Supporting information for

The Amphotericin B-Ergosterol Complex Spans a Lipid Bilayer as a Single-Length Assembly

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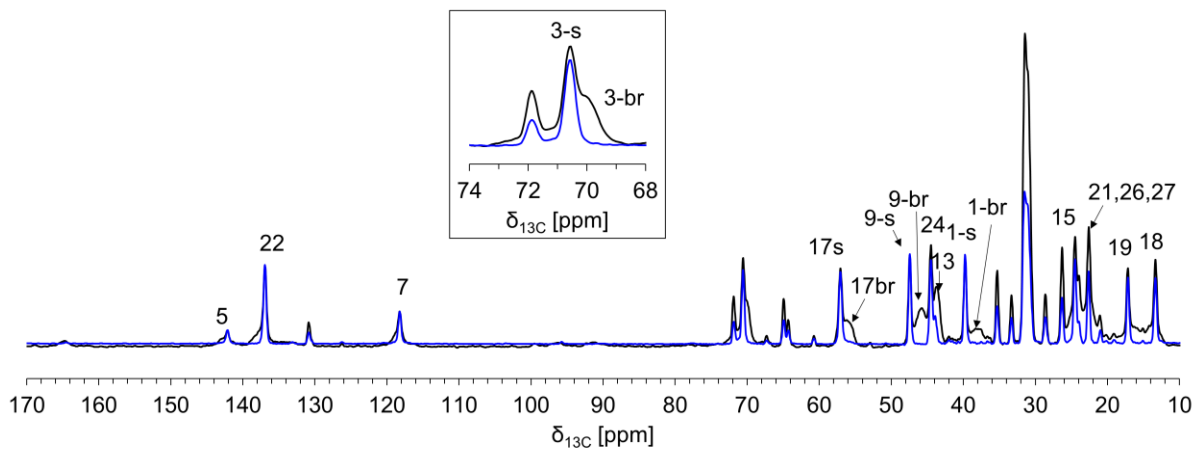

Figure S1. 1D ^{13}C CP-MAS spectra of AmB/skipped-^{13}C-Erg/POPC = 1/1/9 (black) and 0/1/9 (blue) liposomes in the absence of $MnCl_2$.

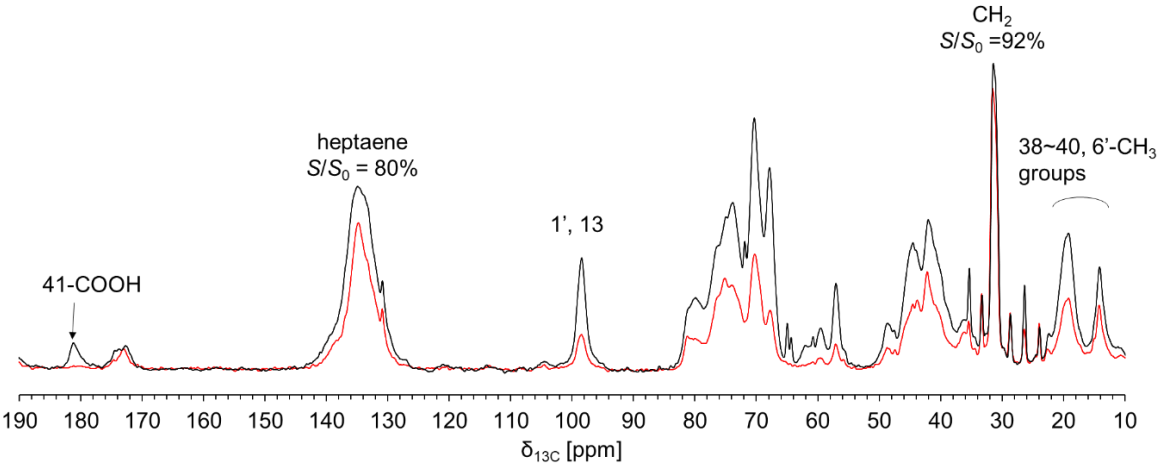

Figure S2. 1D ^{13}C CP-MAS spectra of U-^{13}C-AmB/Erg/POPC =1/3/7 in the absence of $MnCl_2$ (S_0, black) and with 20 mM $MnCl_2$ (S, red). The signal decay at CH_2 (31 ppm) is normalized to 92%.

