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

Supporting Information

How transmembrane peptides insert and orientate in biomembranes: a combined experimental and simulation study

Tongtao Yue,* Mingbin Sun, Shuai Zhang, Hao Ren, Baosheng Ge and Fang Huang*

State Key Laboratory of Heavy Oil Processing, Center for Bioengineering and Biotechnology, China University of Petroleum (East China), Qingdao, 266580, China.

E-mail: yuett@upc.edu.cn, fhuang@upc.edu.cn

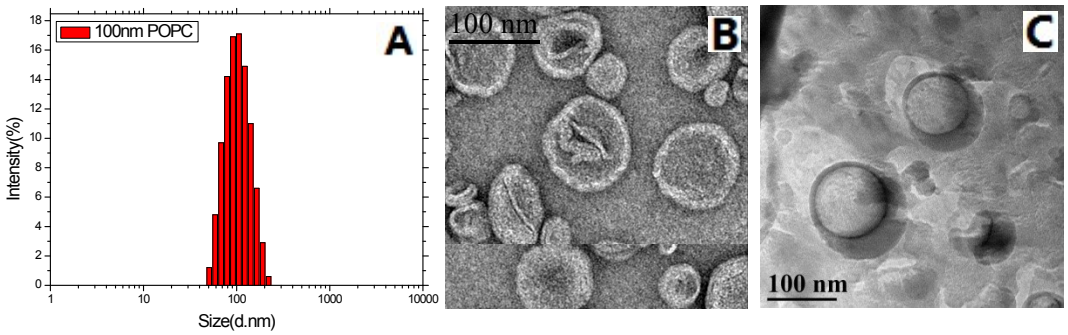

Fig. S1 POPC lipid vesicle characterization. A: DLS size distribution; B: Negative-Stain TEM images; C: Freeze fracture-TEM micrograph.

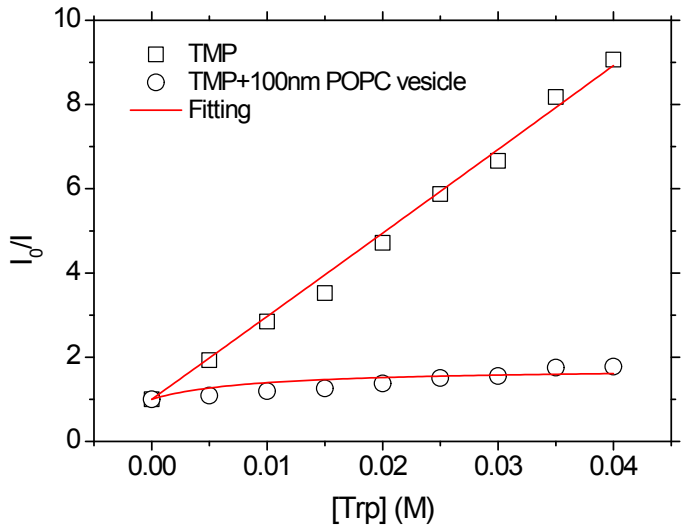

Fig. S2 Fluorescence quenching data for peptides corresponding to the fifth transmembrane α-helix of CXCR4. The quenching constant K_{SV} and percentage of N terminus outside the vesicles are 196.2 M^{-1} and 0.427.

