The computational study on the function of palmitoylation on the envelope protein in SARS-CoV-2

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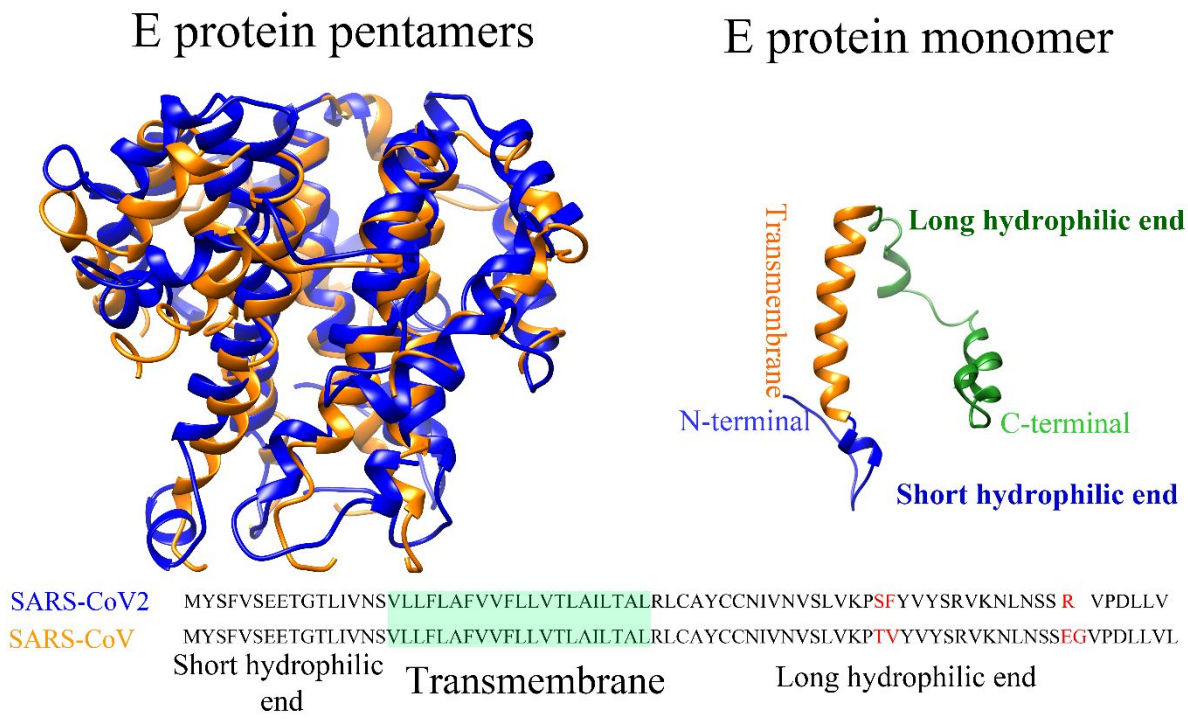


Figure S1: The structure alignment and the sequence alignment of SARS-CoV2 and SARS-CoV. The long and short hydrophilic ends are represented in blue and green in an E protein monomer.

