

## **Supporting Information for**

### **Biophysical mechanisms of membrane thickness dependent MscL gating: An all atom molecular dynamics study**

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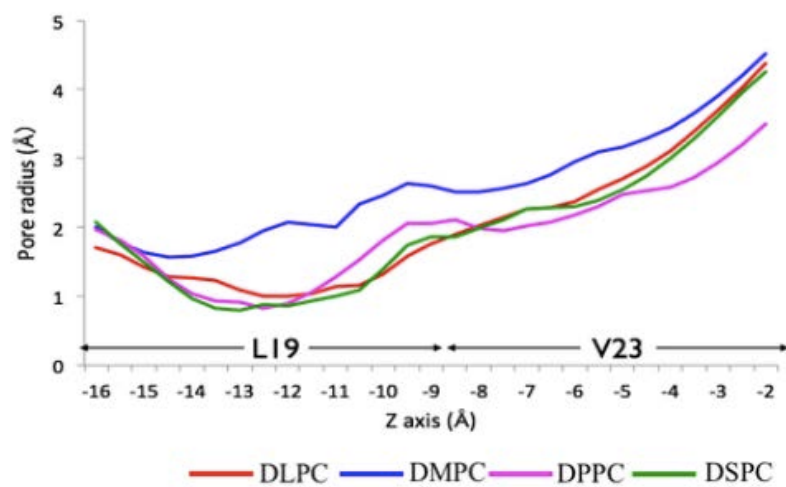
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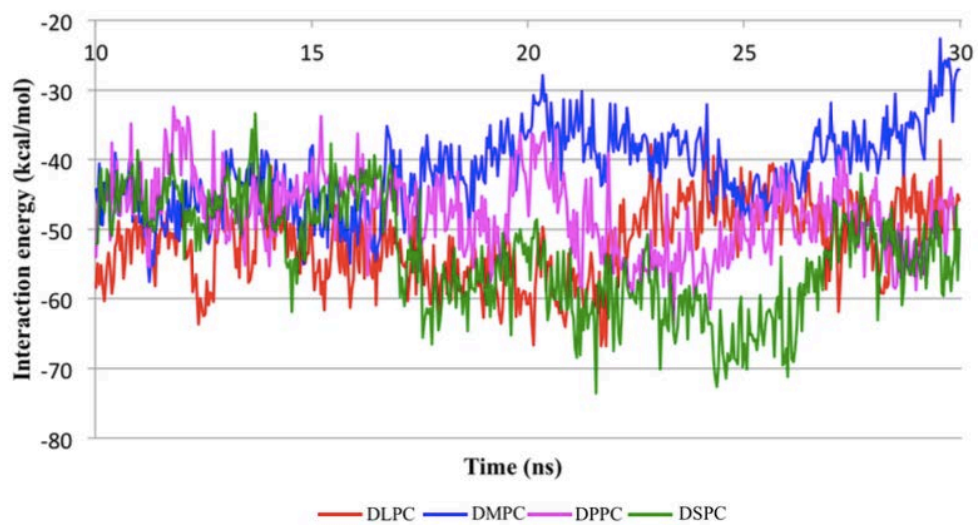
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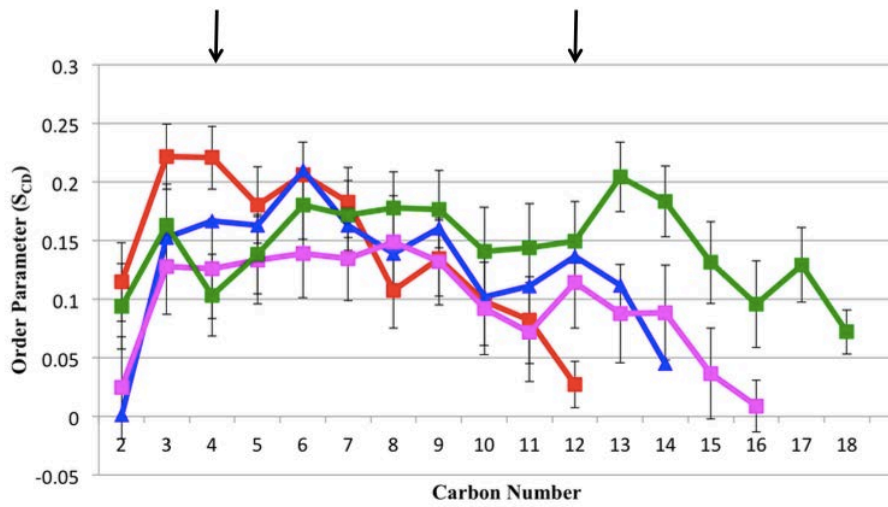
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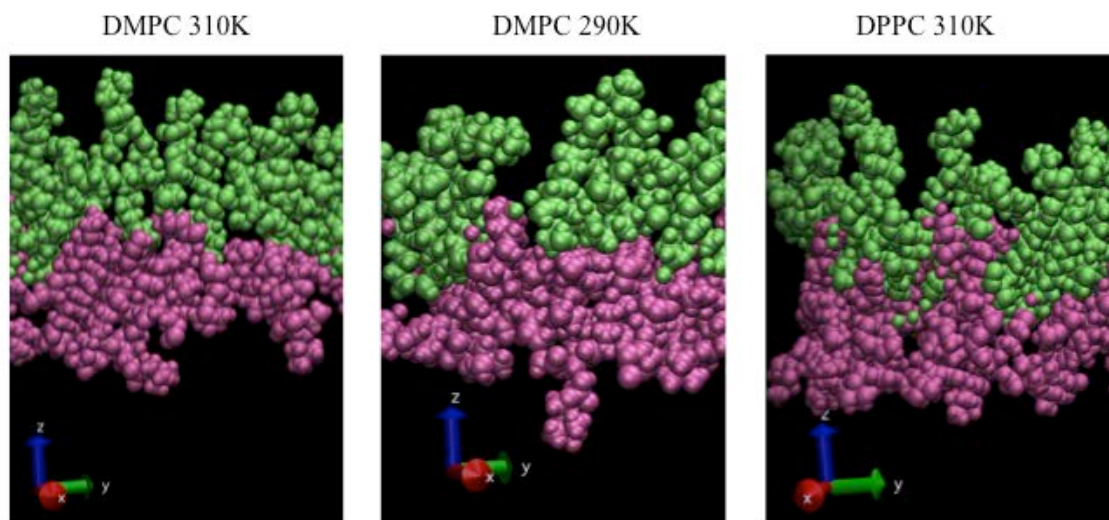
**Figure S1.** Pore radius profile of the gating region consisting of L19 and V23 in the membranes with different thicknesses after 30 ns equilibration. The radius at the narrowest part of the pore ranges 1.0-1.8 Å. Solid curves indicate radius profiles from DLPC (red), DMPC (blue), DPPC (magenta) and DSPC (green) membranes.