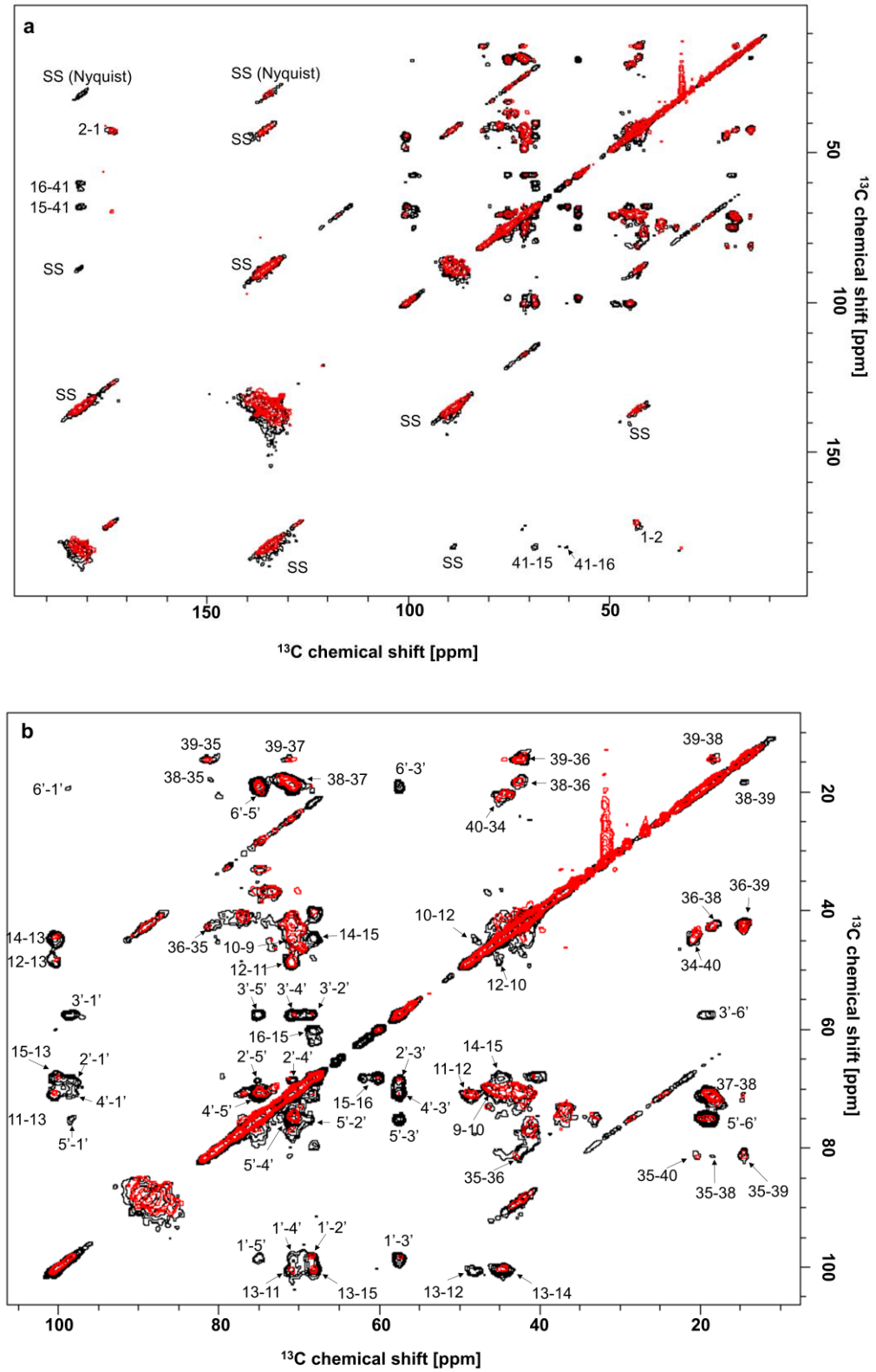

Figure S3. Two dimensional ^{13}C-^{13}C correlation spectra of U-^{13}C-AmB/Erg/POPC=1/3/7 samples with the signal assignments. Hydrated with H_2O without $MnCl_2$ (black) and with 20 mM $MnCl_2$ (red).

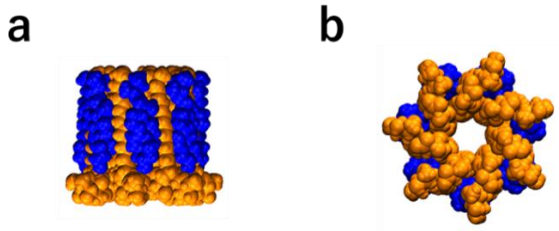

Figure S4. Constructed AmB-sterol complex channel structure in MD simulations. Orange: AmBs, blue: Ergs. (**a**) Side view. (**b**) Top view.

