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Supplemental Information

Simulations of Membrane-Disrupting Peptides I: Alamethicin Pore Stability and Spontaneous Insertion

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Supplemental Materials

Multi-μs simulations of membrane disrupting peptides I: alamethicin pore stability and spontaneous insertion

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Figure S1. Starting configuration of the surface-bound alamethicin. The peptides are colored by residue type (nonpolar residues are orange, polar residues are green, and the charged residue (glutamic acid) is red). Lipids are shown as sticks with the phosphorus atoms as gray spheres.

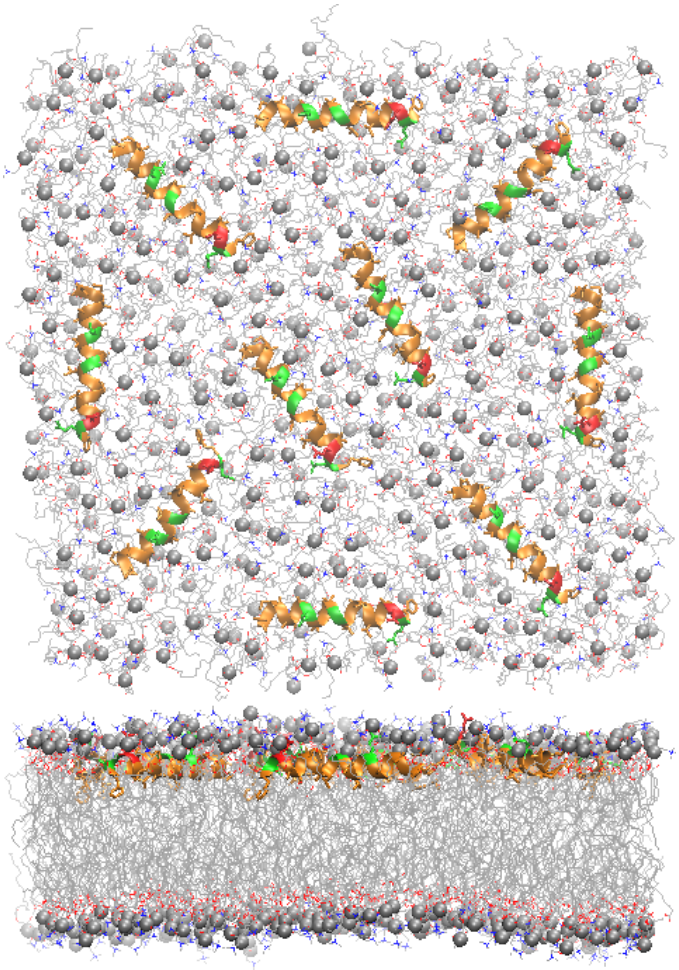


Figure S2. Left) Time series of the peptide fold (α-helix (red), 3-10-helix (green), hydrogen-bonded turn (black), bend (gray), and unstructured loop (white)) for each peptide in the 14 us alamethicin pore simulation. Right) Breakdown of the fold by percentage.

