

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

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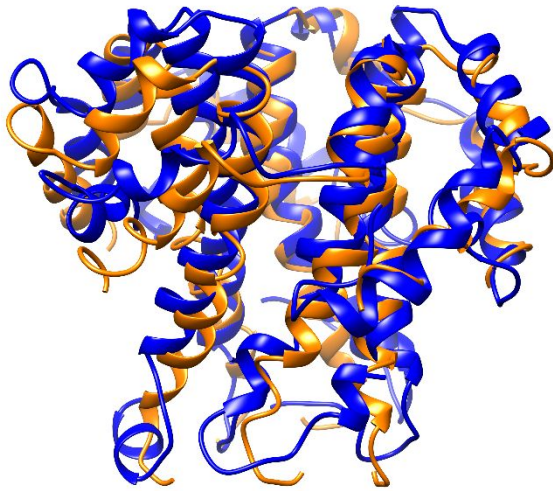
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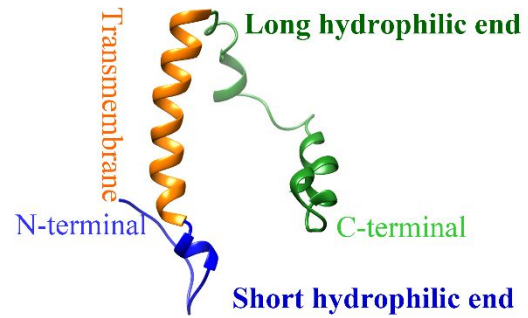
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E protein pentamers



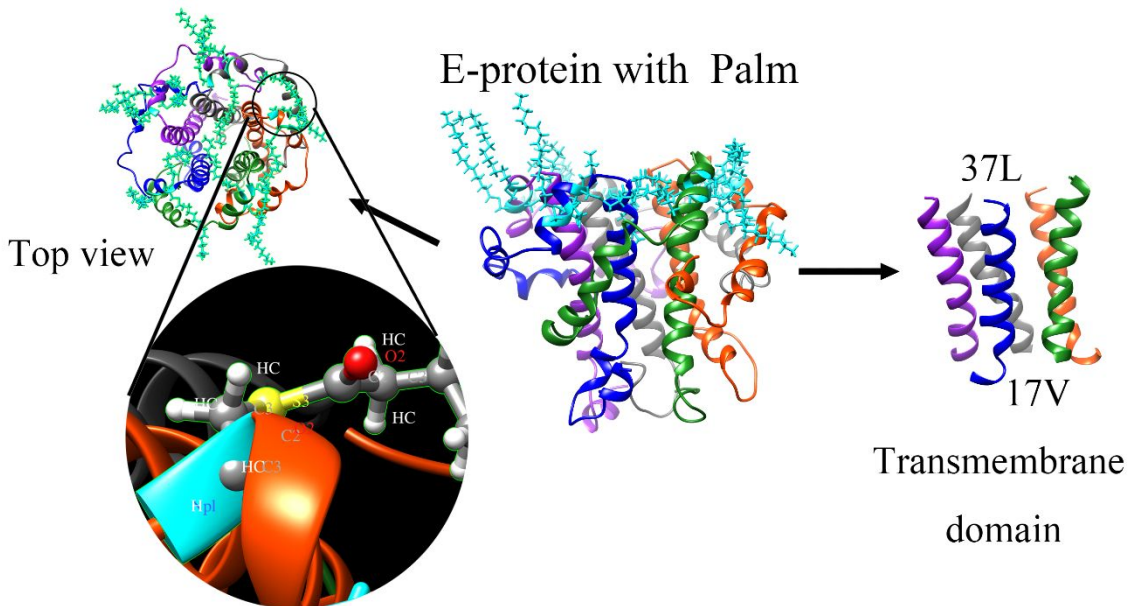
E protein monomer



<p>SARS-CoV2</p> <p>SARS-CoV</p>	<p>MYSFVSEETGLIVNSVLLFLAFVVFLLVTLAILTALRLCAYCCNIVNVS</p> <p>MYSFVSEETGLIVNSVLLFLAFVVFLLVTLAILTALRLCAYCCNIVNVS</p>	<p>VKPSFYVYSRVKLNLSR</p> <p>VKPTVYVYSRVKLNLSSE</p>	<p>VPDLLV</p> <p>EGVPDLLVL</p>
	<p>Short hydrophilic end</p> <p>Transmembrane</p>		<p>Long hydrophilic end</p>