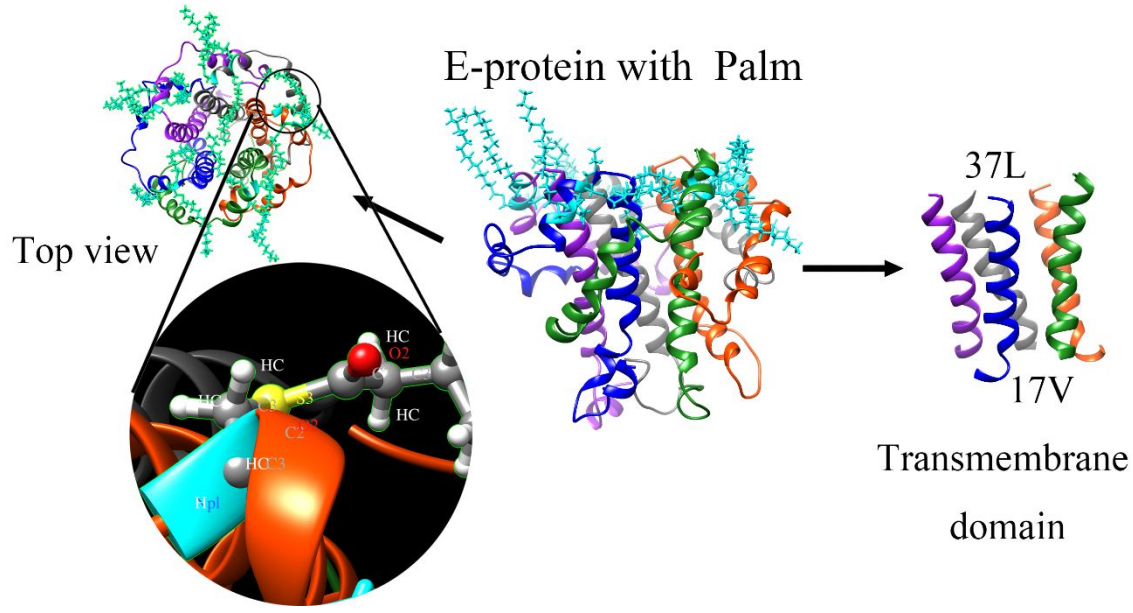
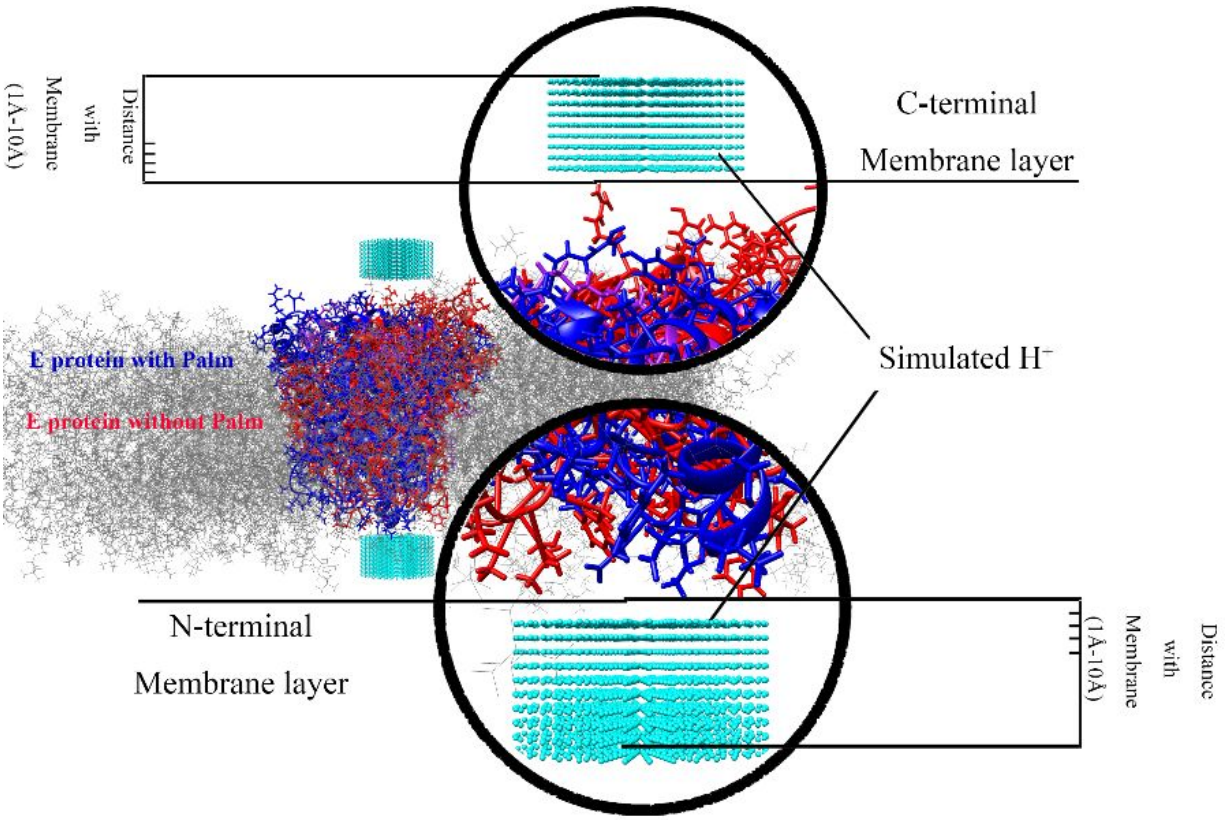


Figure S2: The atomic representation of palmitoylation and the transmembrane domain of E-protein.



