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

Supporting Information of

Insight into the Adsorption Profiles of the *Saprolegnia monoica* Chitin Synthase MIT Domain on POPA and POPC Membranes by Molecular Dynamics Simulation Studies

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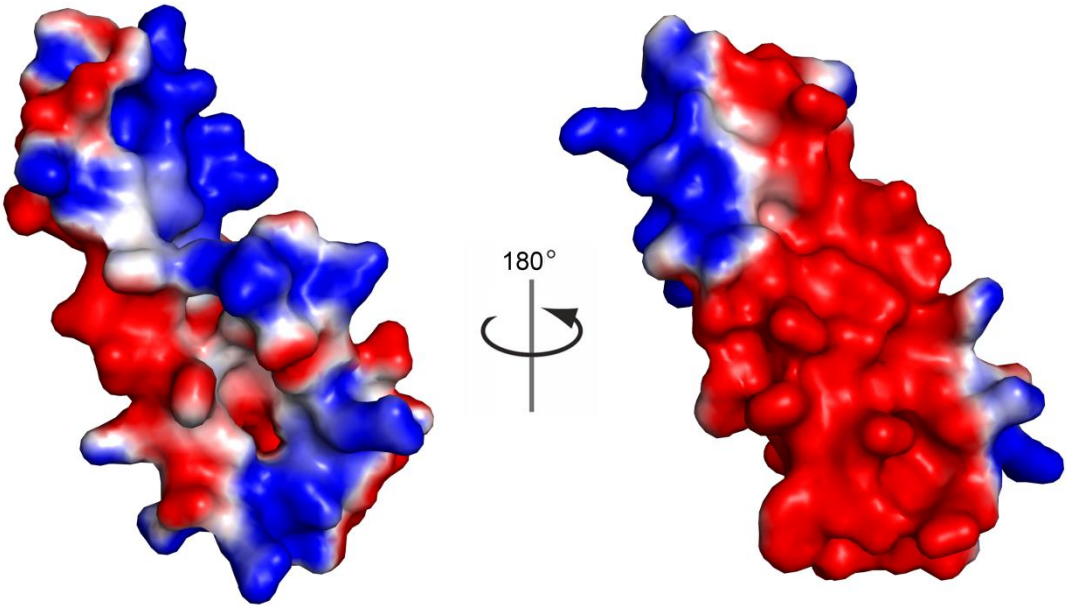
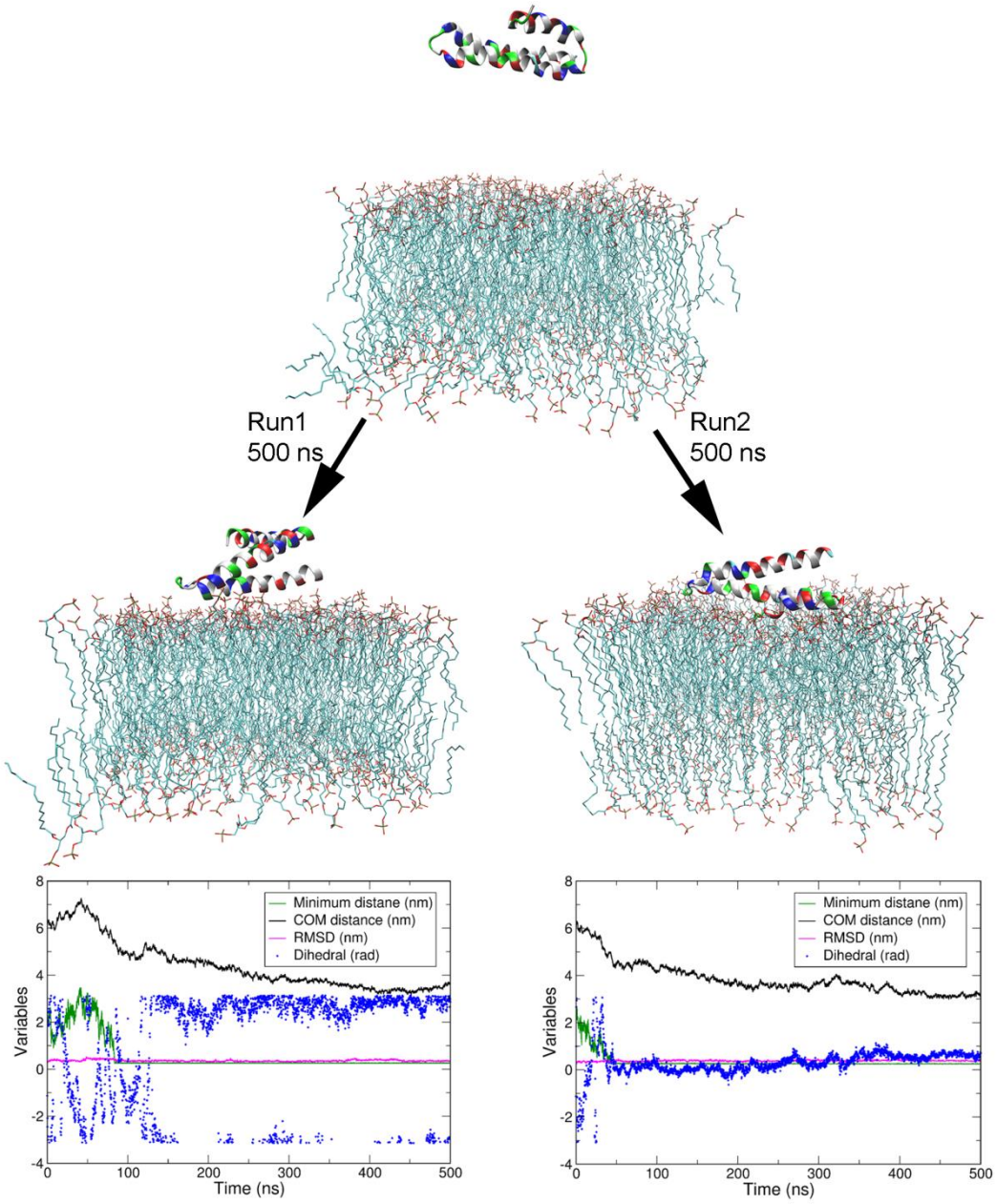
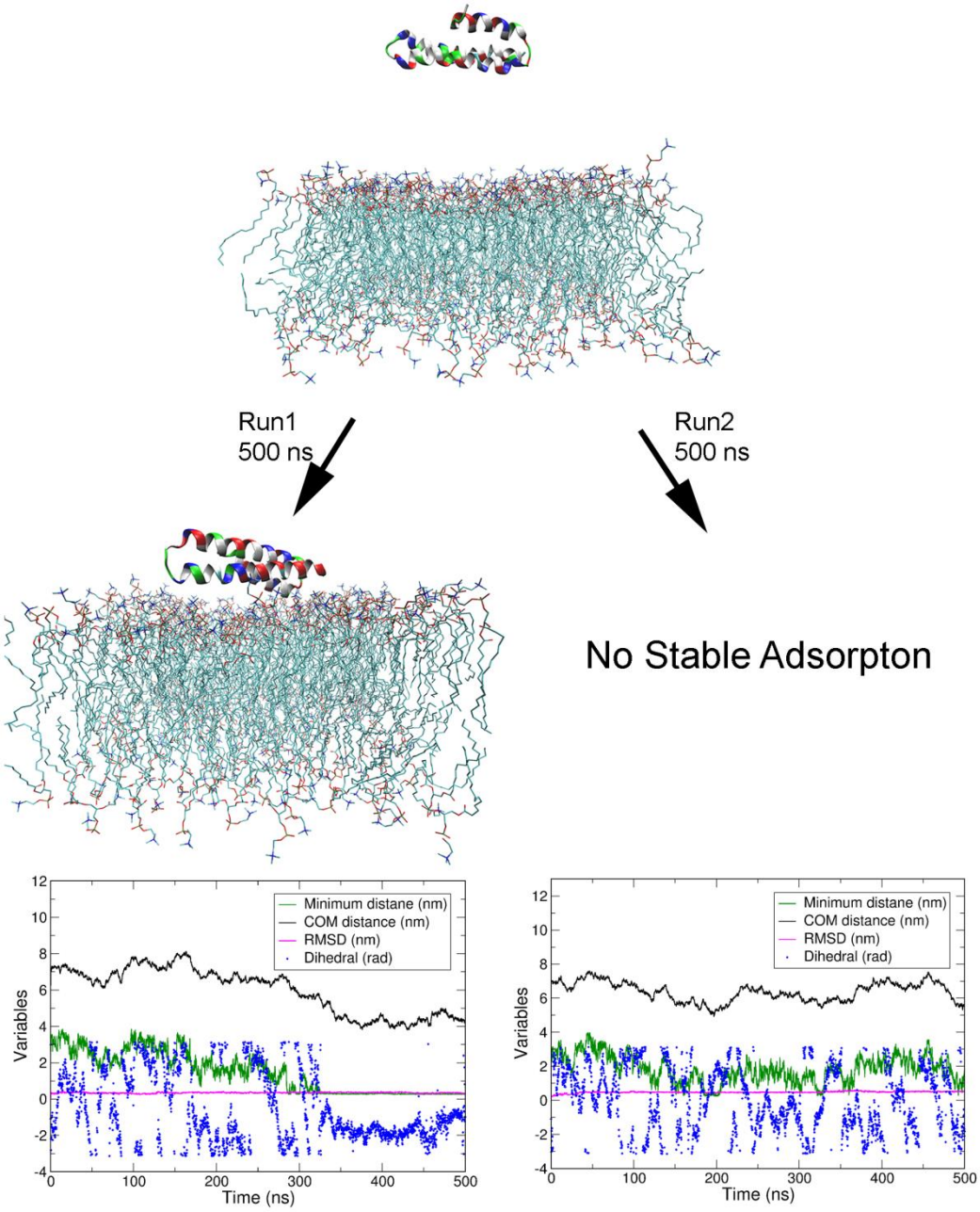