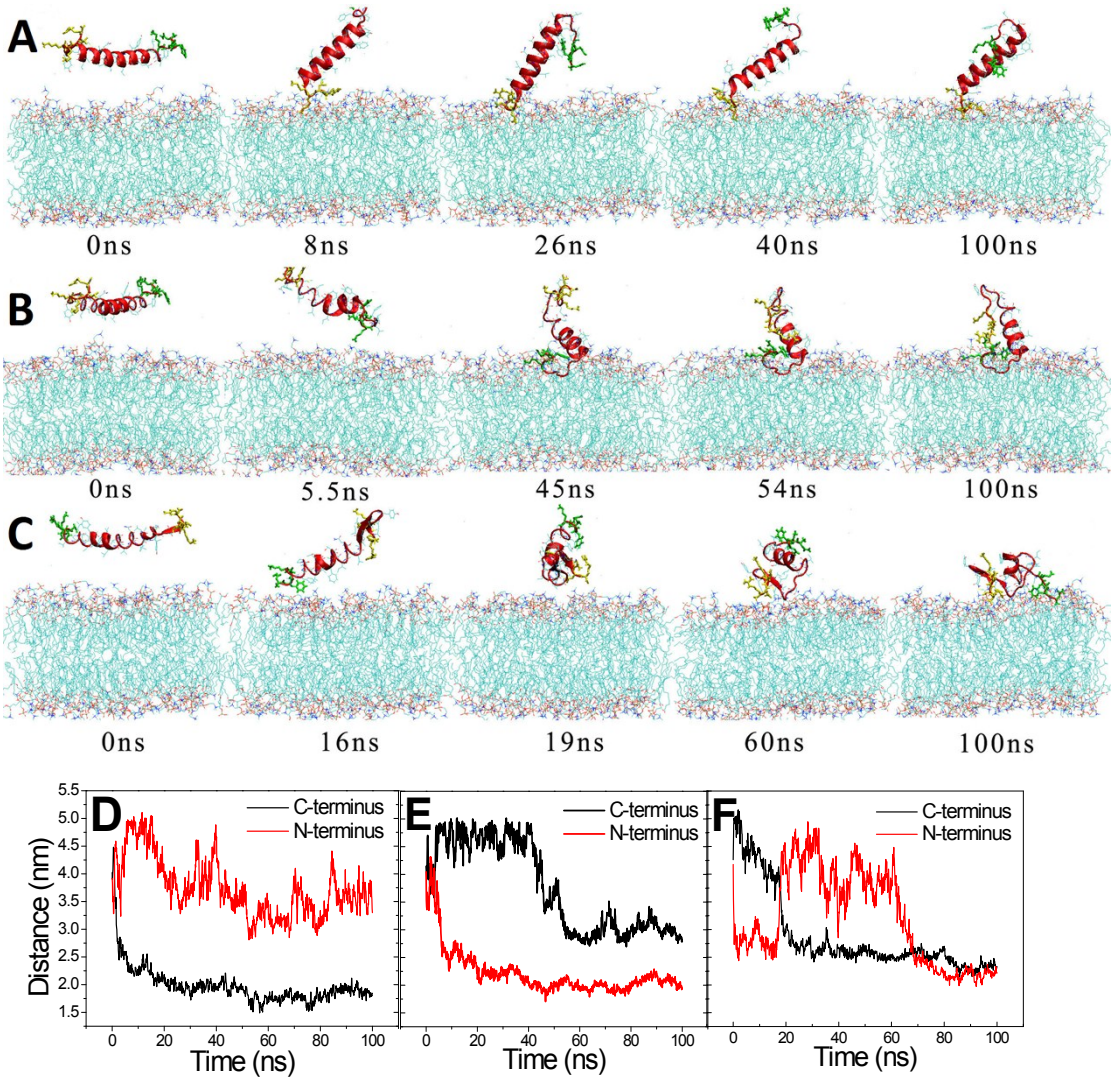

Fig. S3 Three typical pathways of membrane association of the peptide. A-C show the typical snapshots; D-F are corresponding evolutions of distance between each terminus and membrane center.