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24 Figure S3: The diagram of the placement of simulated H^+ ions for electrostatic force testing.

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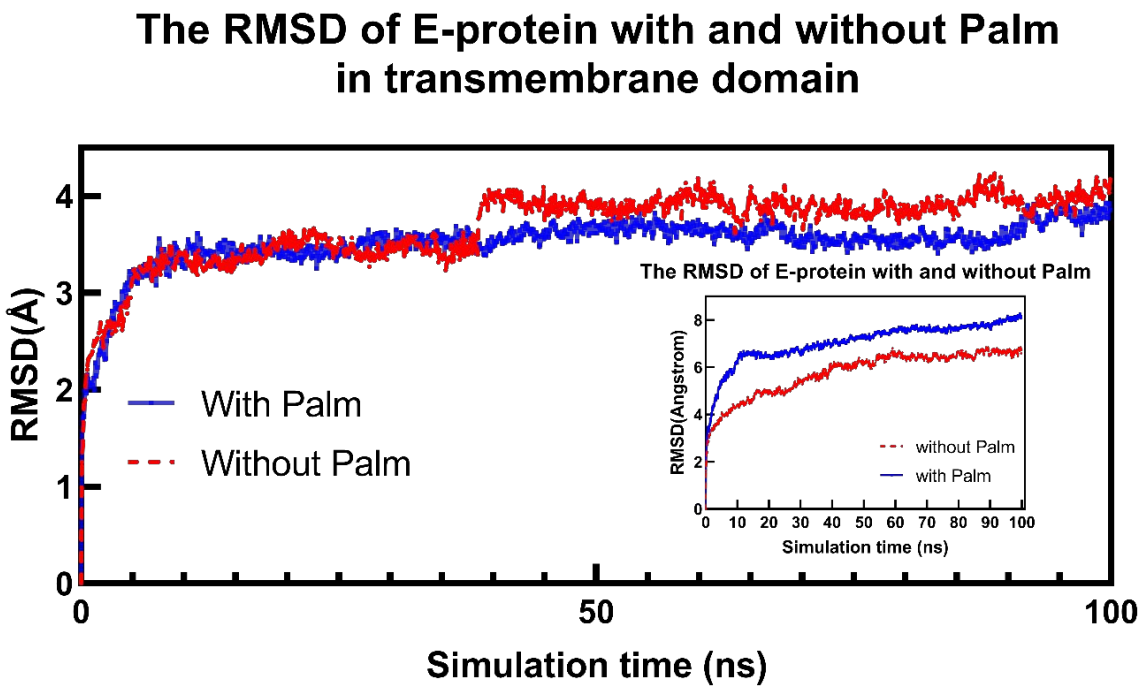

Figure S4: The backbone RMSD of E-protein pentamer with and without Palm during 100 ns simulation