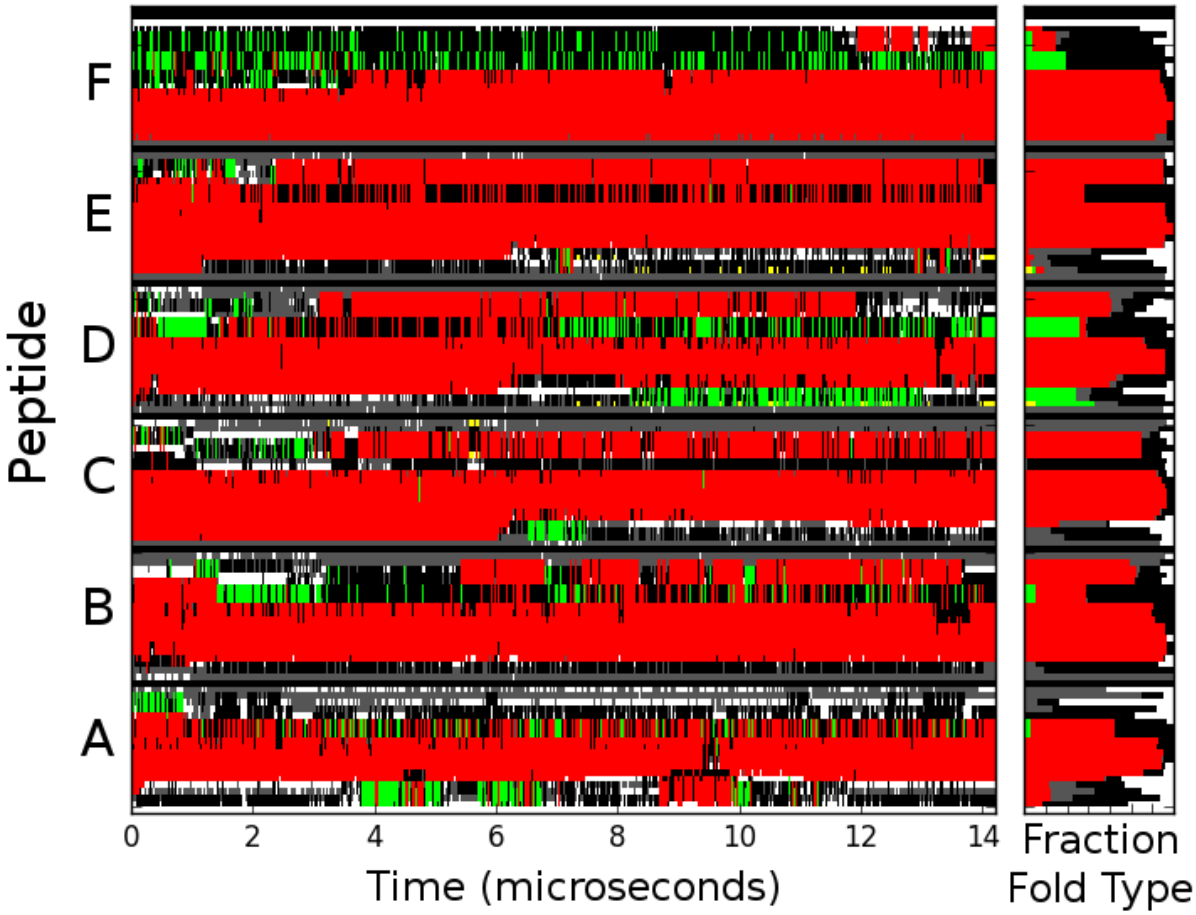


Figure S3. Left) Time series of the peptide fold (α-helix (red), 3-10-helix (green), hydrogen-bonded turn (black), bend (gray), and unstructured loop (white)) for each peptide in the transmembrane alamethicin simulation. Right) Breakdown of the fold by percentage.

