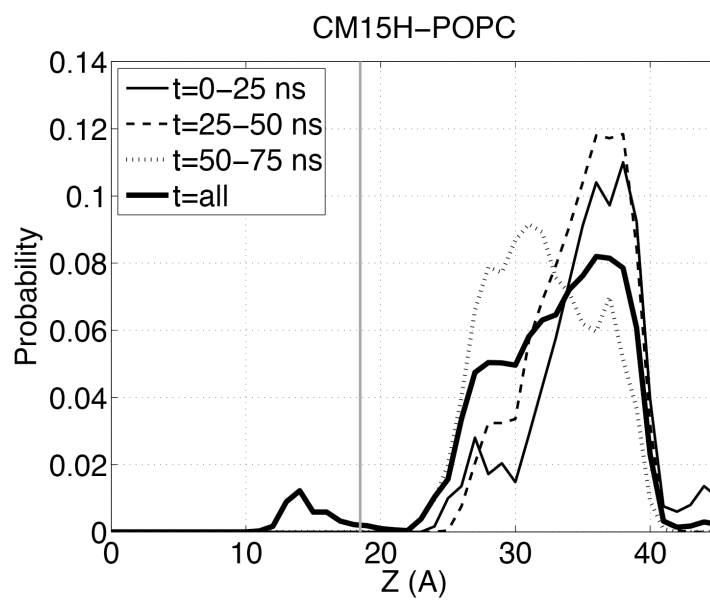


Figure S6: Center-of-mass distribution in the CM15H-POPC simulation.