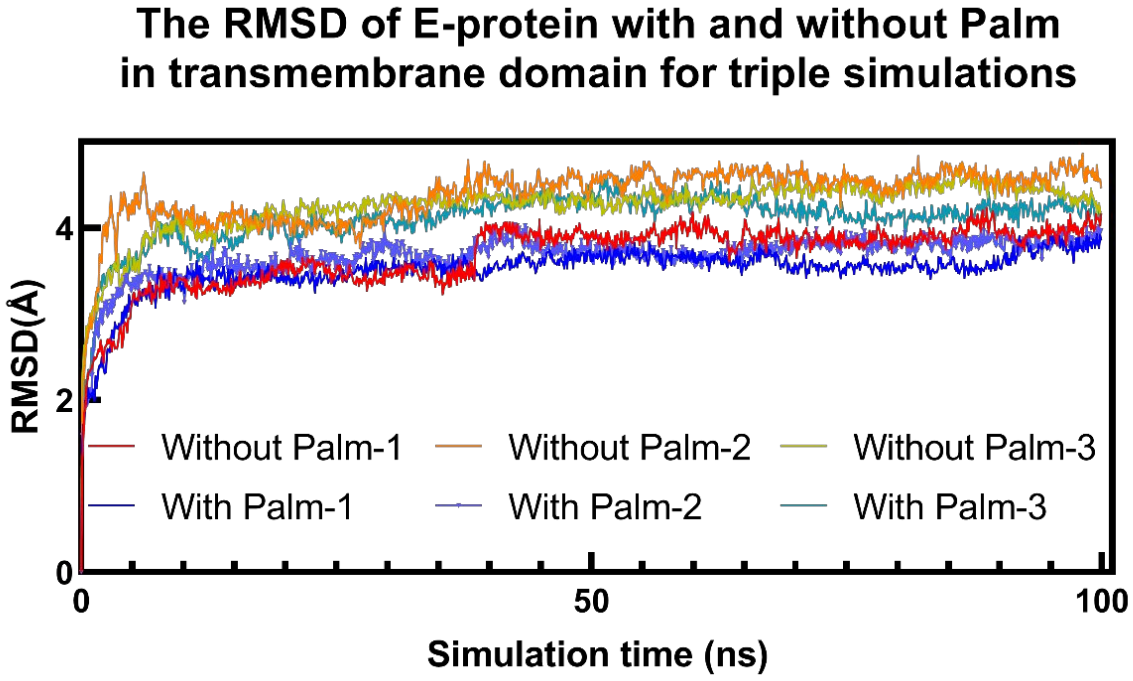

Figure S5: The backbone RMSD of E-protein pentamer with and without Palm during 100 ns for triple simulations

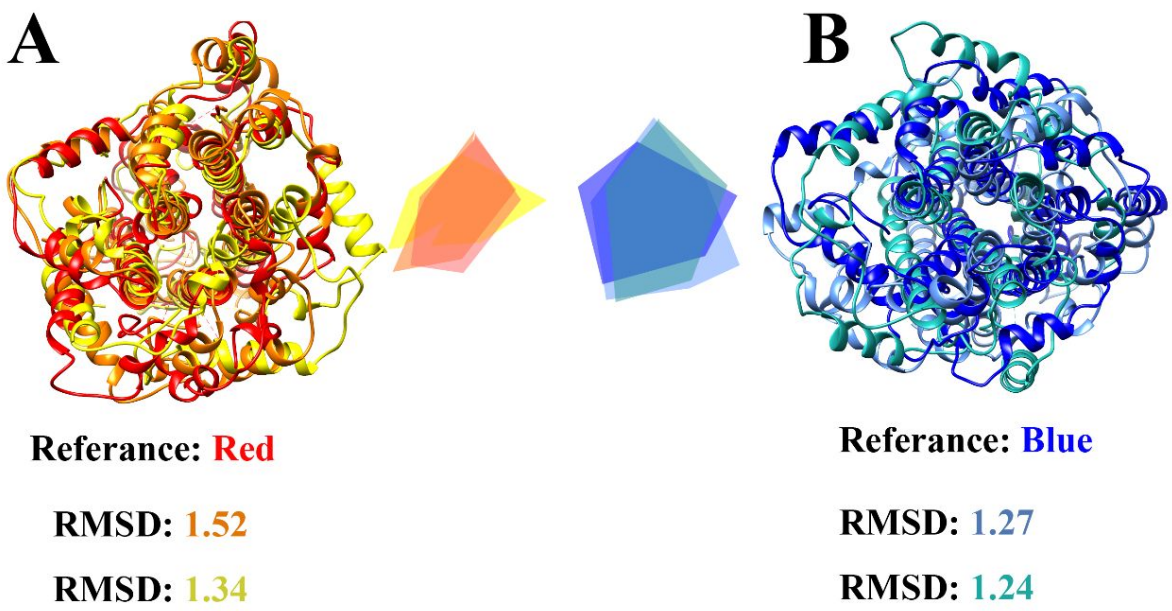

Figure S6: The structural comparison of E-protein pentamer without (A) and with (B) Palm in triple simulations where the RMSD calculation is based on the first simulations (red and blue). The shadows are the general comparison on pores