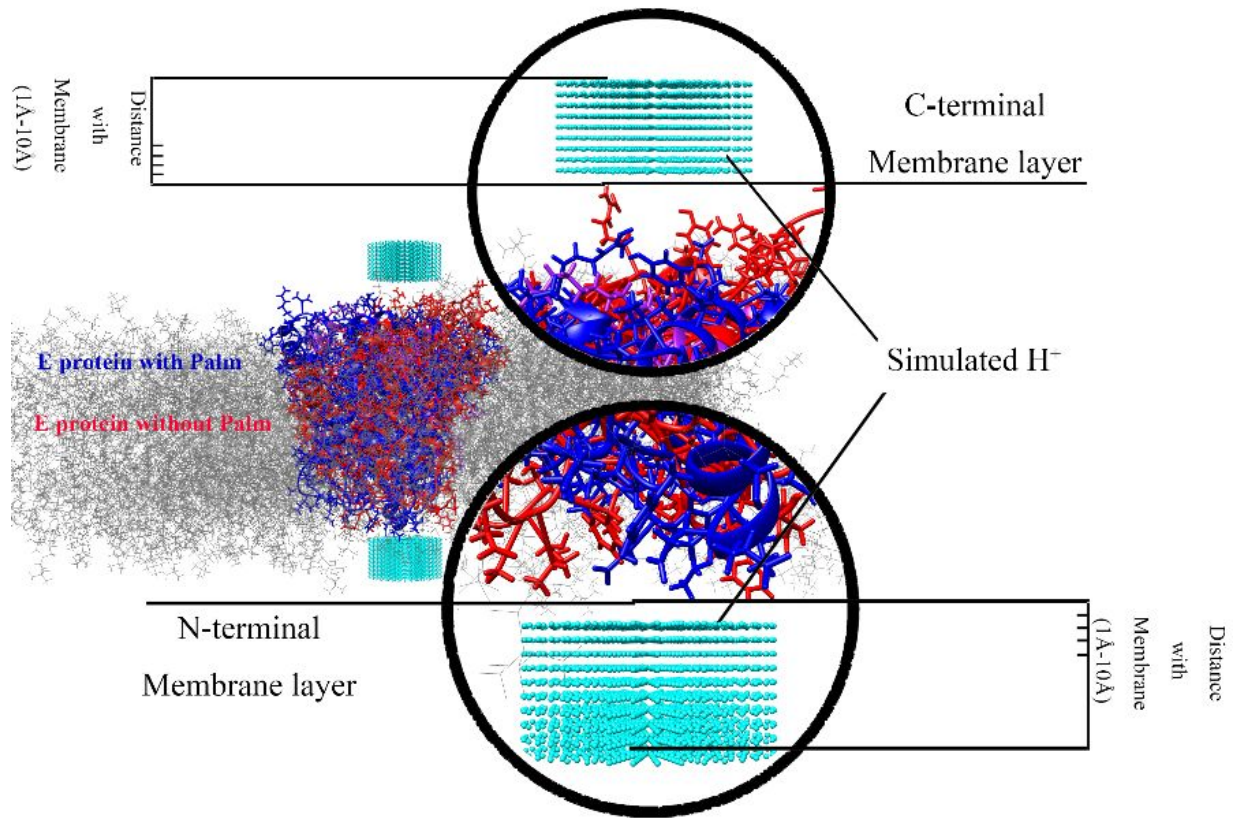
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Figure S1: The structure alignment and the sequence alignment of SARS-CoV2 and SARS-CoV. The long and short hydrophilic ends are represented in blue and green in an E protein monomer.



