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Supplemental Information

Peptide-Lipid Interaction Sites Affect Vesicles' Responses to Antimicrobial Peptides

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Supplementary Material for

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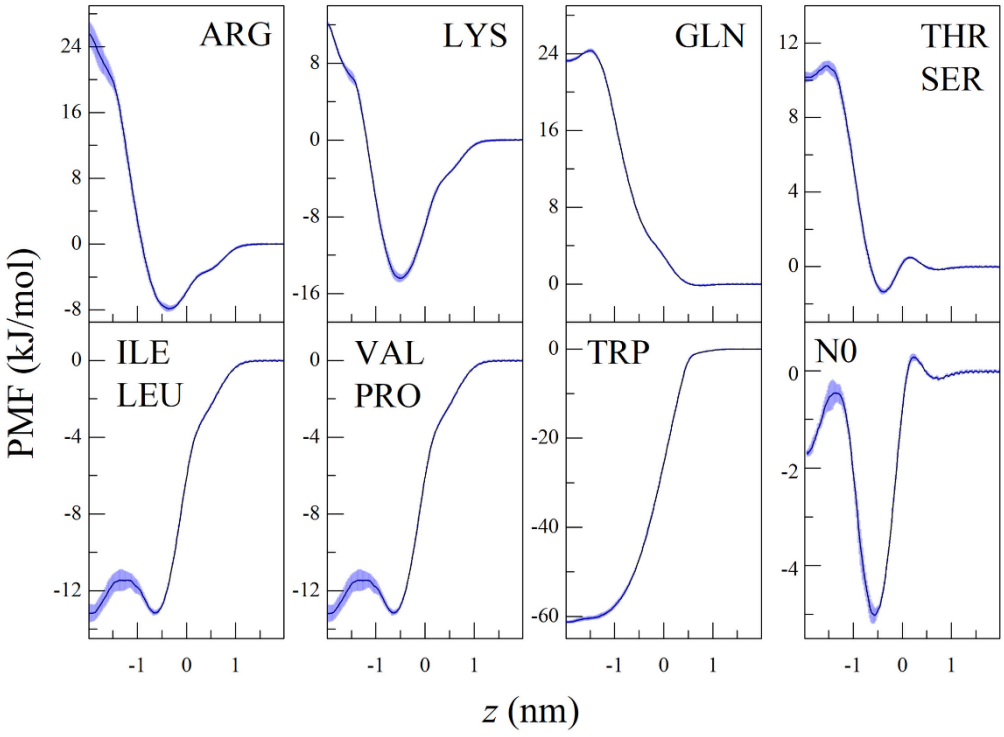

Figure S1. PMF for moving typical amino acid side-chain analogues and backbone bead (N0) across a DOPC bilayer as a function of the distance *z* from the phosphate group in bilayer normal direction calculated by using Dry MARTINI force field.

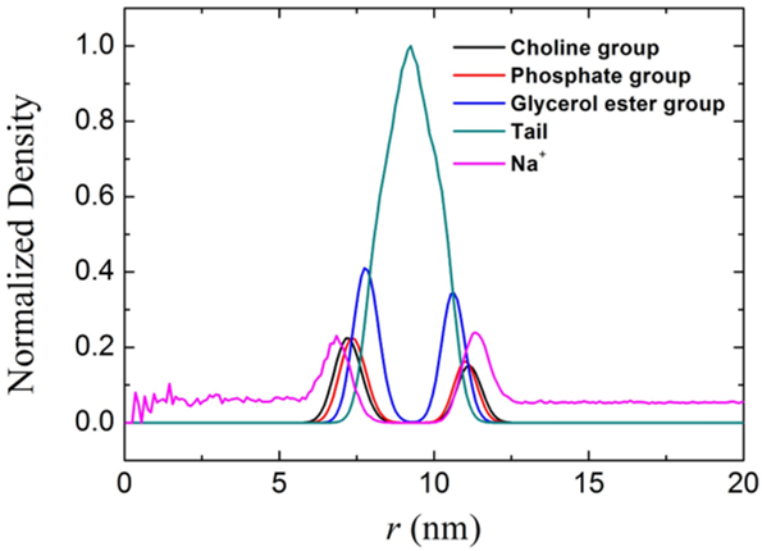

Figure S2. Normalized density distribution profiles of lipid beads and counter ions as a function of distance relative to the vesicle center for a vesicle containing 3200 DOPC/DOPG lipids. The density of the counter ions is magnified 100 times for a clear view.