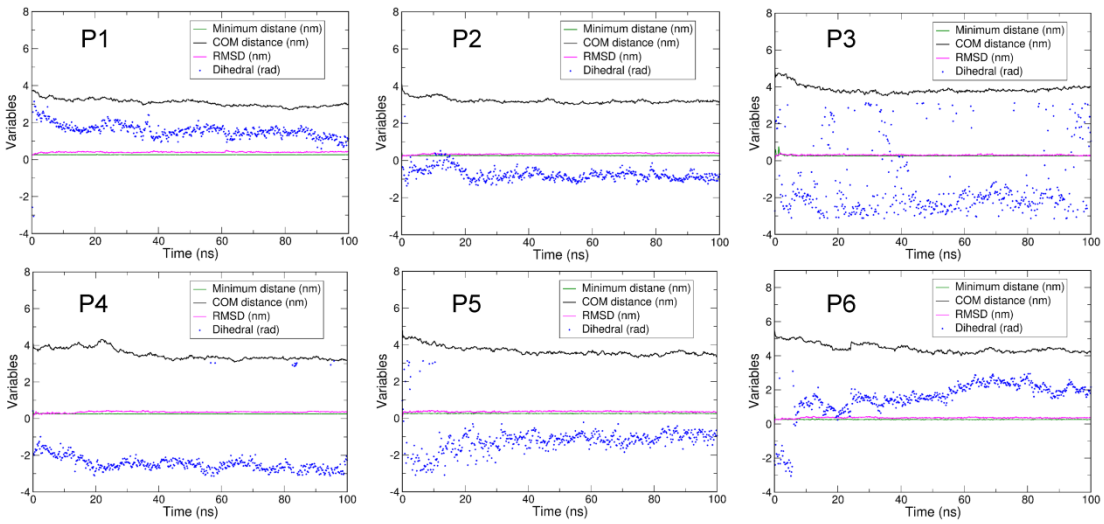
Supplementary Fig. S1. Electrostatic potential surface (EPS) of SmChs1-MIT obtained with APBS[1]. Blue regions, +1 kT; red regions, -1 kT.