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

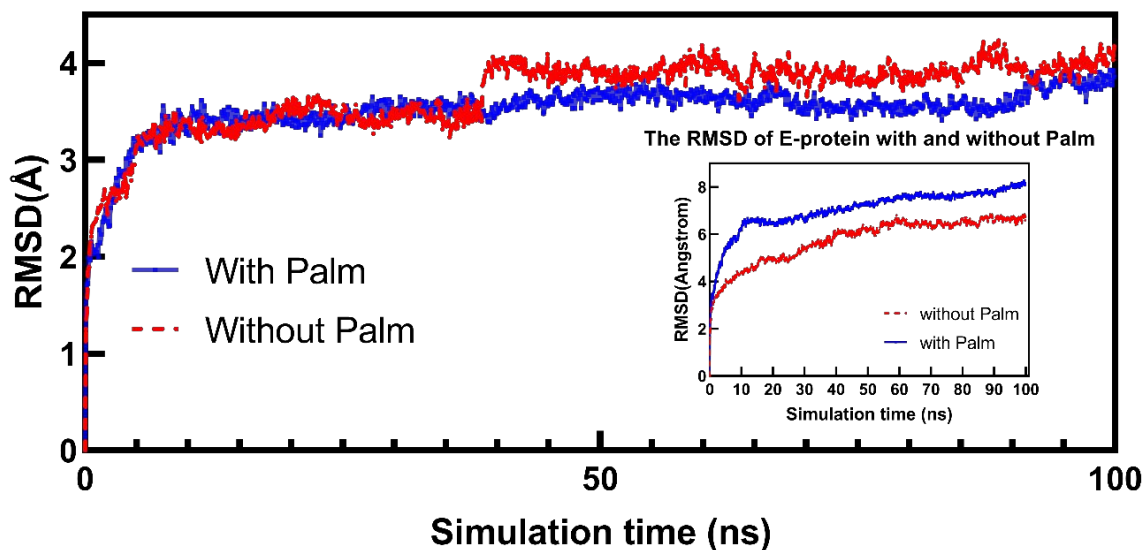


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24 Figure S3: The diagram of the placement of simulated H^+ ions for electrostatic force testing.

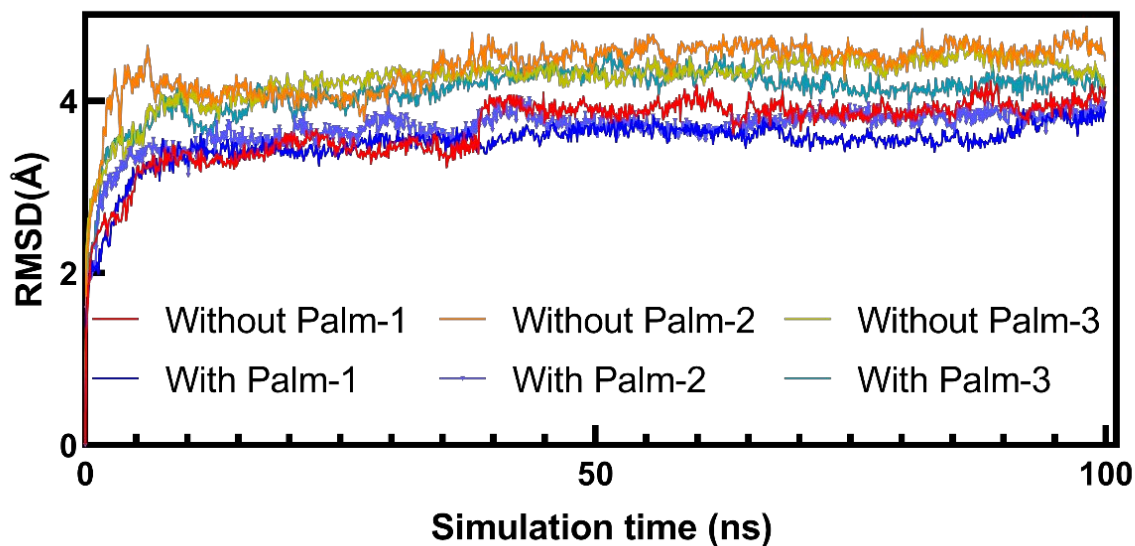
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The RMSD of E-protein with and without Palm in transmembrane domain

