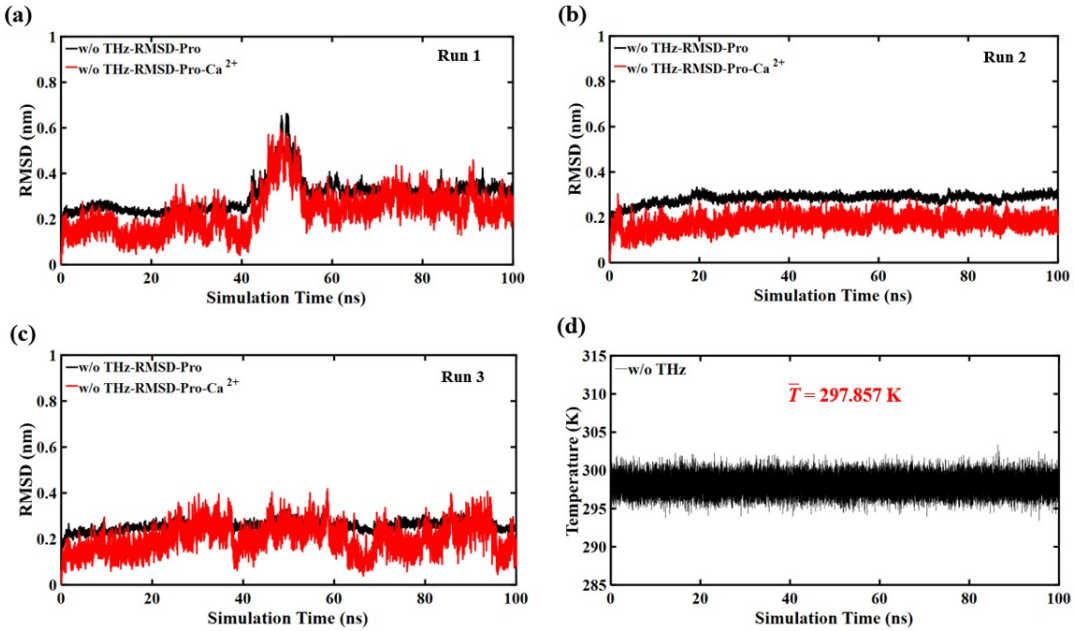

Figure S1. (a-b) The RMSD of the protein backbone and Ca^{2+} relative to the protein during the MD simulation. (c) The system temperature during the MD simulation. These figures can be used to determine whether the system has reached a stable state in MD simulations.

