Embedding A β 42 in Heterogeneous Membranes Depends on Cholesterol Asymmetries

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SUPPLEMENTARY MATERIAL

Figure S1. Results for the ~30% helical $A\beta 42$ peptide for the most asymmetric 30%/70% exo/cyto cholesterol distribution with 40% total cholesterol at 323K. (a) Free energy profile as a function of the distance between the centers of mass of the A β 42 peptide and lipid bilayer (D_{COM}) which shows that the entire peptide is *irreversibly* exposed to the extracellular region and to the membrane surface. (b) Solvent accessible surface area (SASA) at the free energy minimum which shows that the entire peptide is fully exposed to the membrane surface and solvent on the exofacial side.

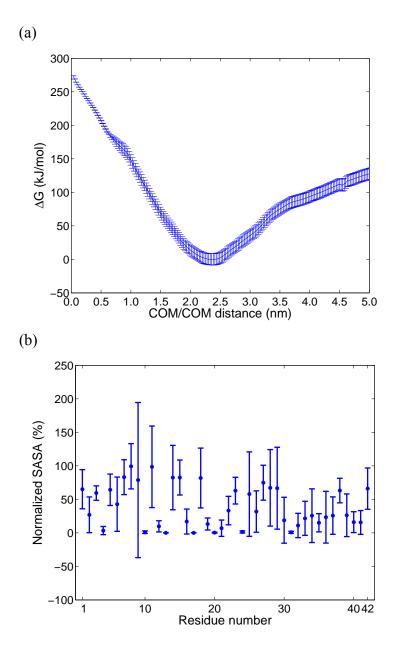


Figure S2. The radial distribution function of the $A\beta$ peptide with different lipid and sterol components for the symmetric 50%/50% exo/cyto cholesterol distribution with total cholesterol of 40%. This plot also includes the PE ligand whose trends are very similar to the PC RDF.