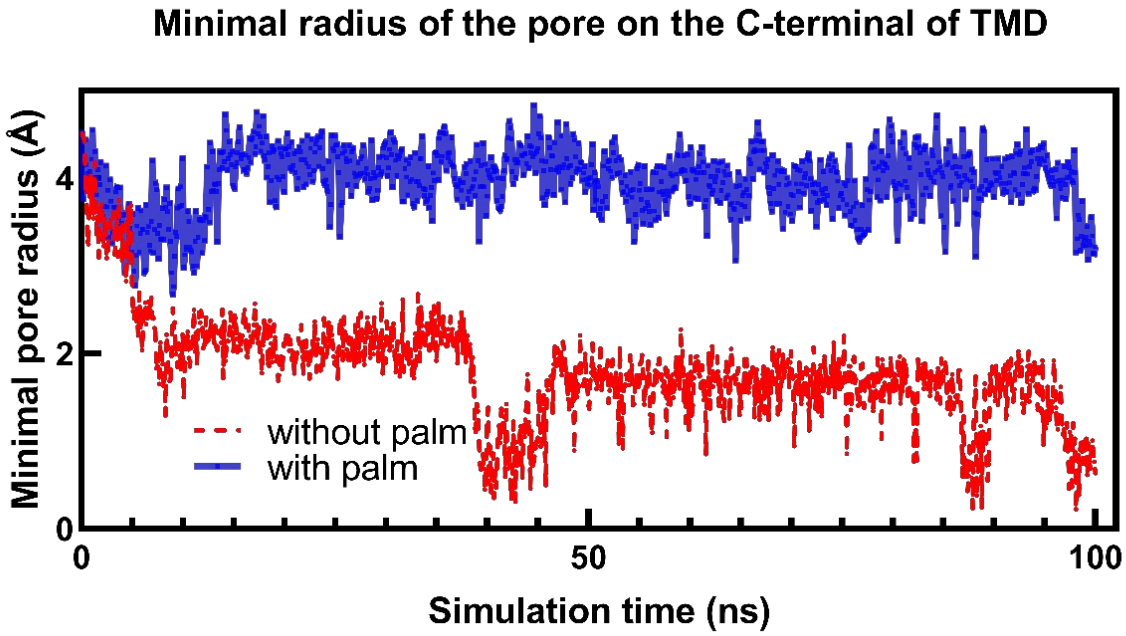

Figure S7: The minimal pore radius of the E-protein pentamer in C-terminal (residue 30-39) of TMD during the whole simulation (by an average of 3 testings)

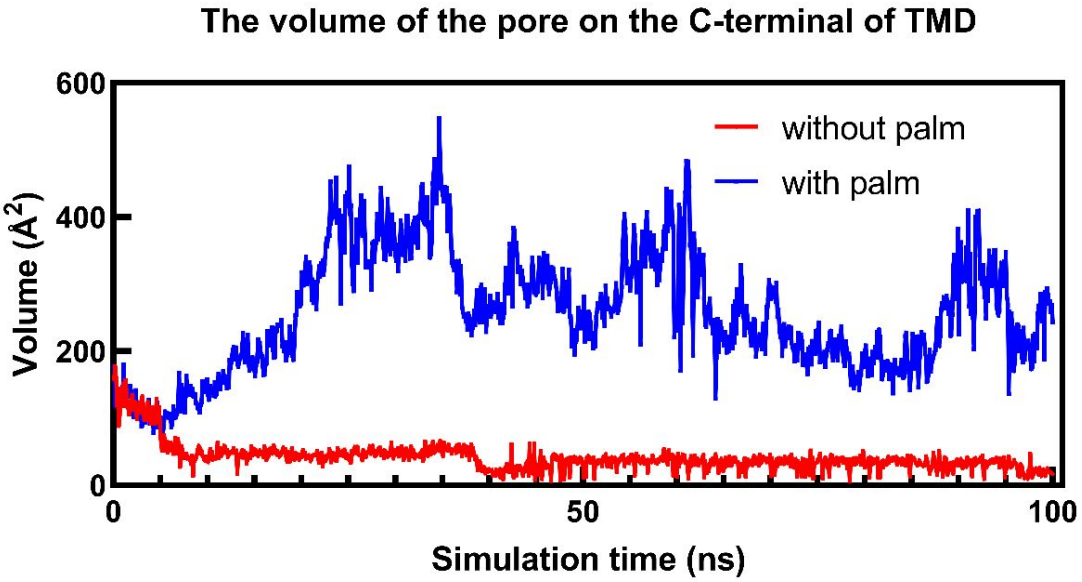

Figure S8: The volume of the E protein pentamer in the C-terminal part of TMD during the whole simulation