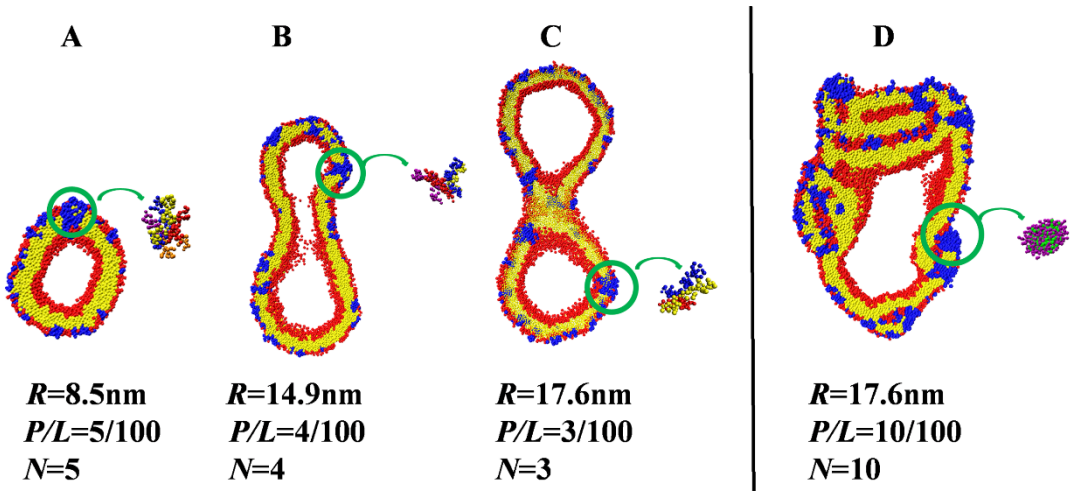

Figure S3. (A)-(C) Melittin-induced membrane pores on different-sized vesicles. The peptides in a largest pore (circled region) are amplified and presented in different colors. (D) Melittin oligomer bound on the exterior surface of a large vesicle. The hydrophilic and charged side-chain beads of the peptides are in purple color, while the hydrophobic side-chain beads and backbone beads are in green color.

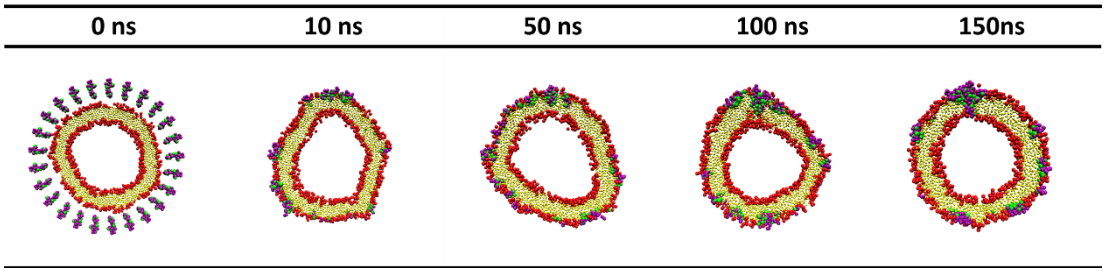

Figure S4. Snapshots of melittin binding, penetration, and insertion in the early stage of peptide-vesicle assembling process (corresponding to Figure 5A). For clear views of these states, the hydrophilic and charged side-chain beads of the peptides are in purple color, the hydrophobic side-chain beads and backbone beads are in green color, the tail beads of the lipids are transparent.

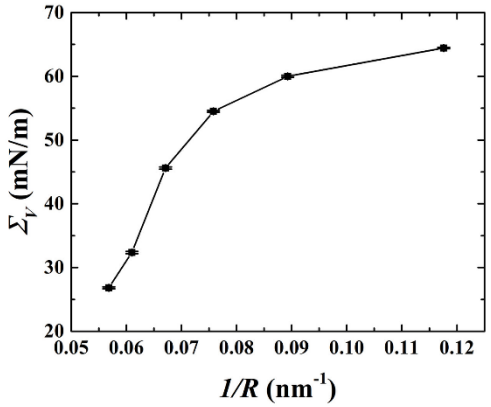

Figure S5. Membrane tension as a function of vesicle's curvature. Each datum was obtained from 500 samples evenly chosen from a trajectory in the last 500 ns.

