Supporting Information

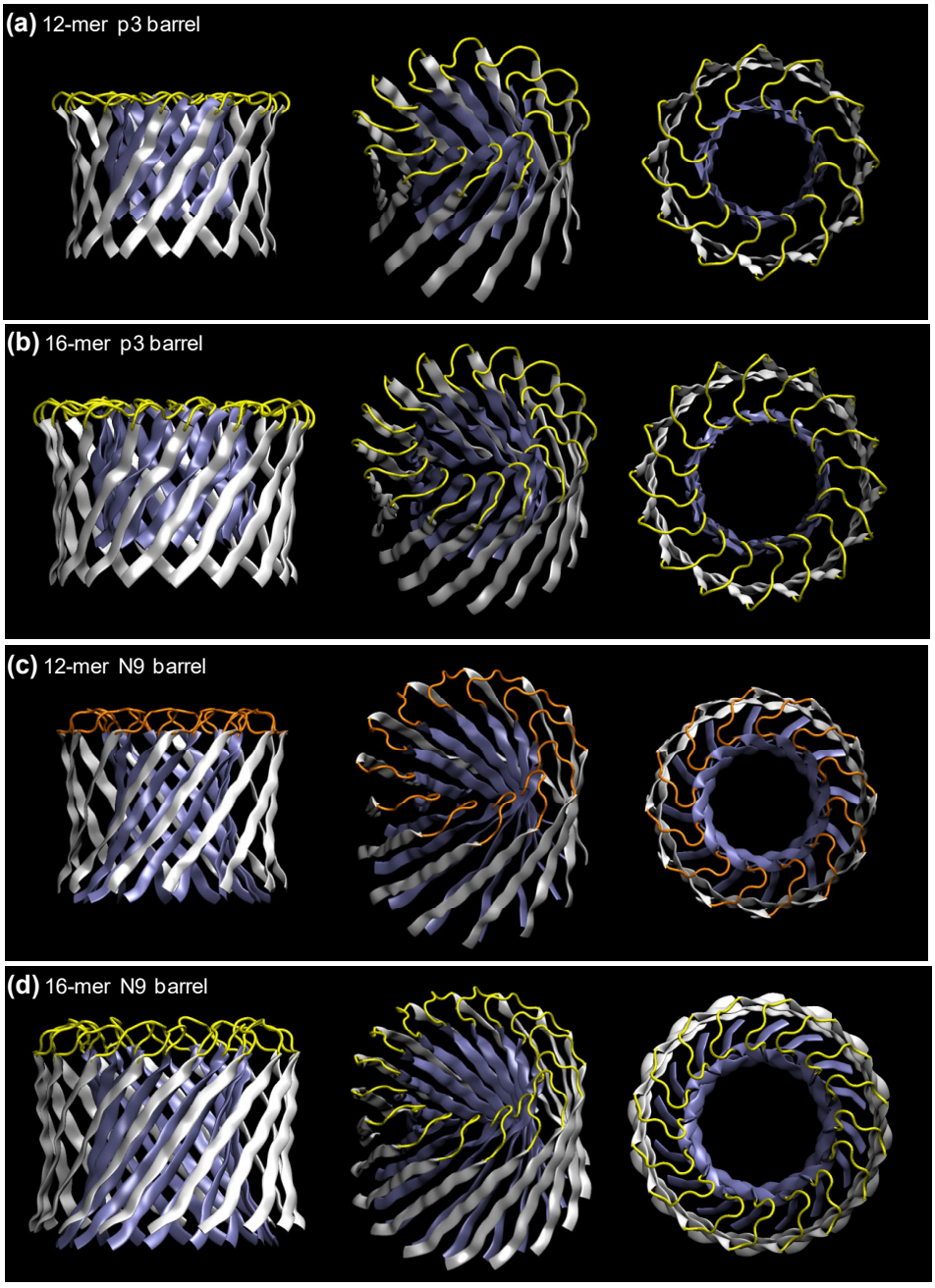

Fig. S1. Building smaller Aβ barrels. Conceptual design of annular structure for the (a) 12-mer p3, (b) 16-mer p3, (c) 12-mer N9, and (d) 16-mer N9 barrels embedded in the lipid bilayers. In

the peptide, the N-terminal β-strands are shown in cyan, the C-terminal β-strands are shown in white, and the loops connecting two strands are shown in yellow.