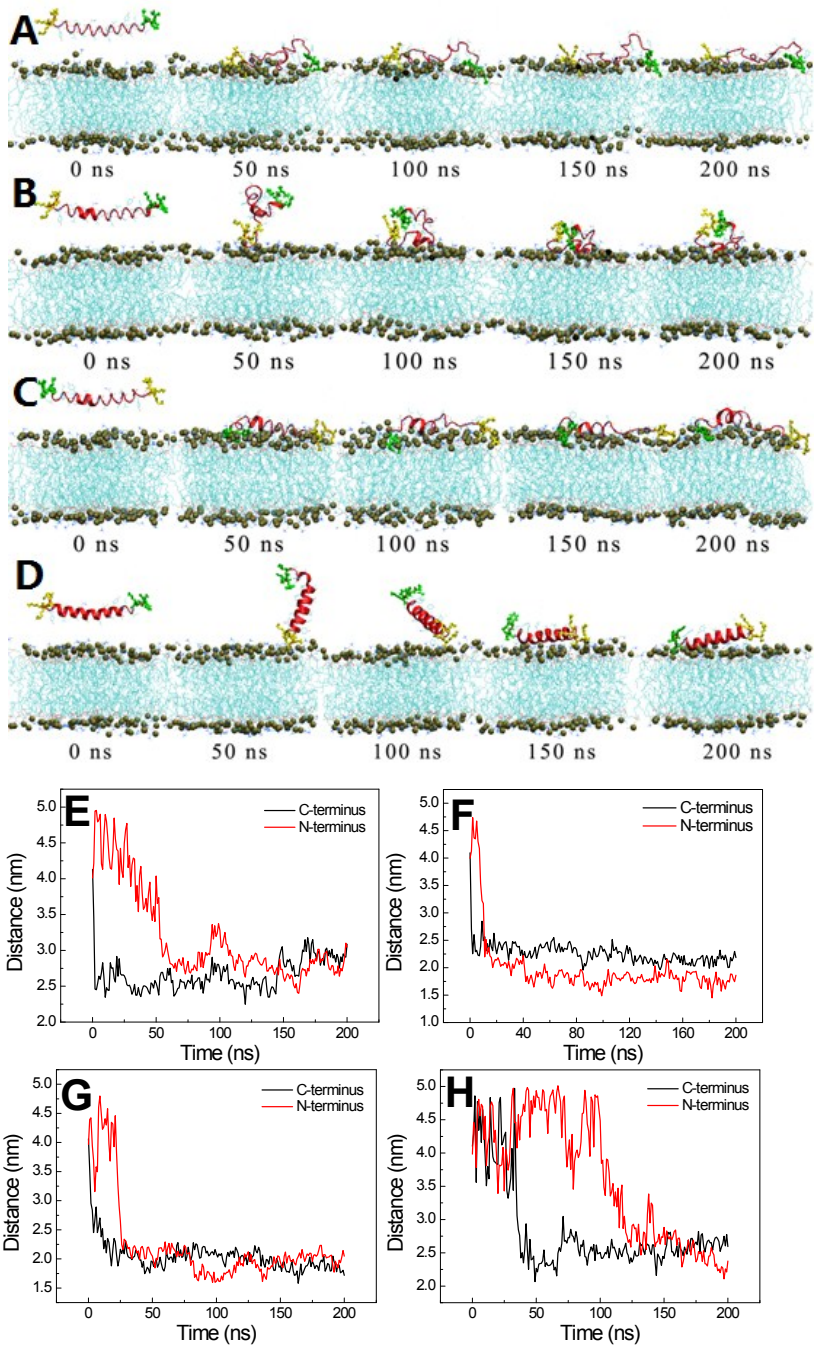

Fig. S4 Four repeat simulations of spontaneous association of peptide with membrane.

A-D show the typical snapshots; E-H are the corresponding evolutions of distance between each terminus and membrane center.

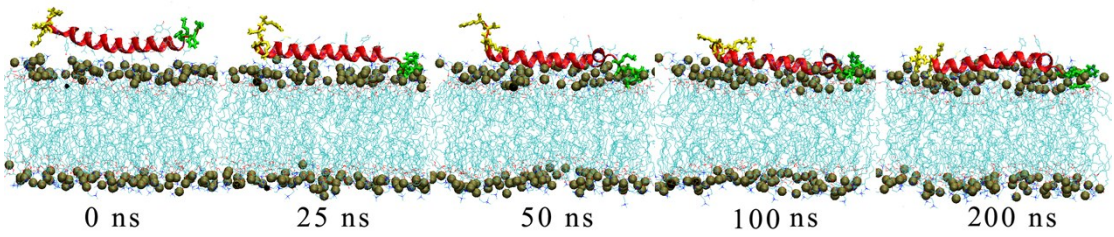

Fig. S5 Repeat simulation of spontaneous peptide-membrane association by using the GROMOS 54a7 force field.