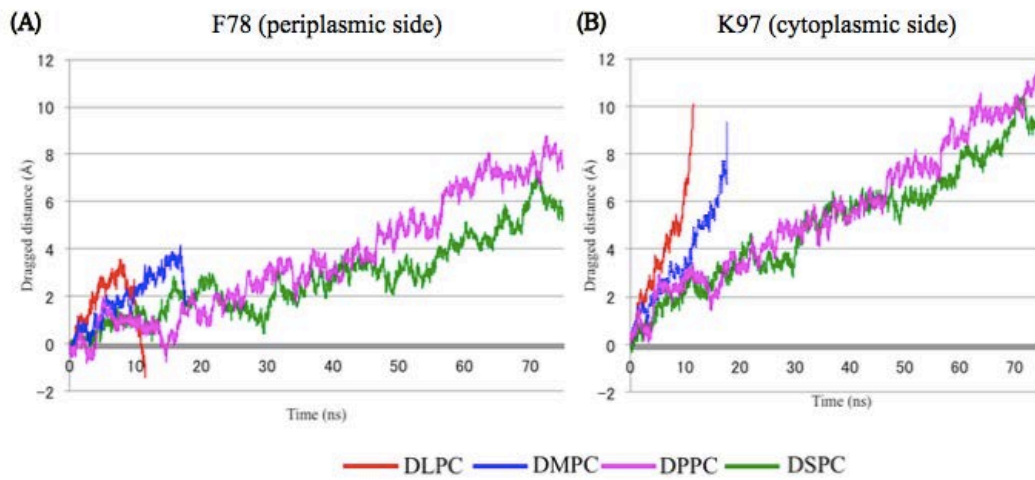
**Figure S2.** Time profiles of interaction energy between F78 of TM2-helix and neighboring lipids in the membranes with different thicknesses for 20 ns after 10 ns equilibration. Solid lines indicate the profiles from DLPC (red), DMPC (blue), DPPC (magenta) and DSPC (green) membranes.