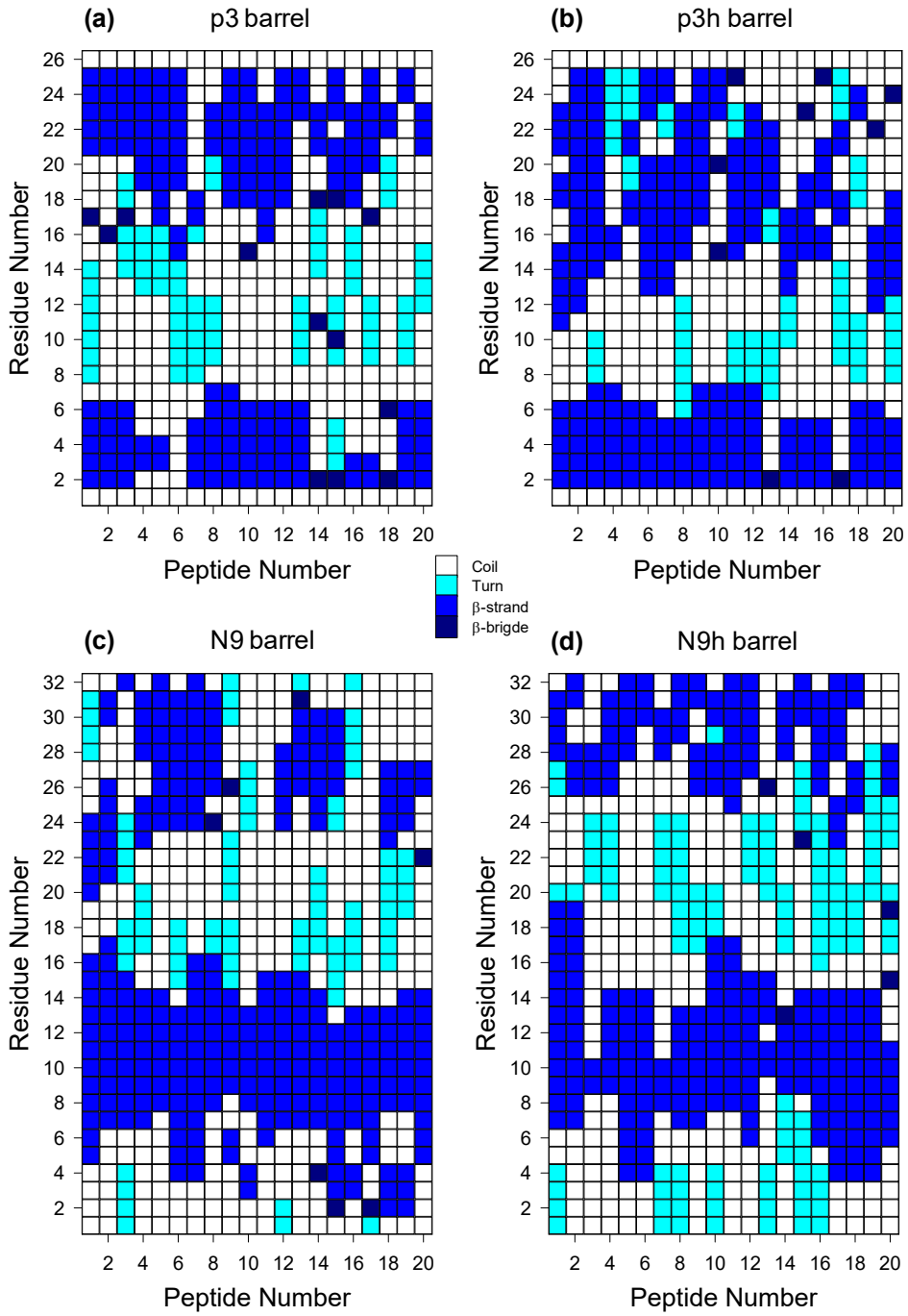

Fig. S2. The β-sheet structures in the barrels. The description of secondary structure by STRIDE for the 20-mer (a) p3, (b) p3h, (c) N9, and (d) N9h barrels.