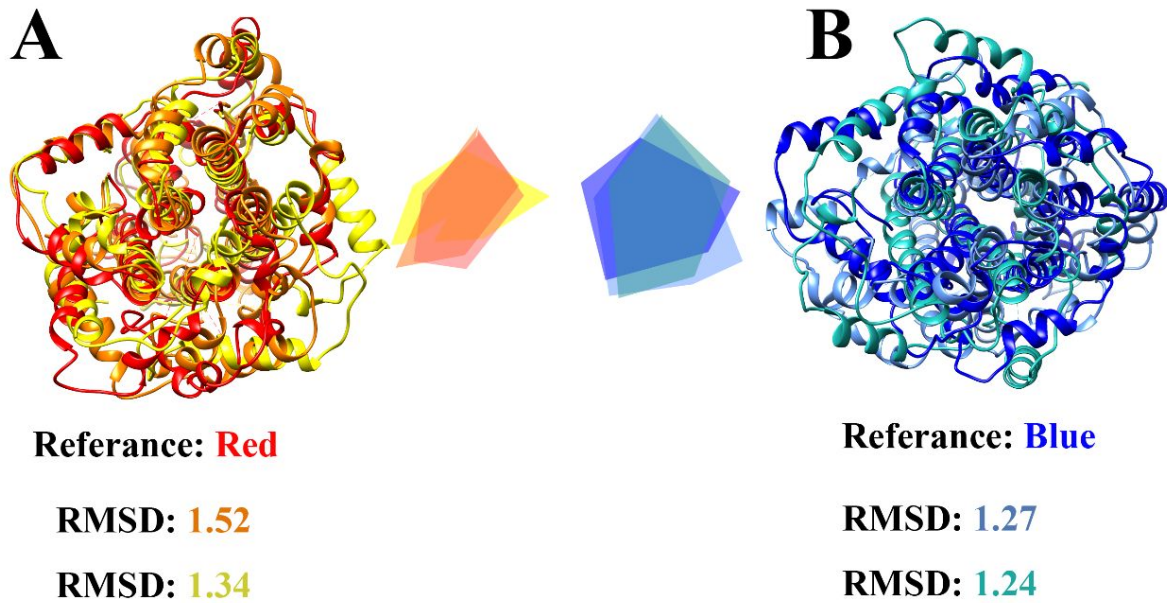


26
27 Figure S4: The backbone RMSD of E-protein pentamer with and without Palm during 100 ns simulation
28

The RMSD of E-protein with and without Palm in transmembrane domain for triple simulations



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

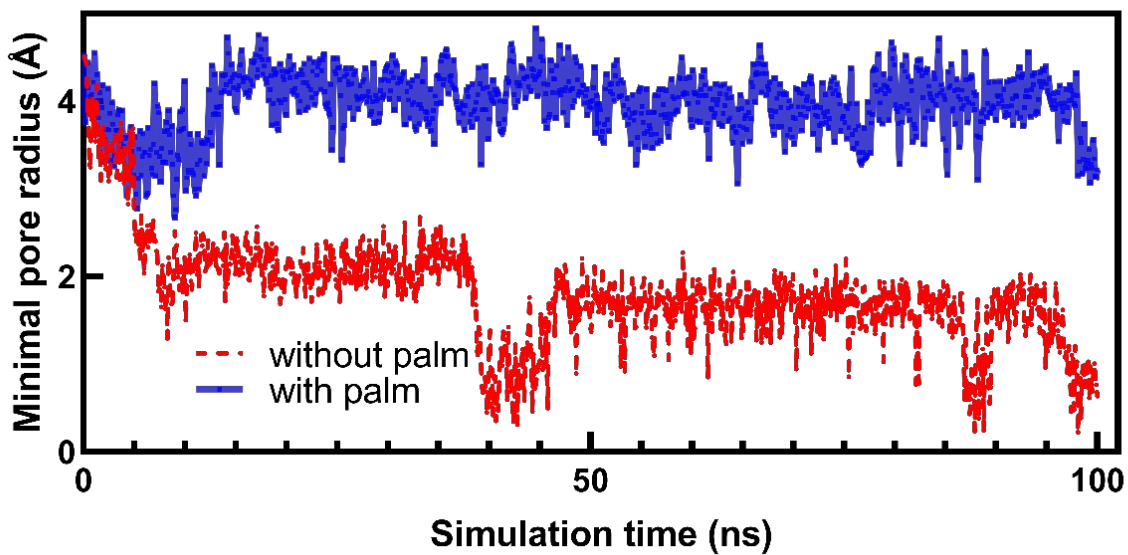


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34 Figure S6: The structural comparison of E-protein pentamer without (A) and with (B) Palm in triple
 35 simulations where the RMSD calculation is based on the first simulations (red and blue). The shadows are
 36 the general comparison on pores