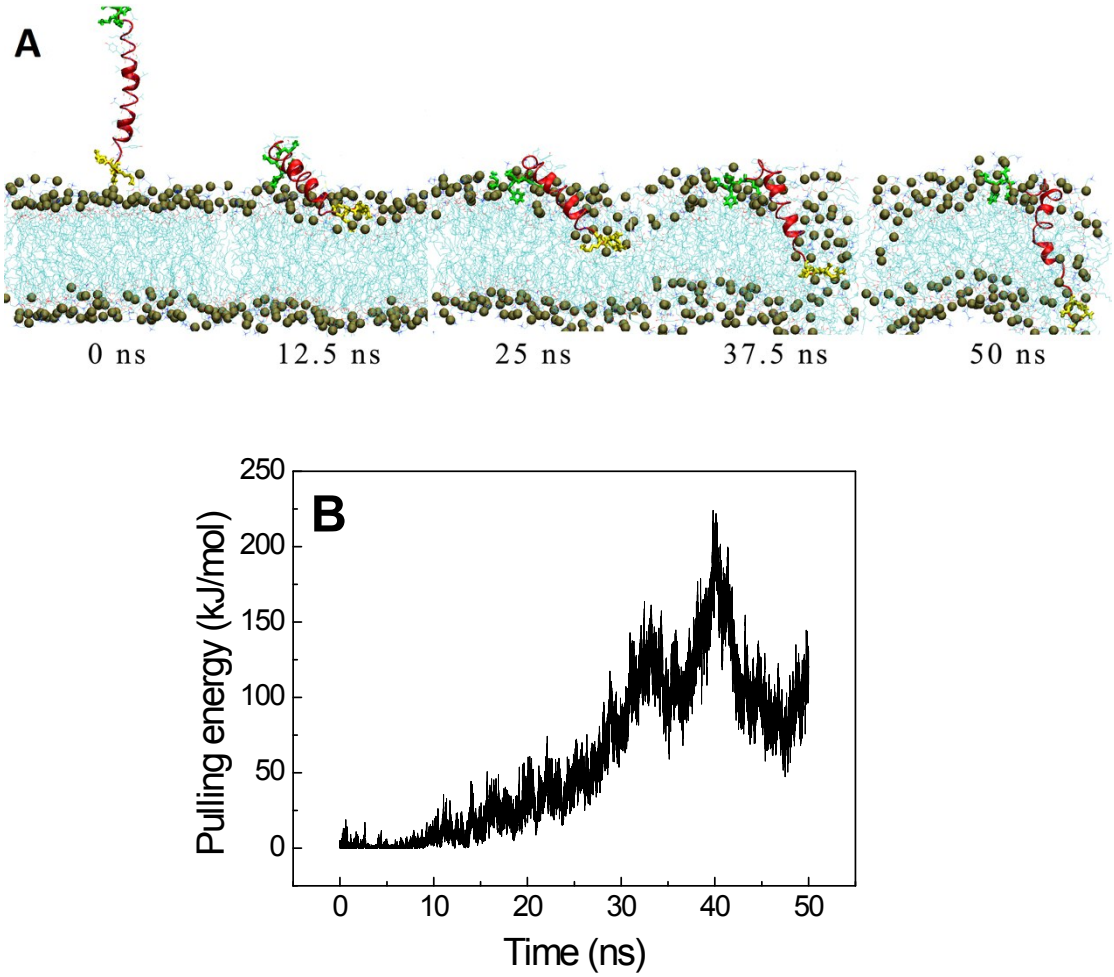

Fig. S6 Pulling simulation that transfer a peptide from water to membrane. A shows the typical snapshots; B shows the time evolution of pulling energy.