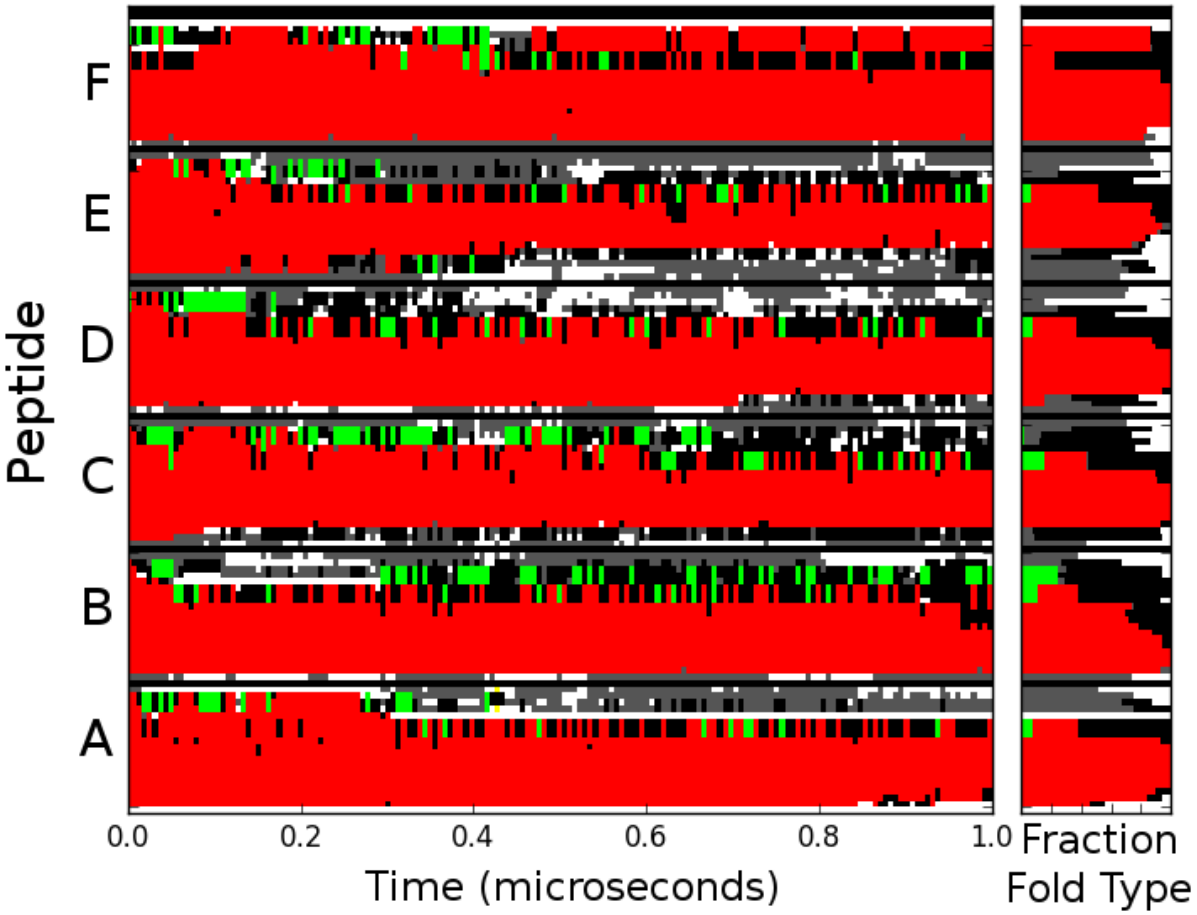


Figure S4. Left) Time series of the peptide fold (α-helix (red), 3-10-helix (green), hydrogen-bonded turn (black), bend (gray), and unstructured loop (white)) for each peptide in the surface-bound alamethicin simulation. Right) Breakdown of the fold by percentage.