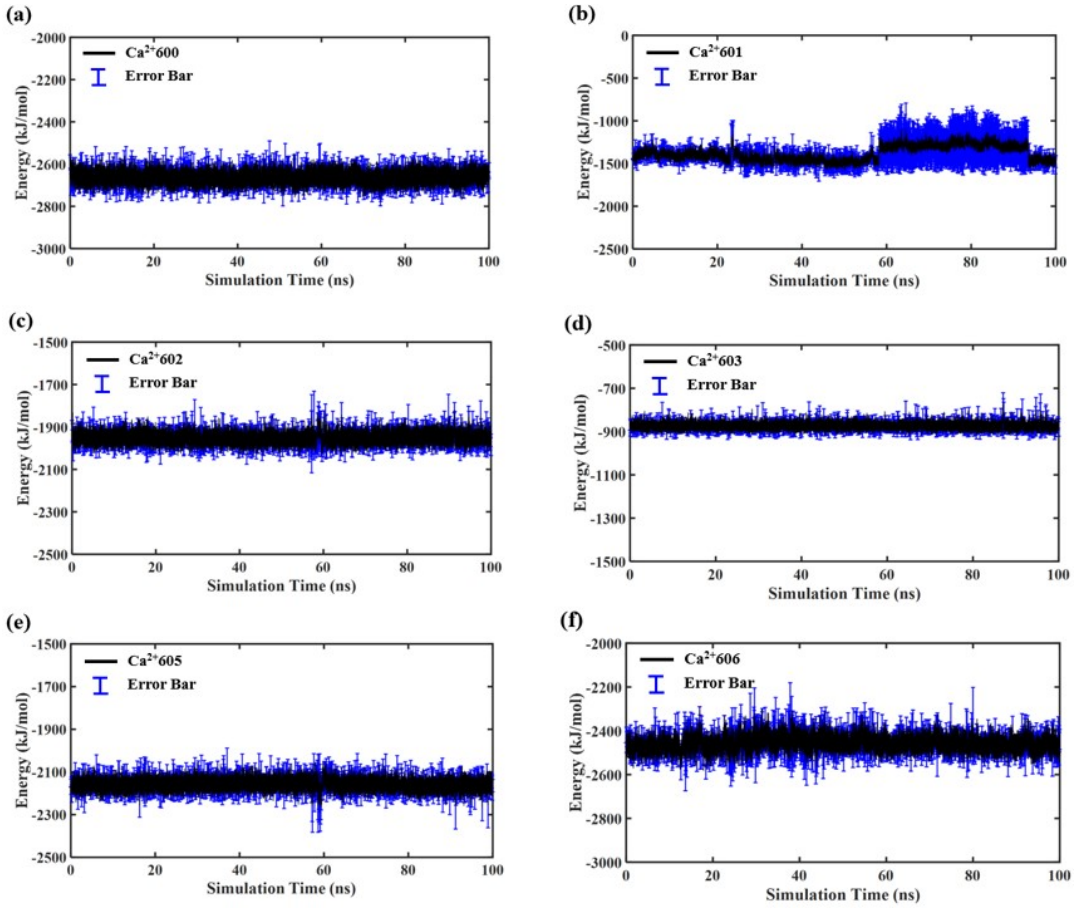

Figure S2. The curves of the interaction energy between each Ca^{2+} and its corresponding binding pocket along with its error bars, as a function of simulation time. All results were obtained through three independent simulations.

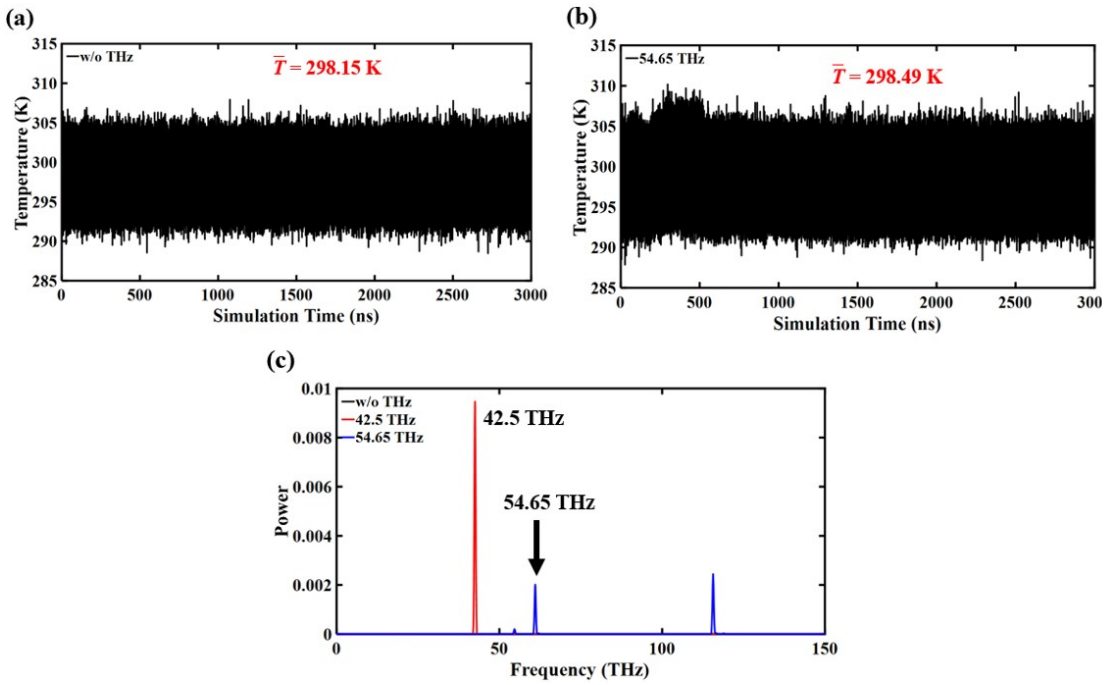

Figure S3. The stability of the entire system in 3 μs MD simulations is measured under (a) no THz and (b) 54.65 THz conditions by system temperature and (b) the accessible contact area of C2AB. Three independent simulations are performed for each condition, and the curves are averaged from all simulations. In the whole simulation process, the temperature is in a relatively stable. Figure (c) is the vibration spectrum of Tip3p water under different MD conditions. At 42.5 THz, it shows the strong absorption of THz wave by water, while at 54.65 THz, it is not significant.