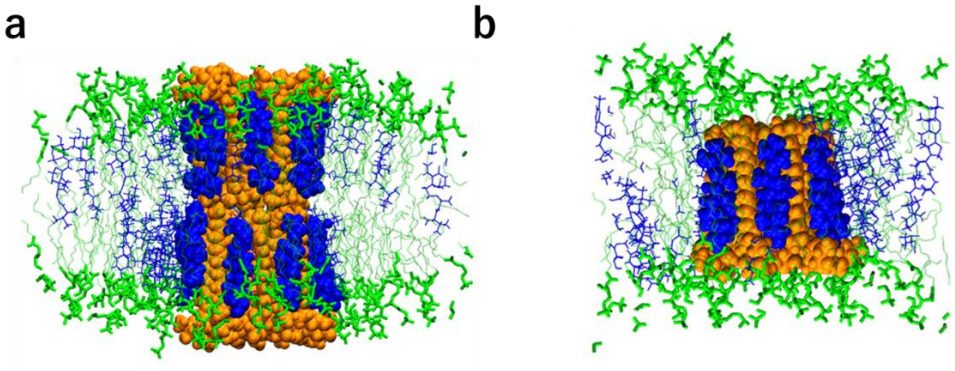

Figure S5. An example of the initial configurations for MD simulation. (**a**) Double-length assembly. (**b**) Single-length assembly. Orange: AmBs, blue: Ergs, green: POPCs. No water is shown for clarity. The structure of the AmB-Erg complex represented by VDW is the same for all three MD runs, though the lipid membranes (POPC and Erg) represented by lines are generated independently for different MD simulations.

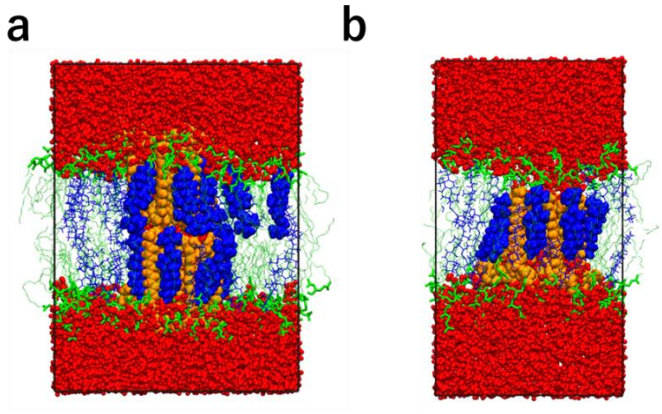

Figure S6. A snapshot of the final configuration from one of the 1μs NPT MD simulations. (**a**) Double-length assembly. (**b**) Single-length assembly. Orange: AmBs, green: POPCs, blue: Ergs, and red: water molecules. VDW representation is used for AmBs and the initially associated Ergs.

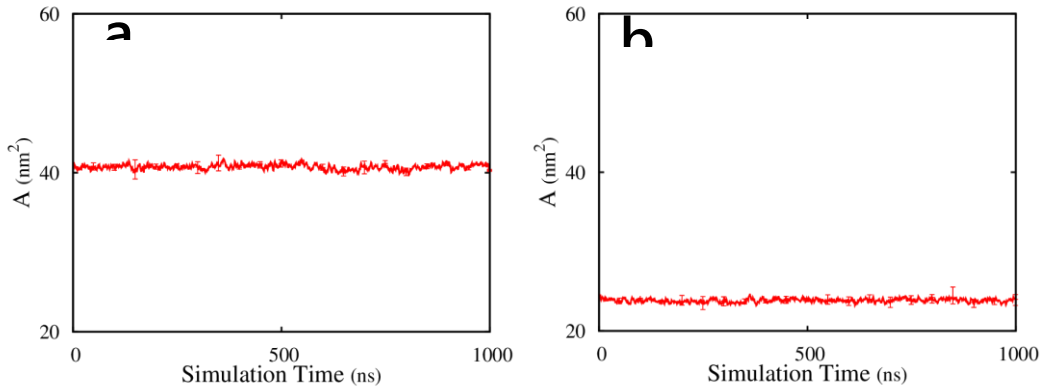

Figure S7. The time variation of membrane area ($A=L_xL_y$) during 1μs MD simulation. (**a**) Double-length assembly. (**b**) Single-length assembly. The averaged area for three MD simulations is plotted.

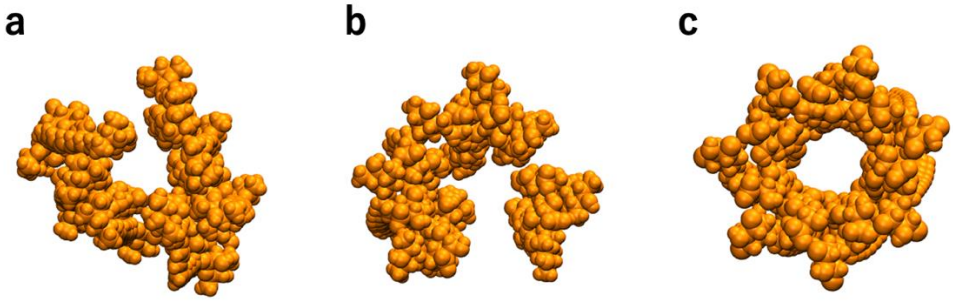

Figure S8. Top view of the AmB channel after 1μs MD simulation. (**a,b**) From the MD trajectory with double-length assembly, where the channel was not stable to be closed; AmB channel in the (a) upper and (b) lower leaflets of the lipid membrane. In this MD simulation, AmB channel could not keep channel structure where a few AmB molecules were separated and the channel were opened toward the lipid membrane. (**c**) Single-length assembly. In all MD simulations with the single-length assembly, the AmB channel was stable, where AmBs were arranged in an axis-symmetric.