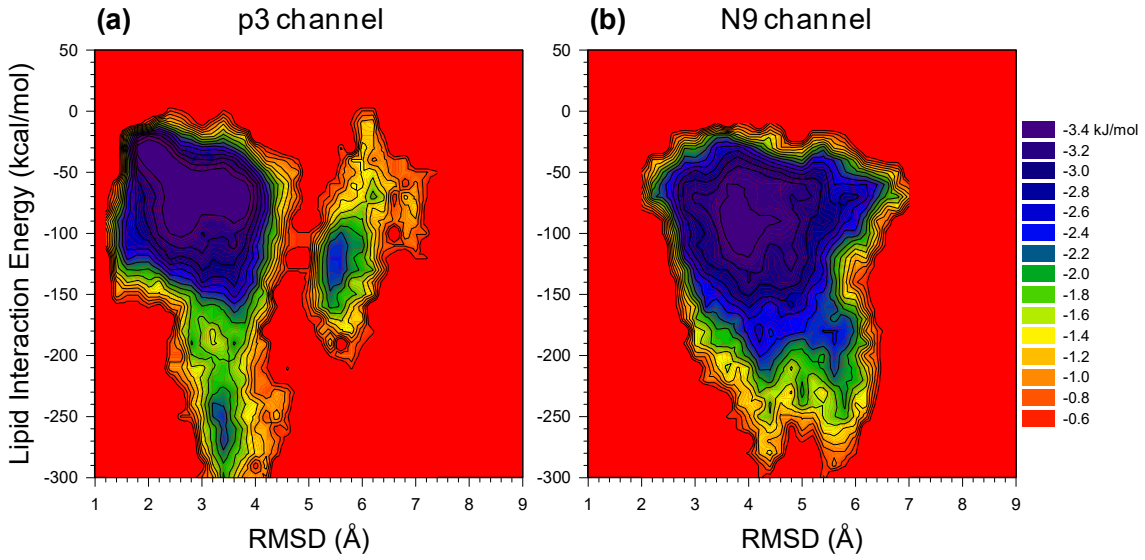

Fig. S3. Comparison of lipid interaction energies to Aβ channels. The relative free energy surface for the peptide-lipid interaction as a function of the root mean squared deviation (RMSD) from the starting point for the 20-mer (a) p3 and (b) N9 channels from previous simulations.

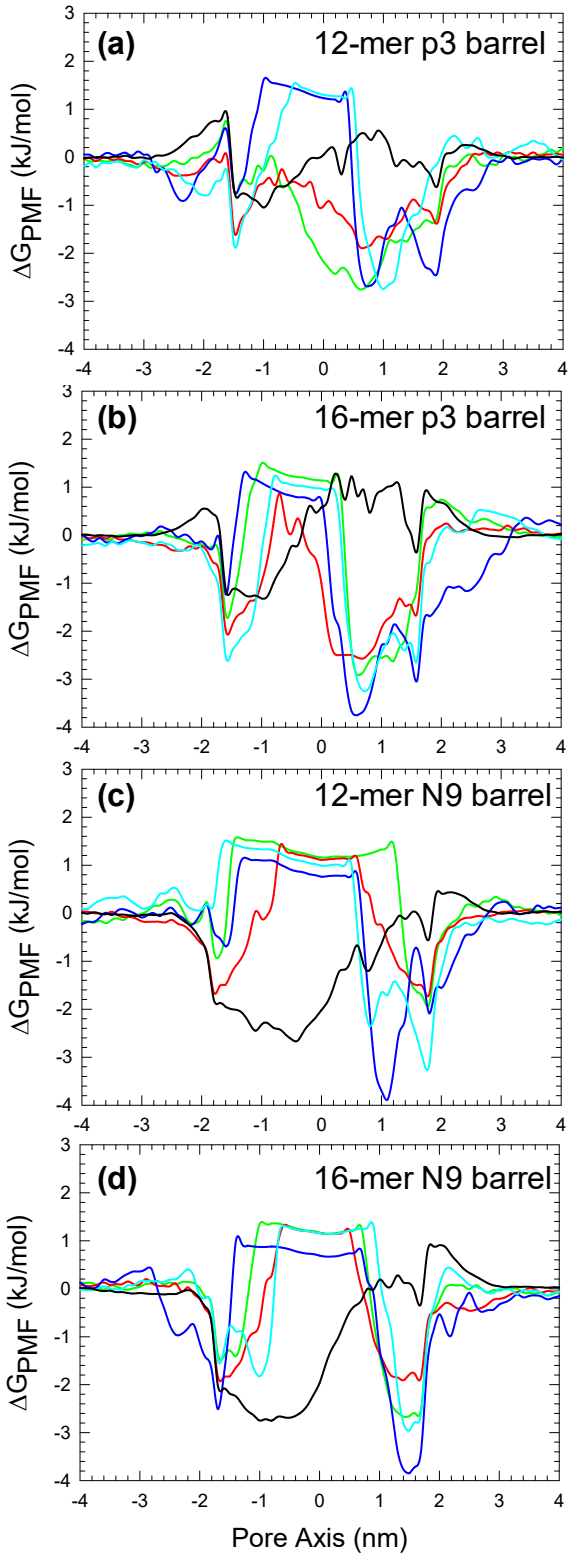
(a)
12-mer p3 barrel
(b)
16-mer p3 barrel
(c)
12-mer N9 barrel
(d)
16-mer N9 barrel
ΔGPMF (kJ/mol)
Pore Axis (nm)

Fig. S4. Ion-permeable Aβ barrels. Potential of mean force (PMF), ΔG_{PMF}, calculated using the equation $\Delta G_{\mathrm{PMF}} = -k_B T \ln\left(\rho_z / \rho_{\mathrm{bulk}}\right)$, where k_{B} is the Boltzmann constant, T is the simulation temperature, ρ_{z} is the ion density at the position z along the pore axis, and ρ_{bulk} is the ion density in the bulk region, representing the relative free energy profile for Mg^{2+} (green lines), K^{+} (red lines), Ca^{2+} (blue lines), Zn^{2+} (cyan lines), and Cl^{-} (black lines) as a function of the distance along the pore center axis for the (a) 12-mer p3, (b) 16-mer p3, (c) 12-mer N9, and (d) 16-mer N9 barrels.