Supporting Information for

Structural Convergence Among Diverse Toxic β-Sheet Ion Channels

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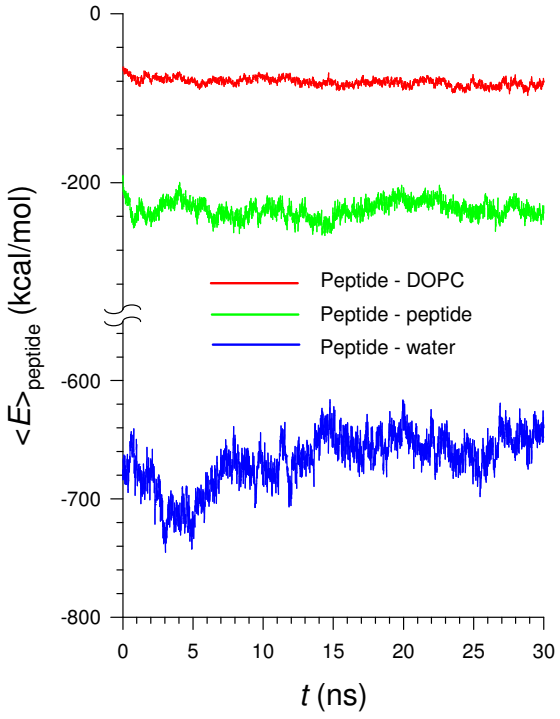

Figure S1. Time series of averaged peptide interaction energy with DOPC lipids (red line), other peptides (green line), and water (blue line) for the 20-mer p3 ($A\beta_{17-42}$) channel.

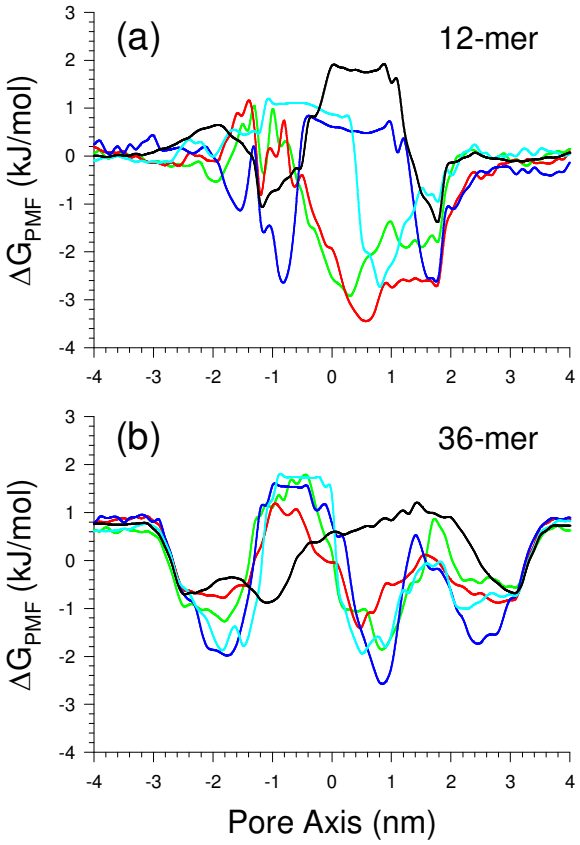

Figure S2. Potential of mean force (PMF), ΔG_{PMF}, calculated using the equation $\Delta G_{PMF} = -k_B T \ln(\rho_z/\rho_{bulk})$, where k_B is the Boltzmann constant, T is the simulation temperature, ρ_z is the ion density at the position z along the pore axis, and ρ_{bulk} is the ion density in the 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 and (b) 36-mer p3 ($A\beta_{17-42}$) channels. The PMF results for the 16- and 36-mer were obtained from the simulations in the zwitterionic DOPC bilayer.