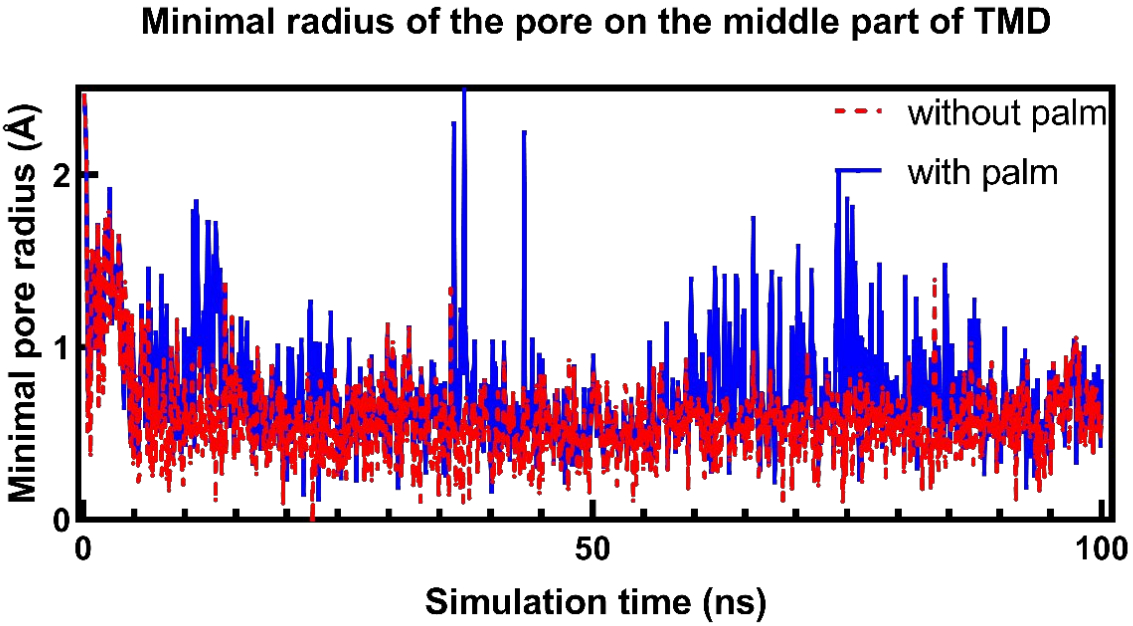

Figure S9: The minimal pore radius of the E-protein pentamer in the middle part (residue 21-30) of the TMD during the simulation.

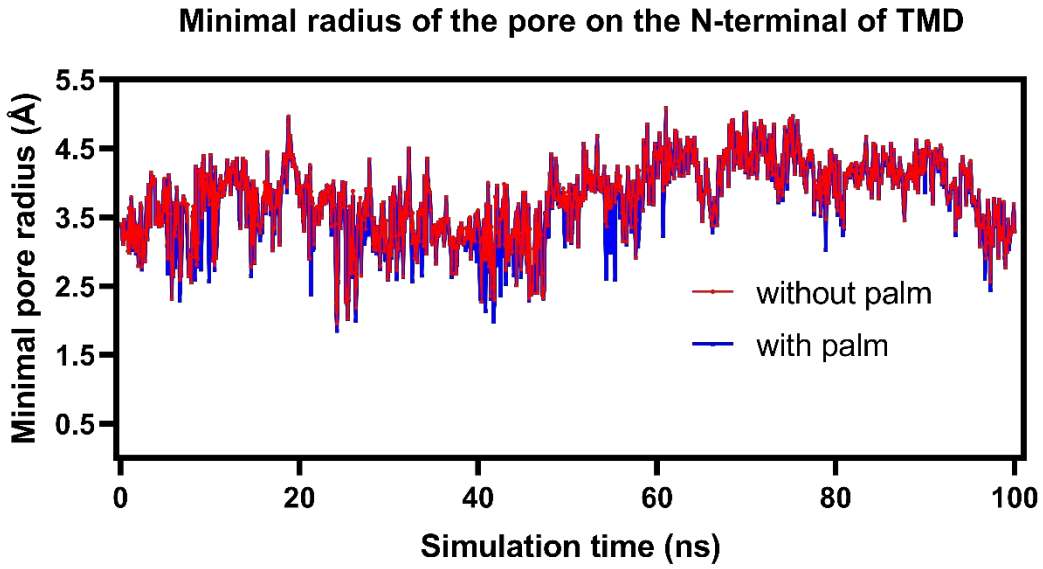

Figure S10: The minimal pore radius of the E-protein pentamer in the N-terminal (residue 10-20) during the simulation.