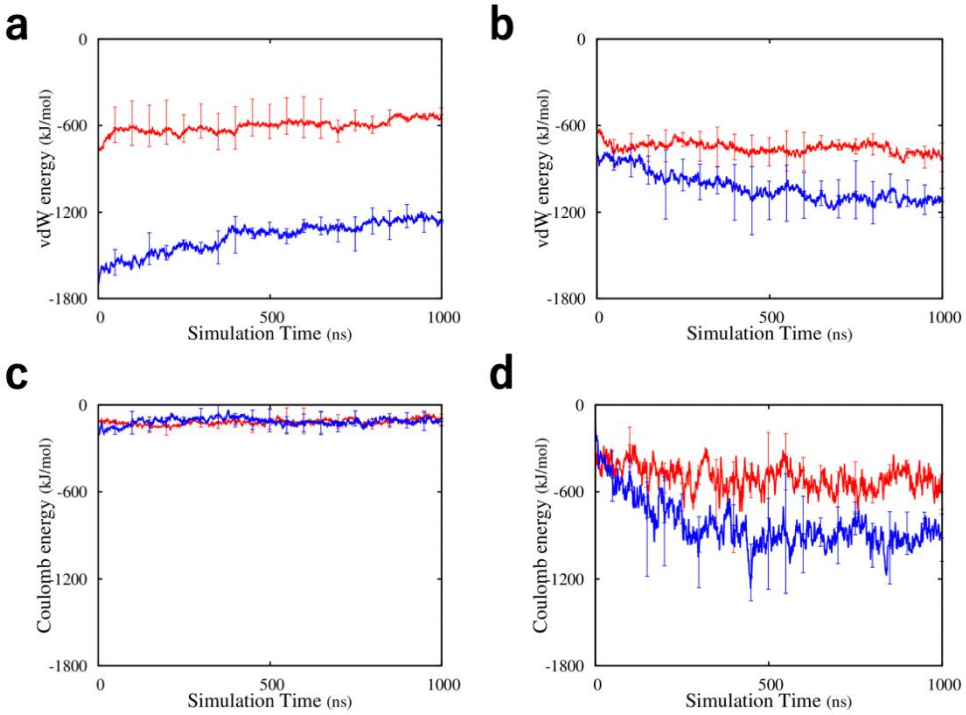

Figure S9. van der Waals (vdW) and Coulomb interaction energies between the AmB and Erg molecules or between the AmB and POPC molecules. *Red-lines*; single-length assembly. *Blue-lines*; double-length assembly. **(a,b)** vdW energy between (a) AmB and Erg, (b) AmB and POPC. **(c,d)** Coulomb energy between (c) AmB and Erg, (d) AmB and POPC.

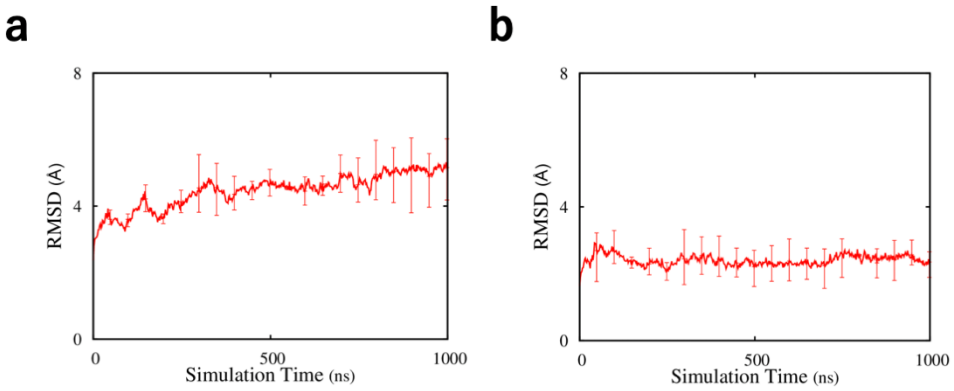

Figure S10. Root mean square deviation (RMSD) of the AmB channel from the initial configuration. (**a**) Double-length assembly. (**b**) Single-length assembly. The averaged RMSD for three MD simulations are plotted. The error bars denote the maximum and minimum values in three MD simulations.