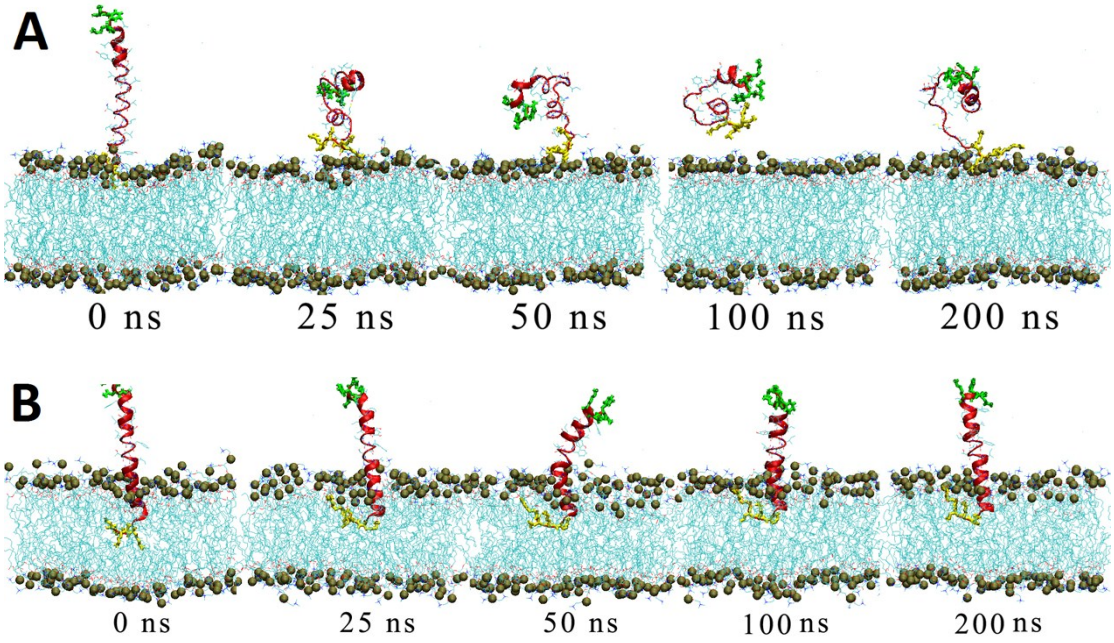

Fig. S7 Extended sampling simulations illustrating the energetically trapped partial insertion state under external restraining force.