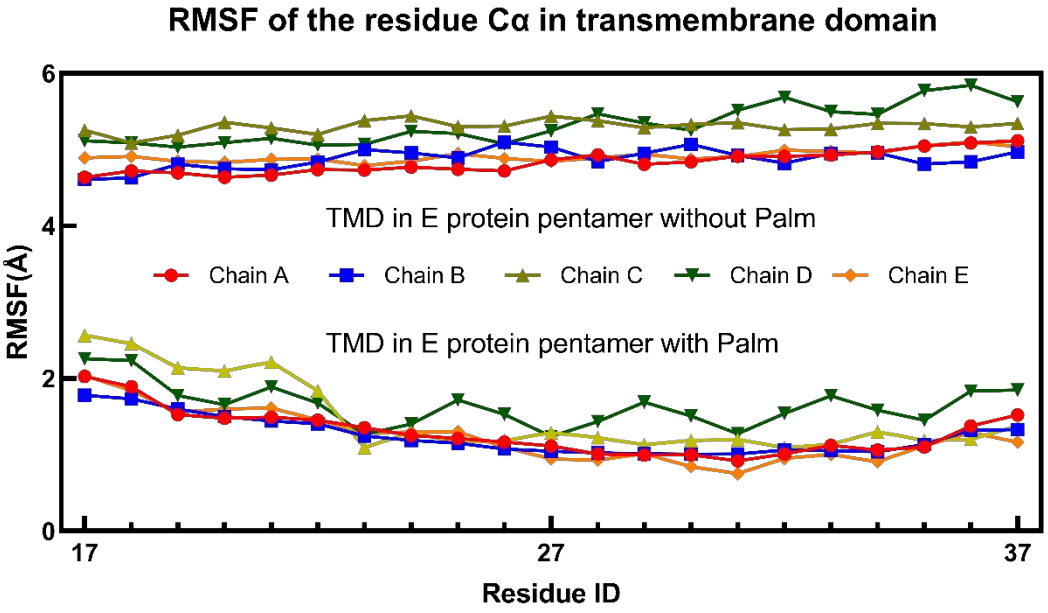

Figure S11: The RMSF of the residues (residues 17 to 37) in the transmembrane domain of E-protein pentamer.

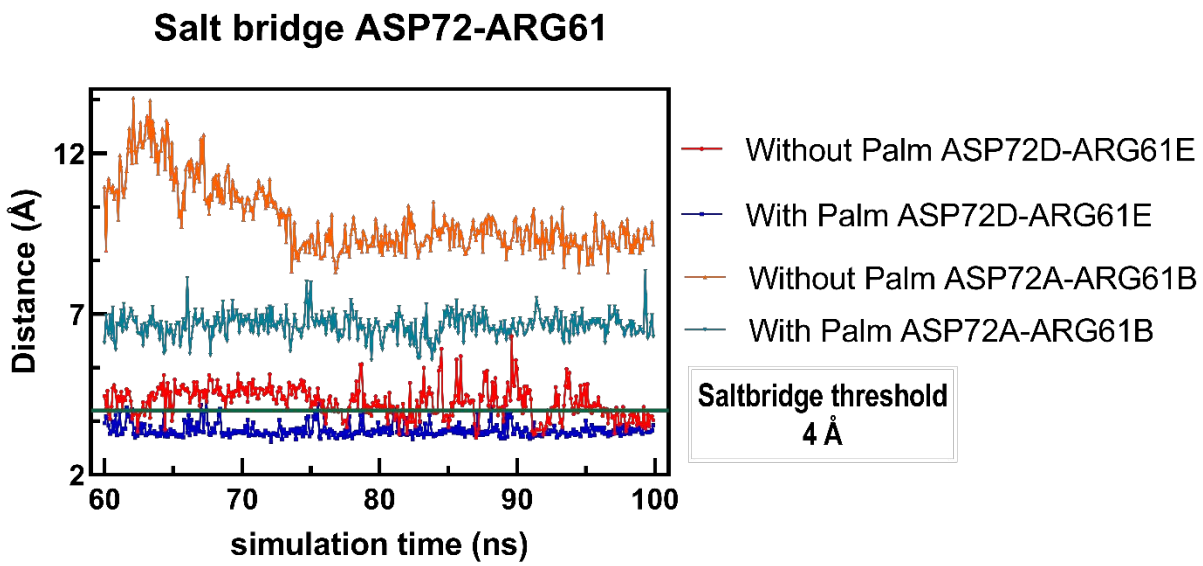

Figure S12: The distance of the salt bridges of ASP72D-ARG61E and ASP72A-ARG61B in both non-palmitoylated E protein pentamer and palmitoylated E protein pentamer. (Technically, ASP72A-ARG61B is not a salt bridge).

