Evaluation of the binding mechanism of human defensin 5 in a bacterial membrane: A simulation study

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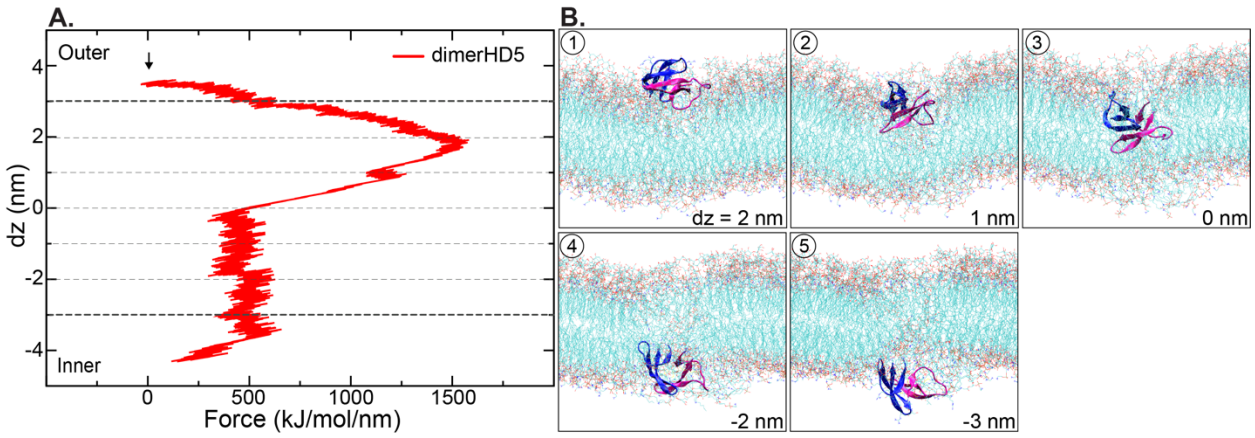

Figure S1. (A) Pull force profiles from constant velocity SMD simulations of HD5 through LPS membrane. (B) The initial snapshot at 5 positions, corresponding to the z-axis position of 2 nm, 1 nm, 0 nm, -2 nm, and -3 nm. Blue and magenta color represents chain *a* and chain *b* of HD5.

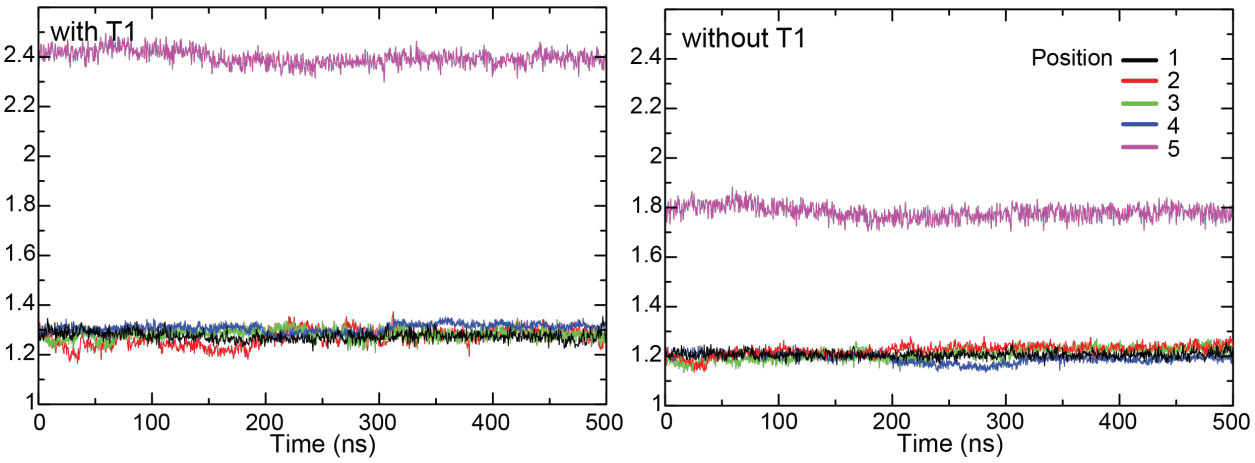

Figure S2. C-alpha RMSDs of all system when the X-ray structure (PDB code: 1ZMP) is used as a reference structure.