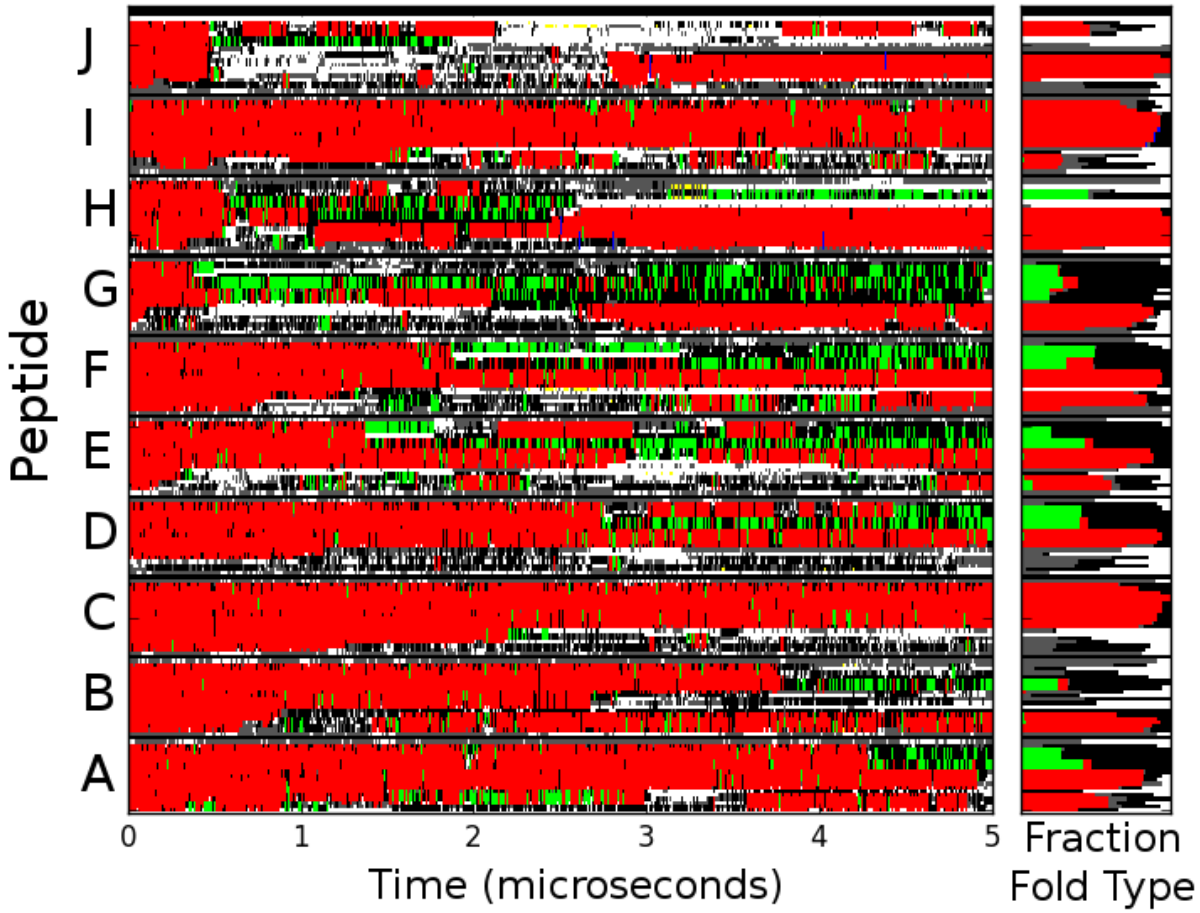


Figure S5. Transmembrane alamethicin peptides in parallel (top) and antiparallel (bottom) orientations after 1 μs. The peptides are colored by residue type (nonpolar residues are orange, polar residues are green, and the charged residue (glutamic acid) is red). Lipid phosphorus atoms are gray spheres. Waters are transparent vdW spheres. Lipids are omitted for clarity.