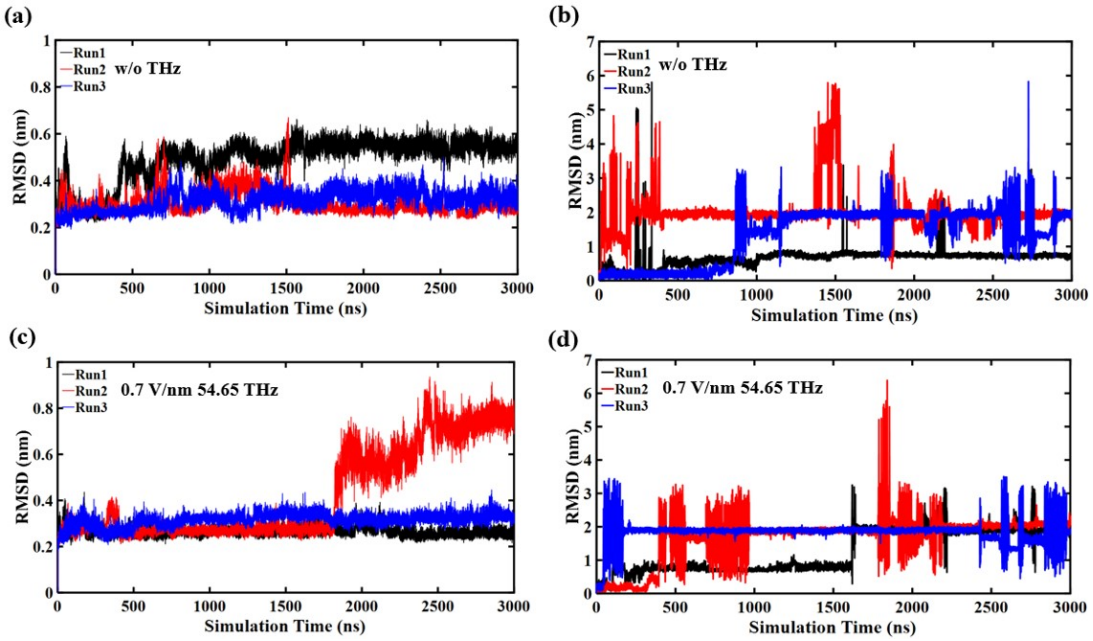

Figure S4. The RMSD of the protein under (a) w/o THz, (c) 54.65 THz and the RMSD of the Ca^{2+} in the pocket relative to the pocket (b) w/o THz, (d) 54.65 THz. For (b) and (d), the RMSD at 1 to 2 nm means that Ca^{2+} have been out of the pocket.

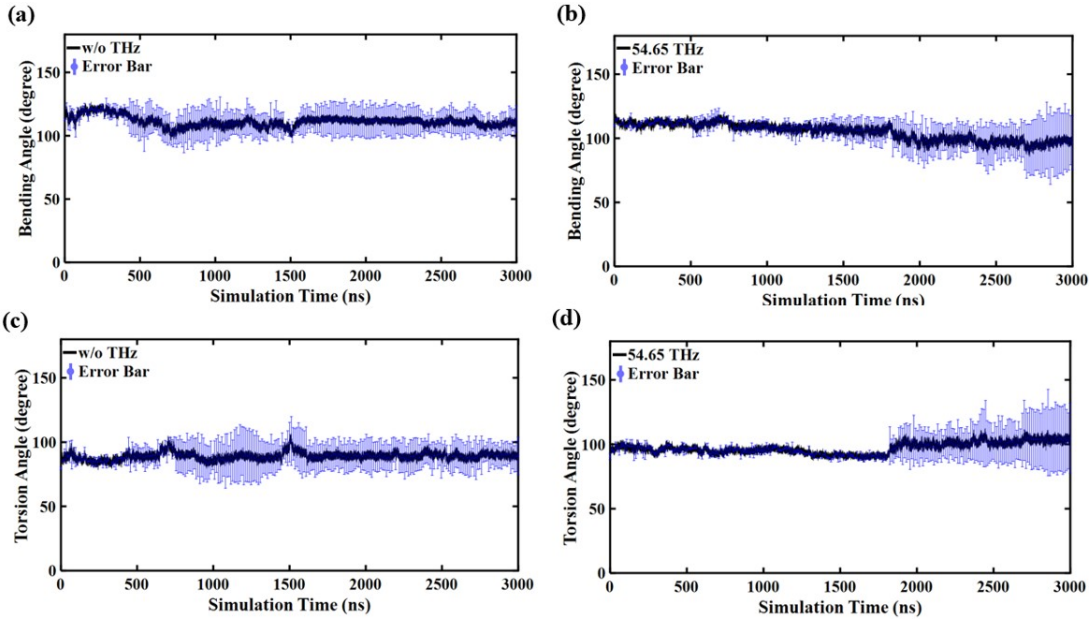

Figure S5. The curves of bending and torsion angles of region C2AB from three independent simulations and their corresponding error ranges vary with simulation time. Due to the conformational changes induced by THz waves, significant fluctuations appeared in the later stage of the simulation, reflected by an increase in the length of the error bars compared with the earlier simulation.

Table S1. The RMSF value of calcium binding pocket amino acids correspond to the initial simulation part.

	Calc	**Exp**
Lys327	0.1223	0.1598
Asp328	0.1418	0.1978
Asp334	0.1221	0.1855
Asp386	0.1112	0.1531
Asp387	0.1431	0.1743
Asp388	0.1477	0.179
Ser391	0.1806	0.1683
Arg392	0.2611	0.203
Asp394	0.1309	0.173
Met459	0.1328	0.1686
Asp460	0.141	0.1762
Asp520	0.111	0.1656
Tyr521	0.1395	0.1631
Asp522	0.1479	0.1662
Glu528	0.2106	0.1756