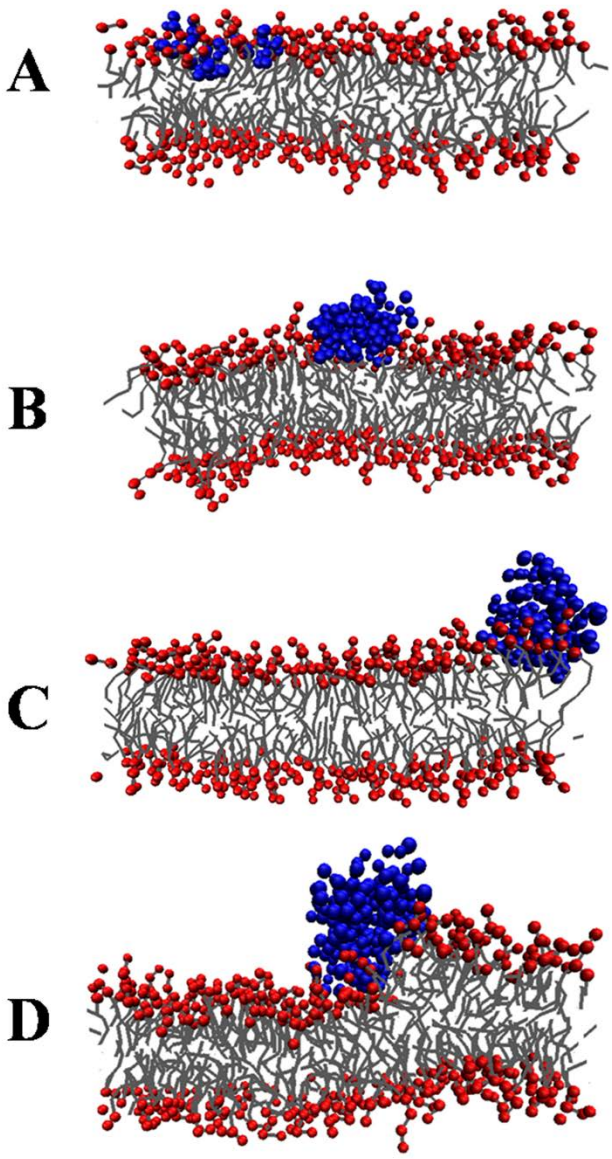

Figure S6. Snapshots of a melittin (A) monomer, (B) dimer, (C) trimer, and (D) tetramer bound on an initially tensionless planar lipid bilayer. For a clear view of the orientation of the lipid tails, bonds present them.

