Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Molecular Mechanisms of Pore Formation and Membrane Disruption by the Antimicrobial Lantibiotic Peptide Mutacin 1140

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Table S1: List of different systems and the lengths of the simulations used in this work.

Membrane Systems	Number of Atoms	Simulation Time (ns)
MU1140 chain on the membrane surface	41190	500
MU1140-Lipid II on the membrane surface	61046	500
MU1140-Lipid II on the HMMM surface	45850	1,000
MU1140 chain in the bilayer	36296	500
One MU1140-Lipid II complex in the bilayer	48813	500 × 2 replicas
Two MU1140-Lipid II complexes in the bilayer	40582	500 × 2 replicas
Four MU1140-Lipid II complexes in the bilayer	54752	500 × 2 replicas

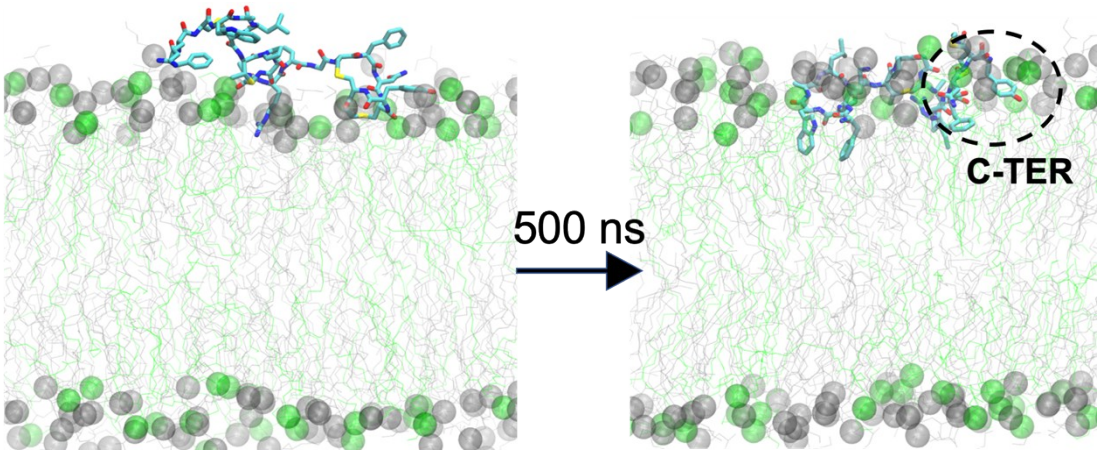

Figure S1. Snapshots of the MU1140 chain on the membrane surface at 0 and 500 ns. The MU1140 chain not complexed with lipid II shows less insertion into the membrane, compared to the one from MU1140-Lipid II complex (Fig. 2a).

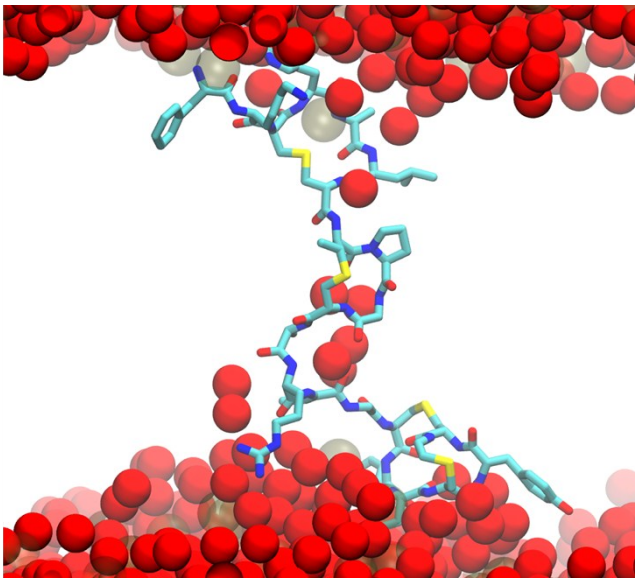

Figure S2. Water permeation by single MU1140 chain in the absence of lipid II interactions (snapshot at 500 ns). When placed in the transmembrane region, a single chain of MU1140 can permeate the water across the bilayer in the same manner as the MU1140 complexed with lipid II. Water molecules are shown as red spheres.

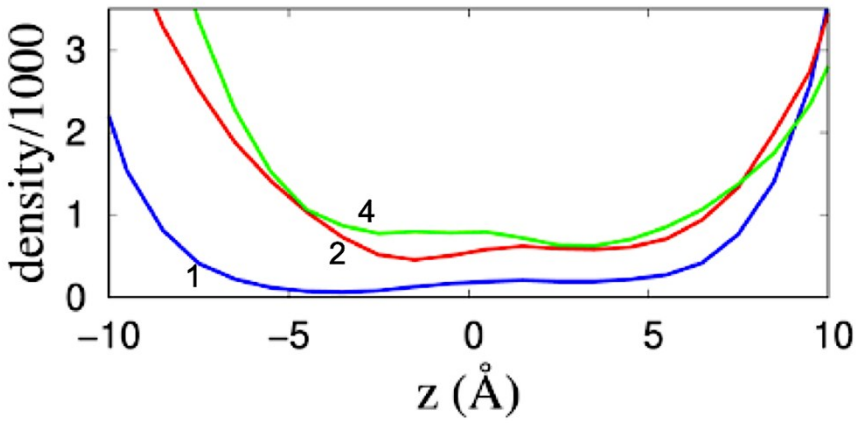

Figure S3. Density profile of the water molecules in the transmembrane region of the lipid bilayer for one, two, and four complexes of MU1140-lipid II (same as Fig. 7d but for a separate replica).