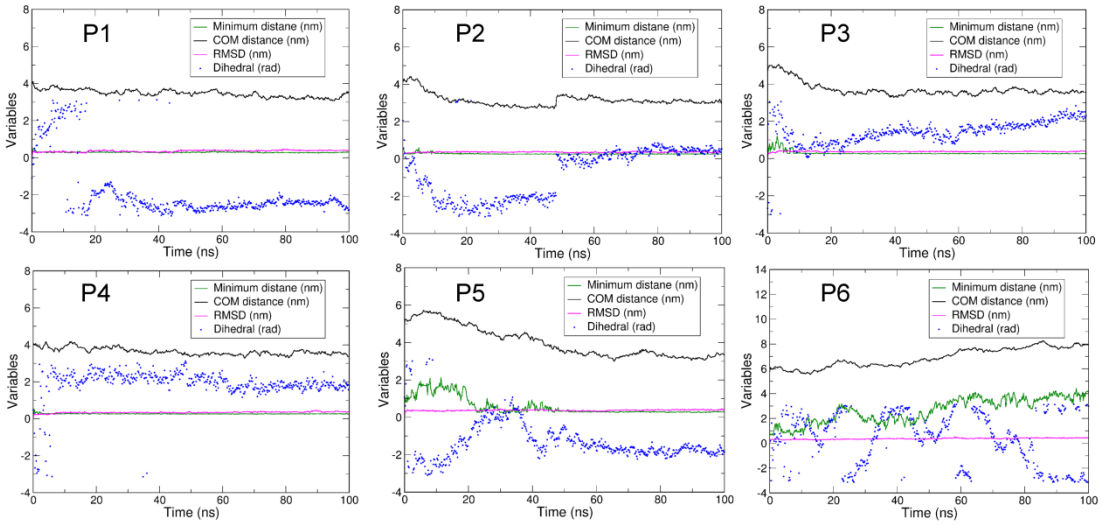
Supplementary Fig. S2. Adsorption profiles of the MIT domain on the POPA membrane in the "distant adsorption" simulations where the minimum distance between the heavy atoms of the protein and the membrane was set to be 2.5 nm in the initial state. The parameters shown in the plots are the minimum distance between the heavy atoms of the protein and the membrane, the distance between the centers of mass of the protein and the membrane, the root mean square deviation (RMSD) of the backbone atoms of the MIT domain, and the dihedral between the centers of mass of loop1, loop2, the whole protein and the membrane.



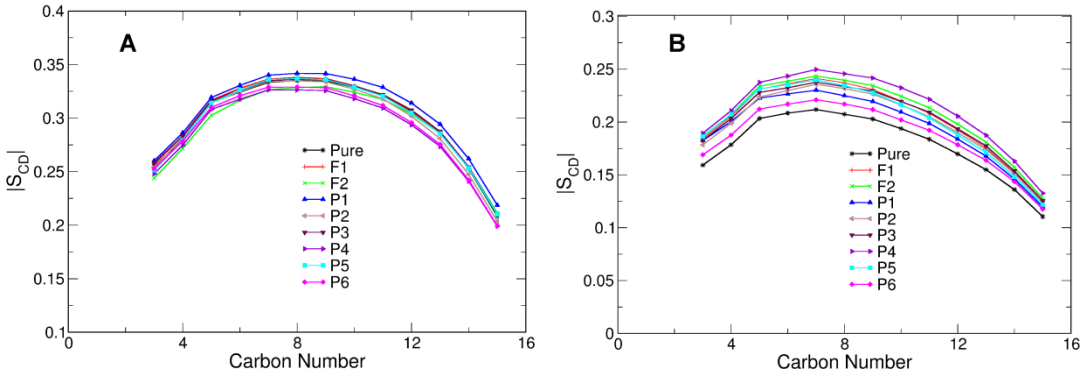
Supplementary Fig. S3. Adsorption profiles of the MIT domain on the POPC membrane in the "distant adsorption" simulations where the minimum distance between the heavy atoms of the protein and the membrane was set to be 2.5 nm in the initial state. The definition of the monitoring parameters is the same as that in **Supplementary Fig. S2**.



