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Scaling and Alpha-helix Regulation of Protein Relaxation in a Lipid Bilayer[1] K. CHENG, Trinity Univ, LIMING QIU, CREIGHTON BUIE, MARK VAUGHN, Texas Tech University — Protein conformation and orientation in the lipid membrane play a key role in many cellular processes. Here we use molecular dynamics simulation to investigate the relaxation and C-terminus diffusion of a model helical peptide: beta-amyloid (Aβ) in a lipid membrane. We observed that after the helical peptide was initially half-embedded in the extracellular leaflet of phosphatidylcholine (PC) or PC/cholesterol (PC/CHOL) membrane, the C-terminus diffused across the membrane and anchored to PC headgroups of the cytofacial lipid leaflet. In some cases, the membrane insertion domain of the Aβ was observed to partially unfold. Applying a sigmoidal fit to the process, we found that the characteristic velocity of the C-terminus, as it moved to its anchor site, scaled with $\theta_{\mathrm{u}}^{-4/3}$, where θ_{u} is the fraction of the original helix that was lost during a helix to coil transition. Comparing this scaling with that of bead-spring models of polymer relaxation suggests that the C-terminus velocity is highly regulated by the peptide helical content, but that it is independent of the amino acid type. The Aβ was stabilized by the attachment of the positive Lys28 side chain to the negative phosphate of PC or 3β oxygen of CHOL in the extracellular lipid leaflet and of the C-terminus to its anchor site in the cytofacial lipid leaflet.

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