Molecular Dynamics Modeling of Pseudomonas Aeruginosa Outer Membranes

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Supplementary Figures

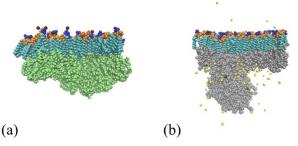


Figure S1. The snapshots of unphysical deformation of (a) Lipid A–DOPE and (b) Lipid A–DOPG membrane. The color scheme of Lipid A functional groups is the same as in Figure 1. Black and yellow atoms represent calcium and sodium ions, respectively. DOPE and DOPG molecules are colored in green and silver, respectively.

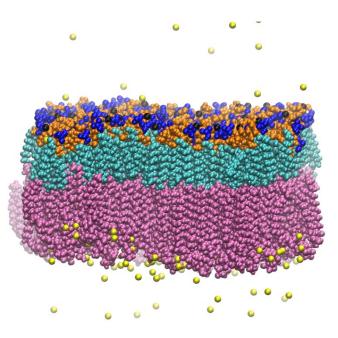


Figure S2. The snapshot of Lipid A–DPPG membrane with 180 DPPG molecules in the lower leaflet.

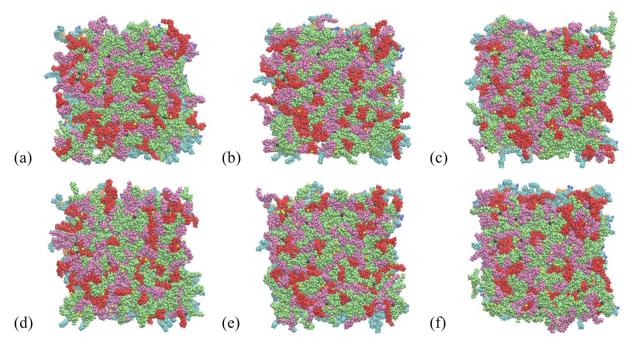


Figure S3. Bottom views of Lipid A – Mixture membrane at (a) 0 ns, (b) 200 ns, (c) 400 ns, (d) 600 ns, (e) 800 ns and (f) 1000 ns. Black and yellow atoms represent calcium and sodium ions, respectively. DPPE, DOPE, DPPG molecules are colored in red, green, and purple, respectively.