Supplementary Fig. S4. Adsorption profiles of the MIT domain on the POPA membrane in the "close adsorption" simulations where the minimum distance between the heavy atoms of the protein and the membrane was set to be 0.5 nm in the initial states. The definition of the monitoring parameters is the same as that in **Supplementary Fig. S2**.



Supplementary Fig. S5. Adsorption profiles of the MIT domain on the POPC membrane in the "close adsorption" simulations where the minimum distance between the heavy atoms of the protein and the membrane was set to be 0.5 nm in the initial states. The definition of the monitoring parameters is the same as that in **Supplementary Fig. S2**.



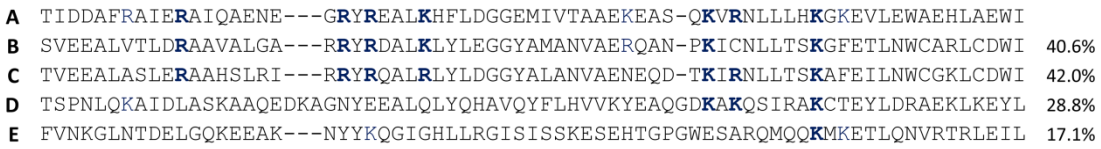
Supplementary Fig. S6. The deuterium order parameters for the *sn*-1 chains of POPA (A) and POPC (B) membranes in different conditions. Pure means that the MIT domain was absent in the system. F1-F2 means the "distant adsorption" simulations where the minimum distance between the heavy atoms of the protein and the membrane was set to be 2.5 nm in the initial state. P1-P6 means the "close adsorption" simulations where the minimum distance between the heavy atoms of the protein and the membrane was set to be 0.5 nm in the initial states.

Supplementary Table 1. The bilayer thickness and area per lipid (A_{lipid}) for POPA and POPC membranes in different systems.

	Thickness (nm) [a]		A_{lipid} (nm^2)	
	POPA	POPC	POPA	POPC
Literature[2]	4.56	4.05	0.520	0.641
Pure	4.49 ±0.03	3.88 ±0.02	0.517 ±0.002	0.644 ±0.007
F1	4.49 ±0.02	3.97 ±0.03	0.523 ±0.003	0.620 ±0.001
F2	4.46 ±0.03	4.04 ±0.02	0.529 ±0.003	0.612 ±0.001
P1	4.48 ±0.02	3.95 ±0.02	0.522 ±0.003	0.626 ±0.005
P2	4.49 ±0.02	3.98 ±0.02	0.518 ±0.002	0.619 ±0.001
P3	4.41 ±0.03	4.00 ±0.02	0.529 ±0.003	0.616 ±0.001
P4	4.55 ±0.02	4.09 ±0.03	0.508 ±0.002	0.600 ±0.001
P5	4.43 ±0.01	3.95 ±0.02	0.520 ±0.002	0.621 ±0.002
P6	4.43 ±0.02	3.86 ±0.02	0.525 ±0.003	0.641 ±0.007

[a] The lipid thickness and area per lipid were measured for the snapshots of the last 10% trajectories of the production simulations using the script developed by Allen et. al.[3]

Supplementary Fig. S7. Alignment of the sequences of the MIT domains from (A) *Saprolegnia monoica* chitin synthase 1, (B) *Phytophthora parasitica* chitin synthase 1, (C) *Albugo laibachii* chitin synthase 1, (D) human Vps4b and (E) human spartin. Conserved residues are highlighted in blue. The sequence identity percentages compared to (A) are presented in the end.



References:

1. N. A. Baker, D. Sept, S. Joseph, M. J. Holst and J. A. McCammon, *Proc. Natl. Acad. Sci. U. S. A.*, 2001, **98**, 10037-10041
2. A. Dickey and R. Faller, *Biophys. J.*, 2008, **95**, 2636-2646.
3. W. J. Allen, J. A. Lemkul and D. R. Bevan, *J. Comput. Chem.*, 2009, **30**, 1952-1958.