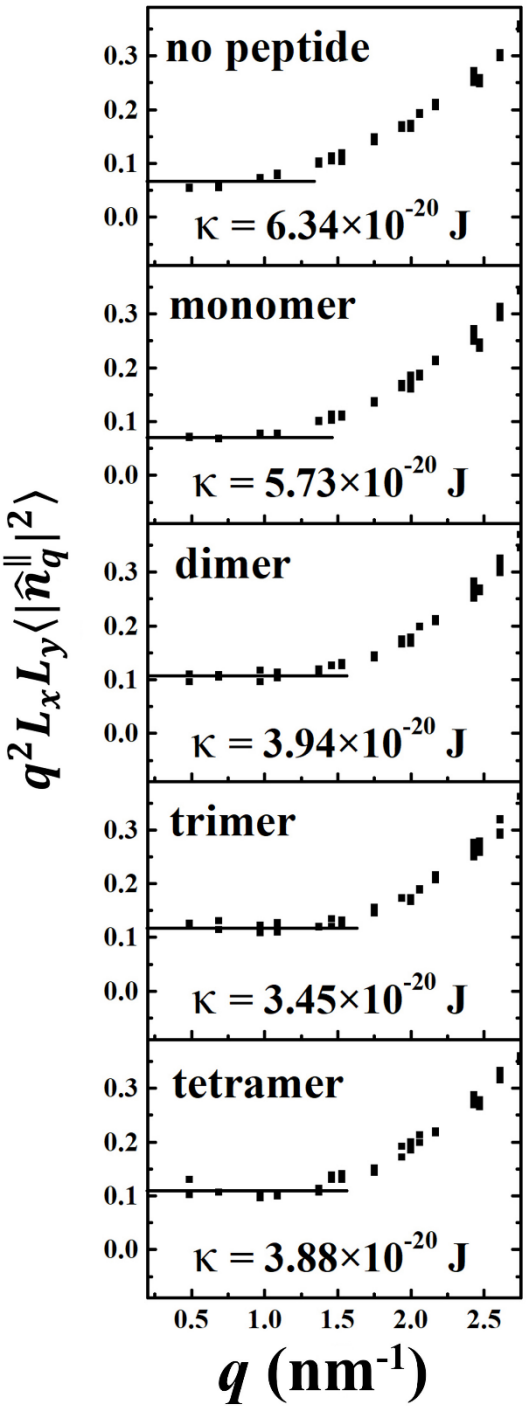

Figure S7. Spectrum of longitudinal lipid orientation fluctuations of an initially tensionless planar lipid bilayer before binding of peptide and after binding of a melittin monomer, dimer, trimer, and tetramer.

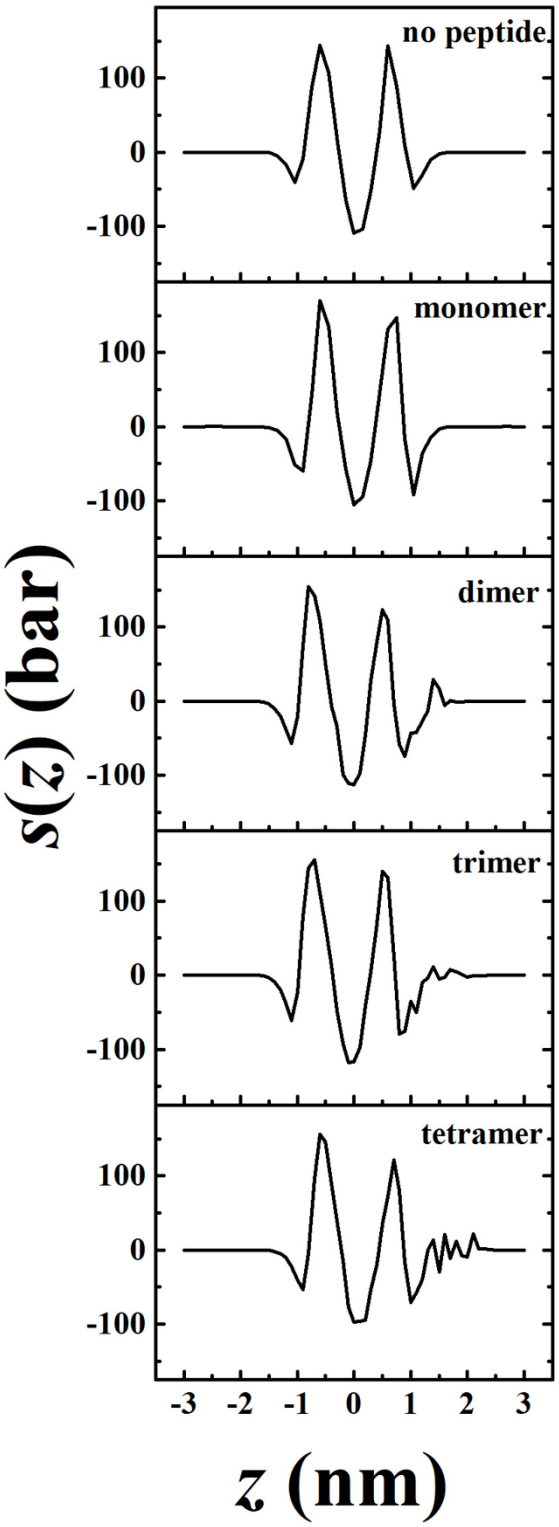

Figure S8. Stress profile of an initially tensionless planar lipid bilayer before binding of peptide and after binding of a melittin monomer, dimer, trimer, and tetramer.