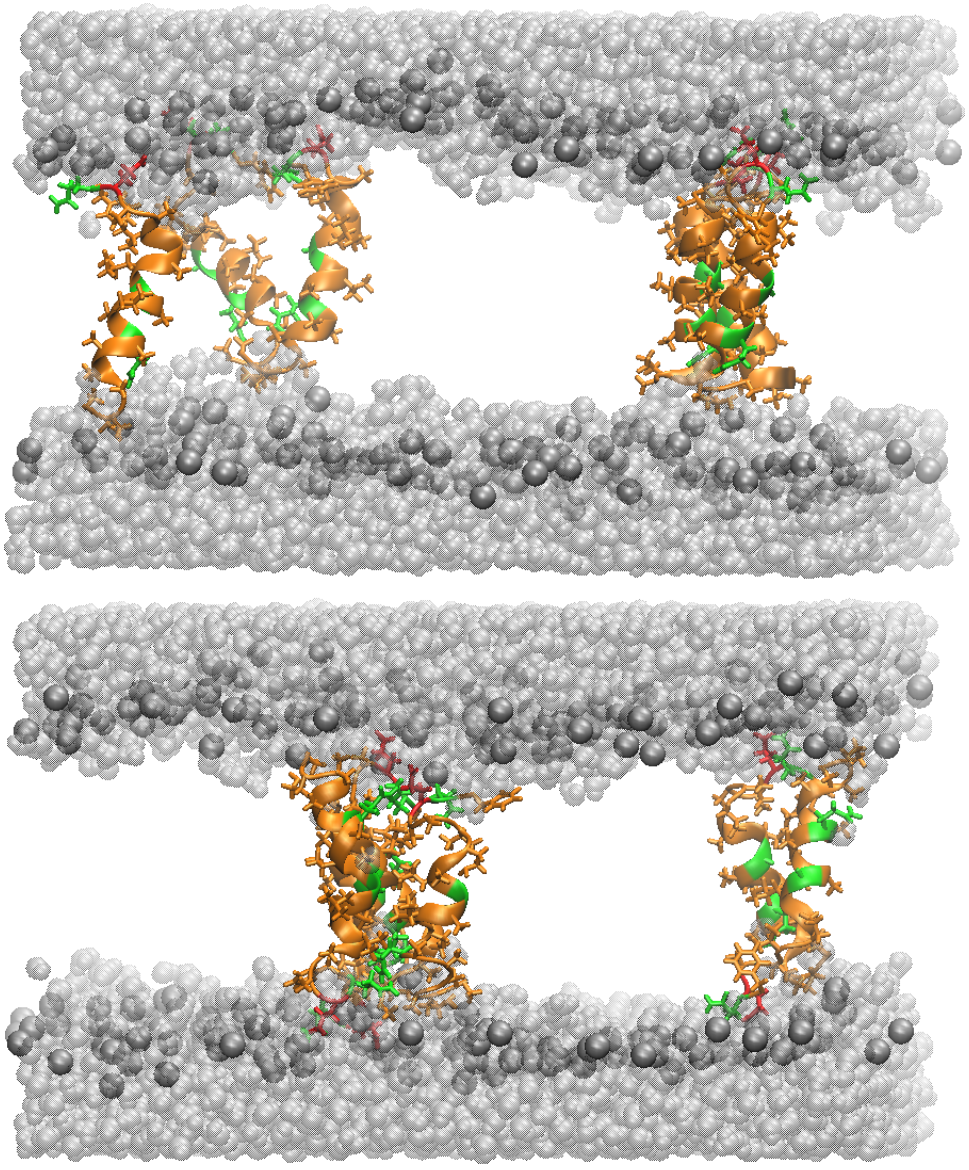
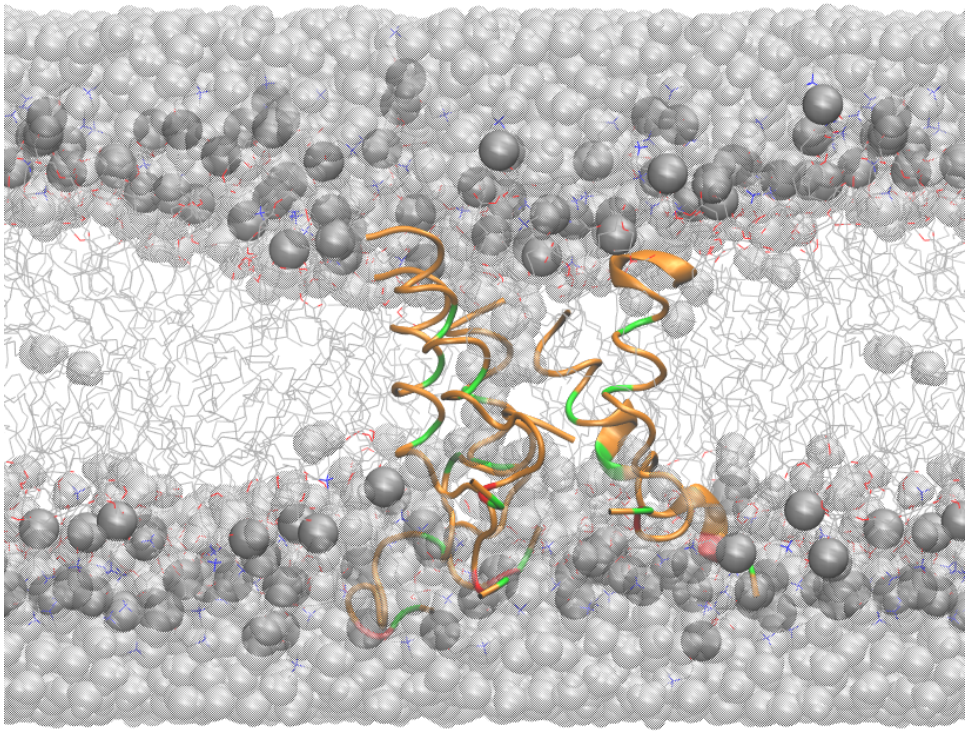