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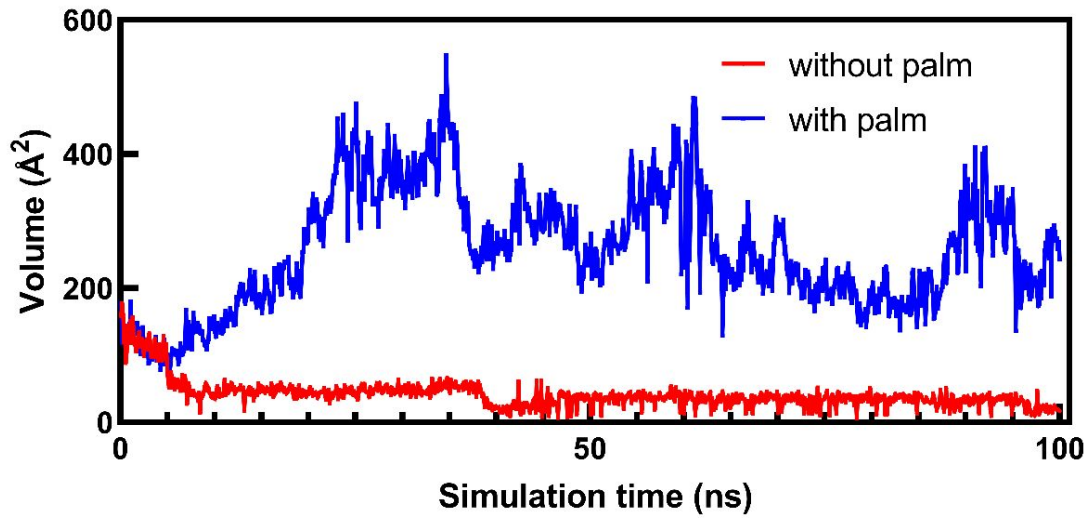
Minimal radius of the pore on the C-terminal of TMD



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

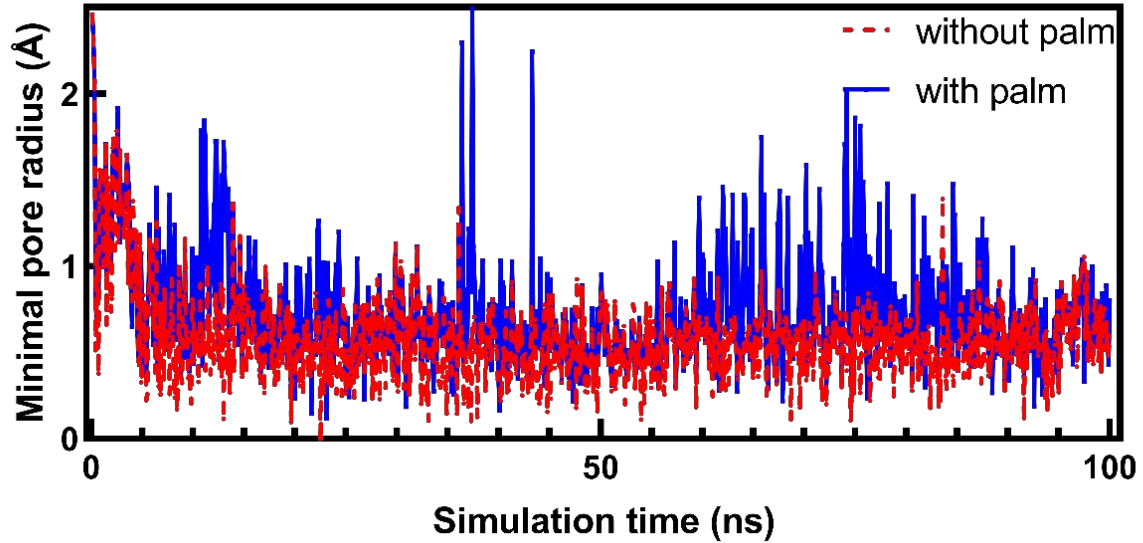
The volume of the pore on the C-terminal of TMD



