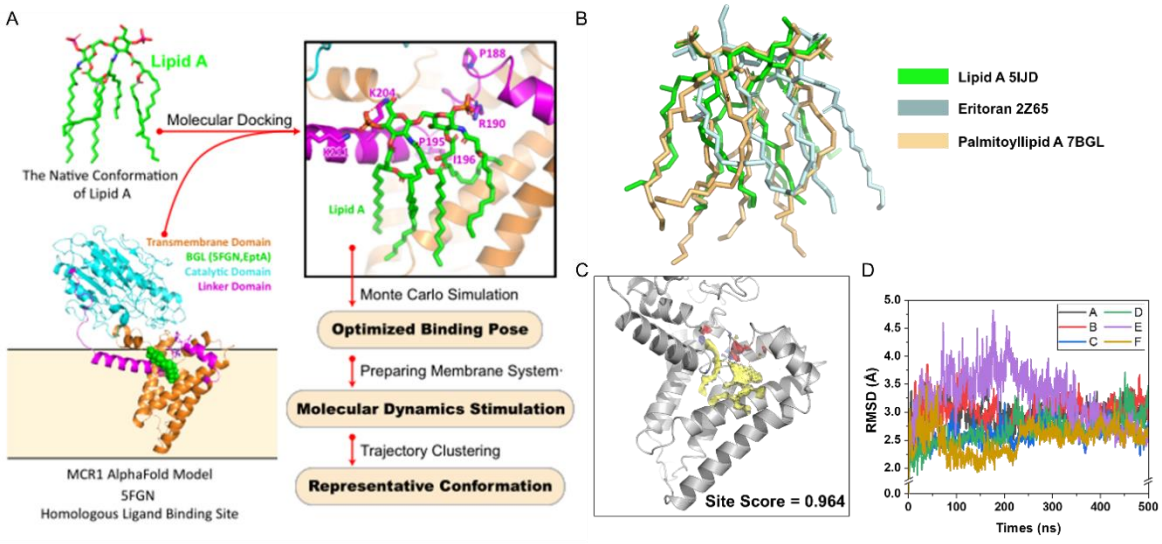

Figure S20. Analysis of the molecular dynamic simulation and binding energy.

Molecular dynamic stimulation was utilized to discover the potential LPS binding cavity on the surface of MCR-1, and the workflow was designed as shown in **(A)**. Structural comparison within lipid A (PDB code: 5IJD) and its analogues: Eritoran (PDB code: 2Z65) and Palmitoyllpid A (PDB code: 7BGL) are shown in **(B)**. **(C)** The potential lipid A binding site on the surface of MCR-1 was discovered by SiteMap of Maestro. **(D)** shows the RMSD fluctuations for multiple trajectories of MCR1-lipid A.