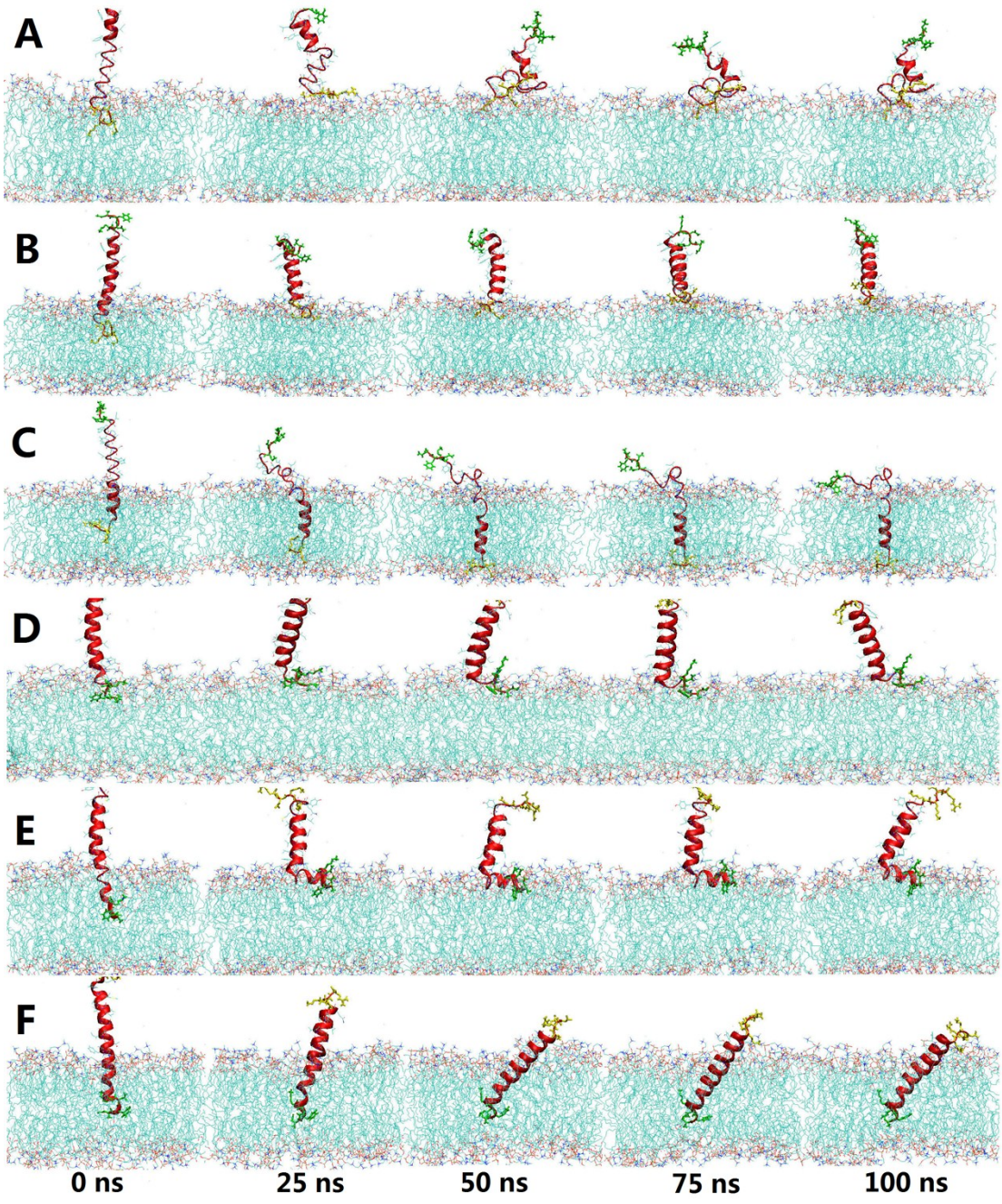

Fig. S8 Typical snapshots of membrane-peptide association starting from configurations with different orientations (A-C for C terminus downwards and D-F for N terminus downwards) and different initial insertion depths. The initial insertion depth (d) are A: 3.5nm; B: 3.2nm; C: 2.9 nm; D: 3.5 nm; E: 2.6 nm; and F: 2.4 nm.

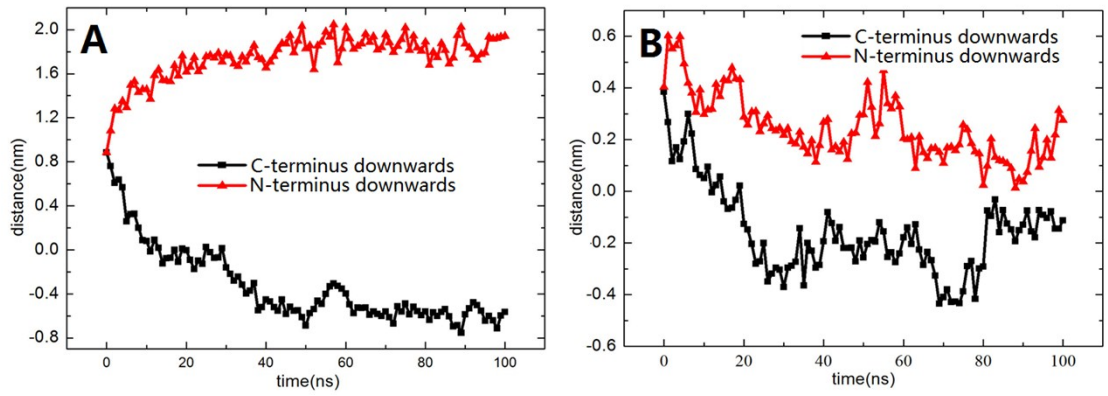

Fig. S9 Time evolution of distance between inserting terminus and membrane center with different insertion orientations. The initial insertion depths were set to 2.9 nm (A) and 2.4 nm (B), which are critical insertion depths for insertion orientation of C-terminus downwards and N-terminus downwards, respectively.

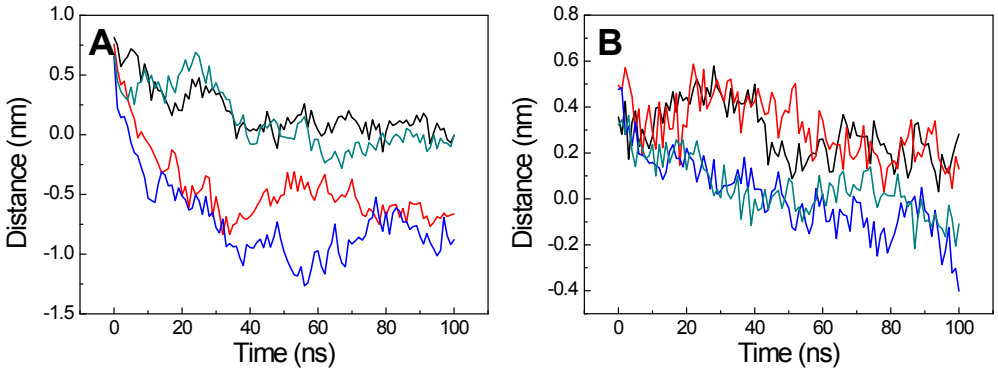

Fig. S10 Repeat simulations determining the critical insertion depth for two orientations. A and B are the evolutions of distance between each terminus and membrane center.