41

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

Minimal radius of the pore on the middle part of TMD

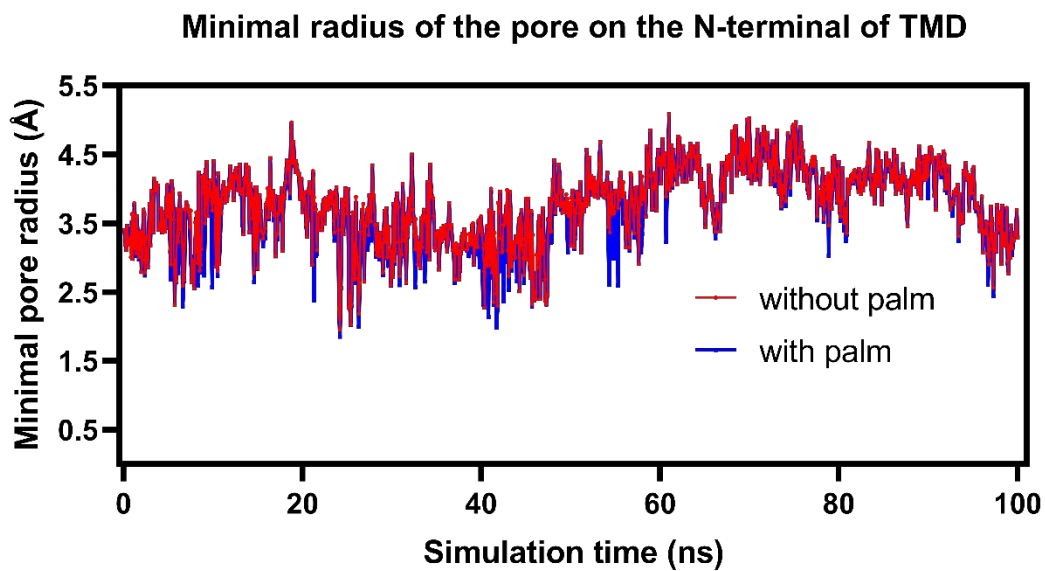


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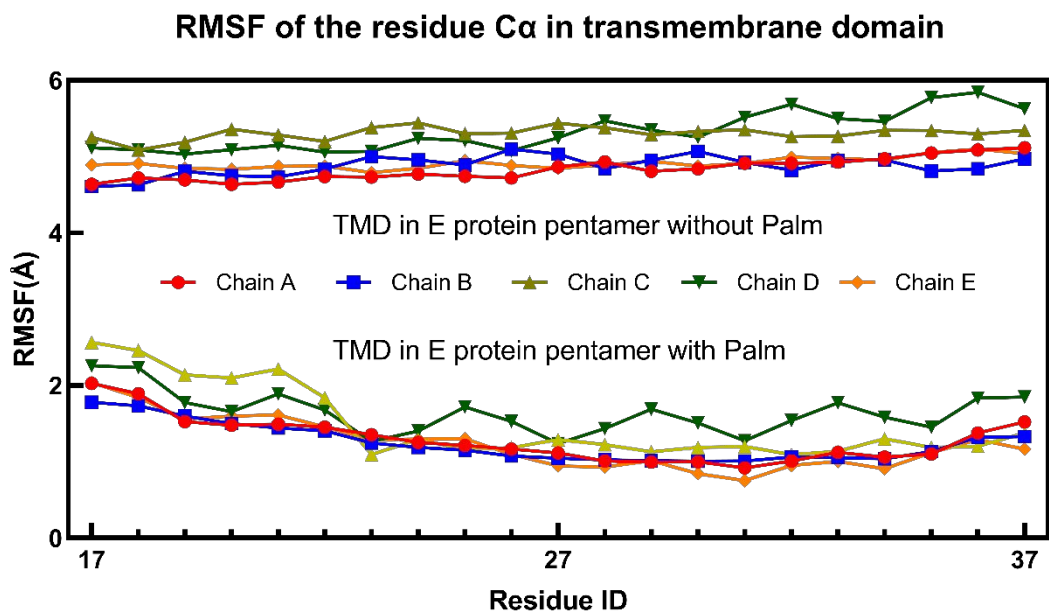
45 Figure S9: The minimal pore radius of the E-protein pentamer in the middle part (residue 21-30) of the
46 TMD during the simulation.