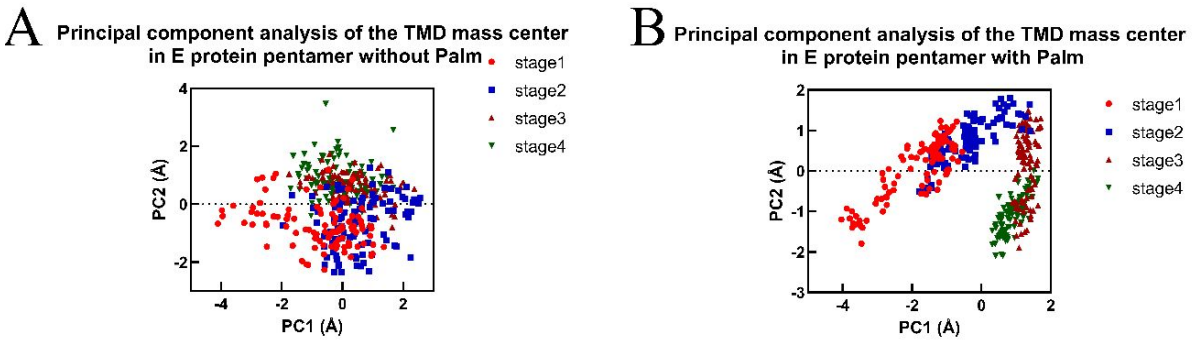

Figure S13: The PCA of the mass center of the transmembrane domain of E-protein pentamer with and without Palm. The stages 1, 2, 3, 4 represent the simulations between 0-25ns, 25-50ns, 50-75ns, 75-100ns.

Table S1: The rotation of the PCA for non-palmitoylated and palmitoylated E protein pentamer (Figure S13).

	PC1	PC2	PC3		PC1	PC2	PC3
X	0.192947	0.979483	0.058182		-0.67637	0.159331	-0.71913
Y	0.697639	-0.09525	-0.71009		0.652164	-0.32426	-0.68523
Z	0.68998	-0.1776	0.701702		0.342363	0.932453	-0.11541

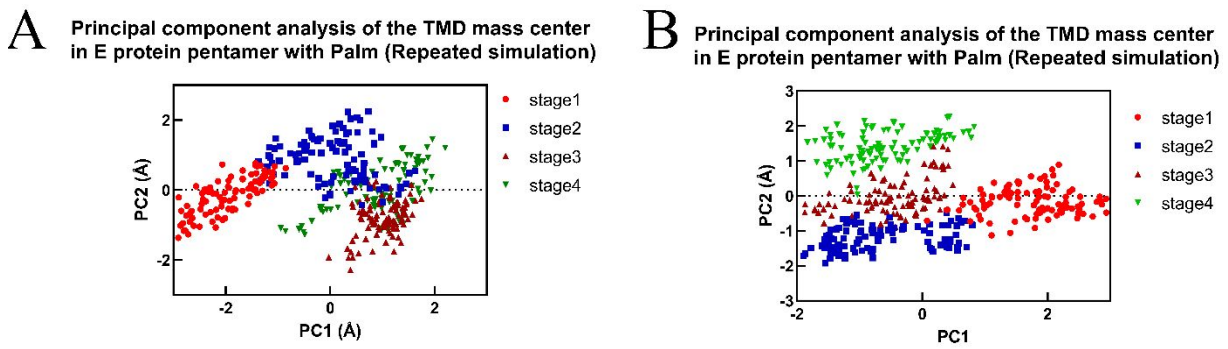

Figure S14: The PCA of the mass center of the transmembrane domain of E-protein pentamer with and without Palm in the repeated simulations. The stages 1, 2, 3, 4 represent the simulations between 0-25ns, 25-50ns, 50-75ns, 75-100ns.