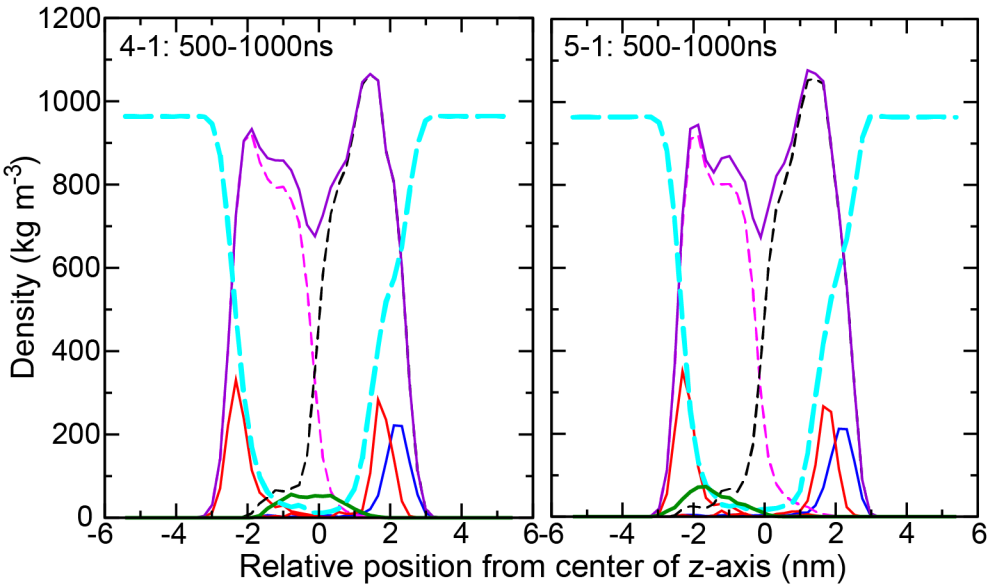

Figure S3. Density profiles of key components from extended 1000 ns simulations. The subgroups are dimeric HD5 (green), membrane (purple), outer leaflet (black dashed line), inner leaflet (magenta dashed line), KDO (blue), Pi (red), and water (cyan dashed line).

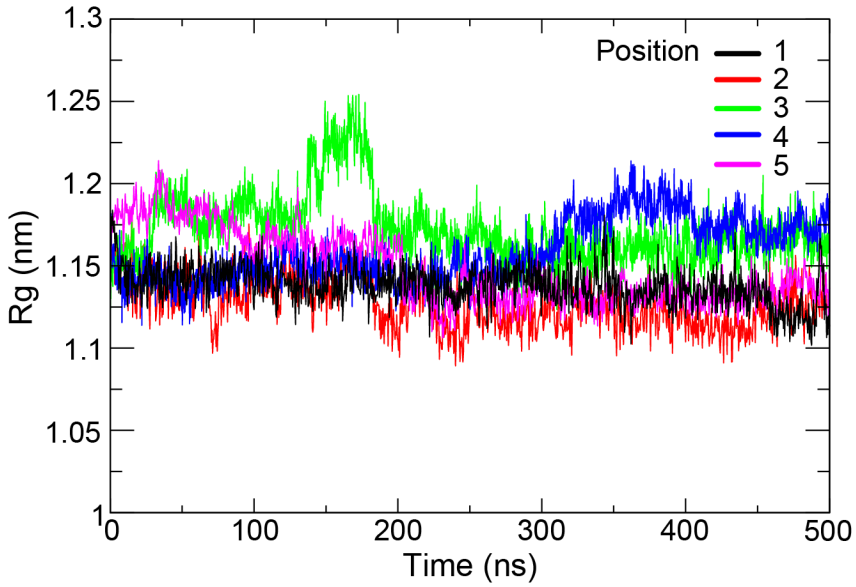

Figure S4. Radii of gyration of HD5 in all systems