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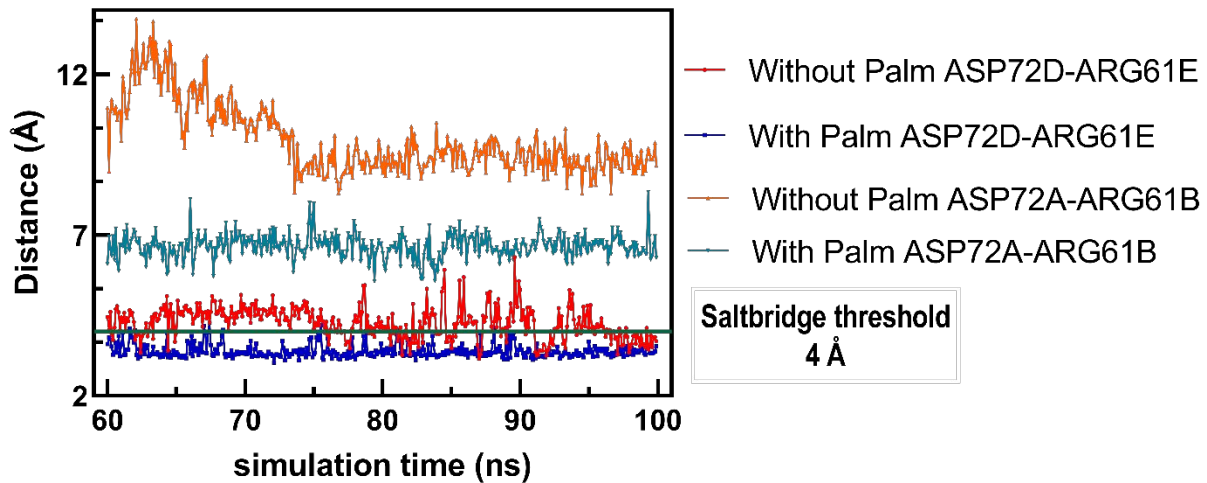


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 50 Figure S10: The minimal pore radius of the E-protein pentamer in the N-terminal (residue 10-20) during
 51 the simulation.
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 54 Figure S11: The RMSF of the residues (residues 17 to 37) in the transmembrane domain of E-protein
 55 pentamer.

Salt bridge ASP72-ARG61

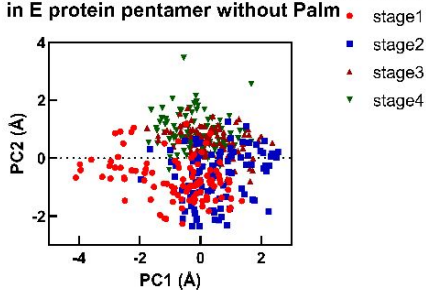


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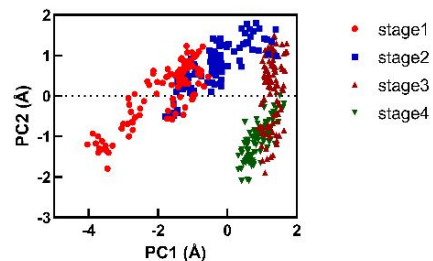
57 Figure S12: The distance of the salt bridges of ASP72D-ARG61E and ASP72A-ARG61B in both non-
58 palmitoylated E protein pentamer and palmitoylated E protein pentamer. (Technically, ASP72A-ARG61B
59 is not a salt bridge).

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A Principal component analysis of the TMD mass center in E protein pentamer without Palm



B Principal component analysis of the TMD mass center in E protein pentamer with Palm



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62 Figure S13: The PCA of the mass center of the transmembrane domain of E-protein pentamer with and
63 without Palm. The stages 1, 2, 3, 4 represent the simulations between 0-25ns, 25-50ns, 50-75ns, 75-
64 100ns.

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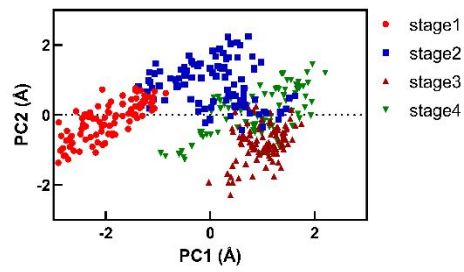
66 Table S1: The rotation of the PCA for non-palmitoylated and palmitoylated E protein pentamer (Figure
67 S13).

	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

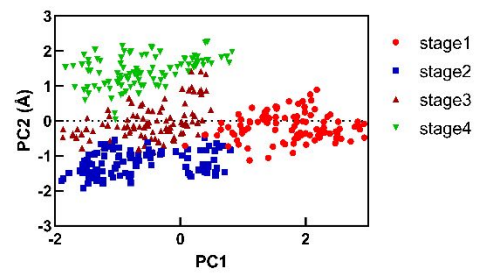
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A Principal component analysis of the TMD mass center in E protein pentamer with Palm (Repeated simulation)



B Principal component analysis of the TMD mass center in E protein pentamer with Palm (Repeated simulation)



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71 Figure S14: The PCA of the mass center of the transmembrane domain of E-protein pentamer with and
72 without Palm in the repeated simulations. The stages 1, 2, 3, 4 represent the simulations between 0-25ns,
73 25-50ns, 50-75ns, 75-100ns.