Figure S6. Alamethicin pore after 1 μs at 413K and with a -0.2 V electric field. The peptides are colored by residue type (nonpolar residues are orange, polar residues are green, and the charged residue (glutamic acid) is red). Lipids are shown as sticks with phosphorus atoms as gray spheres. Waters are transparent vdW spheres.



```
* Stream file for 2-Aminoisobutyric acid
*

read rtf card @app
* Topology for 2-Aminoisobutyric acid
*
31  1

DECL -CA
DECL -C
DECL -O
DECL +N
DECL +HN
DECL +CA
DEFA FIRS NTER LAST CTER
AUTO ANGLES DIHE

RESI AIB          0.00
GROUP
ATOM N    NH1    -0.47  !      | HB1 HB2
ATOM HN   H       0.31  !  HN-N  | /
ATOM CA   CT1     0.16  !      |  CB--HB3
GROUP                   !      | /
ATOM CB   CT3    -0.27  !     CA    HC1
ATOM HB1  HA3     0.09  !      | \  /
ATOM HB2  HA3     0.09  !      |  CC--HC2
ATOM HB3  HA3     0.09  !   O=C   \
GROUP                   !      |    HC3
ATOM CC   CT3    -0.27  !
ATOM HC1  HA3     0.09
ATOM HC2  HA3     0.09
ATOM HC3  HA3     0.09
GROUP
ATOM C    C       0.51
ATOM O    O      -0.51
BOND CB CA  N  HN  N  CA
BOND C  CA  C  +N  CB HB1  CB HB2  CB HB3
BOND CC CA  CC HC1  CC HC2  CC HC3
DOUBLE O  C
IMPR N -C CA HN  C CA +N O
CMAP -C  N  CA  C   N  CA  C  +N
DONOR HN N
ACCEPTOR O C
IC -C   CA   *N   HN    1.3551 126.4900  180.0000 115.4200  0.9996
IC -C   N    CA   C     1.3551 126.4900  180.0000 114.4400  1.5390
IC N    CA   C    +N    1.4592 114.4400  180.0000 116.8400  1.3558
IC +N   CA   *C   O     1.3558 116.8400  180.0000 122.5200  1.2297
IC CA   C    +N   +CA   1.5390 116.8400  180.0000 126.7700  1.4613
IC N    C    *CA  CB    1.4592 114.4400  123.2300 111.0900  1.5461
IC N    C    *CA  CC    1.4592 114.4400 -120.4500 106.3900  1.0840
IC C    CA   CB   HB1   1.5390 111.0900  177.2500 109.6000  1.1109
IC HB1  CA   *CB  HB2   1.1109 109.6000  119.1300 111.0500  1.1119
IC HB1  CA   *CB  HB3   1.1109 109.6000 -119.5800 111.6100  1.1114
IC C    CA   CC   HC1   1.5390 111.0900 -177.2500 109.6000  1.1109
IC HC1  CA   *CC  HC2   1.1109 109.6000 -119.1300 111.0500  1.1119
IC HC1  CA   *CC  HC3   1.1109 109.6000  119.5800 111.6100  1.1114

end

return
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