**Figure S3.** Order parameter for the sn-1 chain of MscL-interacting lipids after 30 ns equilibration. Order parameter profiles along carbon number are shown from DLPC (red), DMPC (blue), DPPC (magenta) and DSPC (green) membranes.



**Figure S4.** Snapshots of DMPC bilayer at 310 K and 290 K, and DPPC at 310 K upon membrane stretching. Green indicates outer leaflet and pink inner leaflet of the bilayer. Interdigitation can be seen only in DPPC at 310 K.



**Figure S5.** Trajectories of F78 (A) and K97 (B) along z (transmembrane)-axis under 75 dyn/cm of membrane tension. The vertical axis shows distance from an original position (0) along z-axis (Å) and the horizontal one time (ns) after the onset of stretching. Solid lines indicate the trajectories from DLPC (red), DMPC (blue), DPPC (magenta) and DSPC (green). Both F78 and K97 move toward periplasmic side in the initial phase, then F78 move back to the cytoplasmic side in DLPC and DMPC membranes.

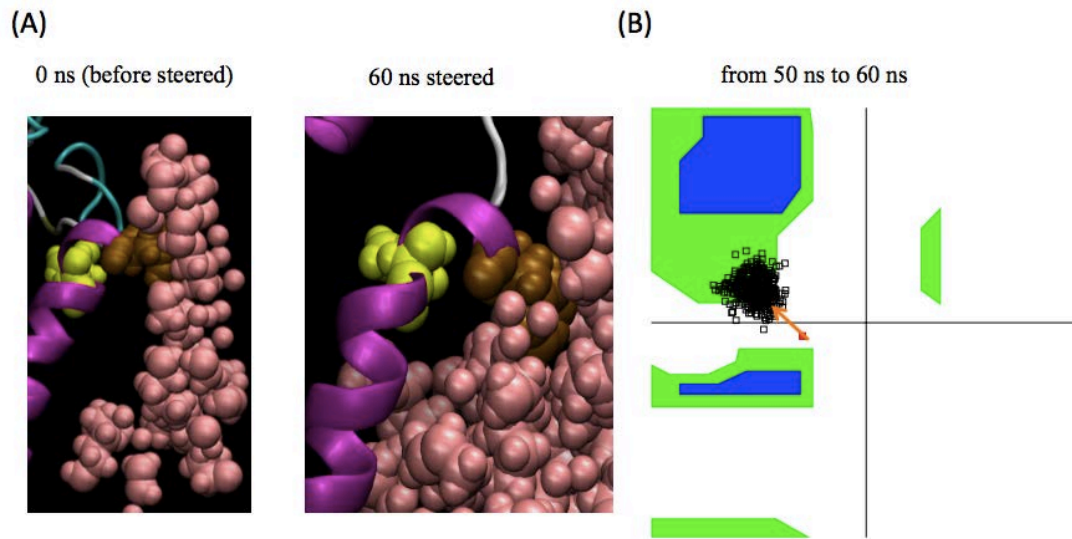


Figure S6 (A) Snapshots of F78 and N81 in DSPC membrane upon membrane stretching. Periplasmic side of the TM2 helix kinked 60 ns after stretching in DSPC membrane: Yellow, N81; Brown, F78; Pink, lipid; Purple, TM2 helix. (B) N81 Ramachandran plot of a subunit during 50 to 60 ns after stretching of DSPC membrane. Red square indicates Ramachandran plot of the subunit at the beginning of stretching.