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Article

Identification of Potential Lead Compounds Targeting Novel Druggable Cavity of SARS-CoV-2 Spike Trimer by Molecular Dy-Namics Simulations

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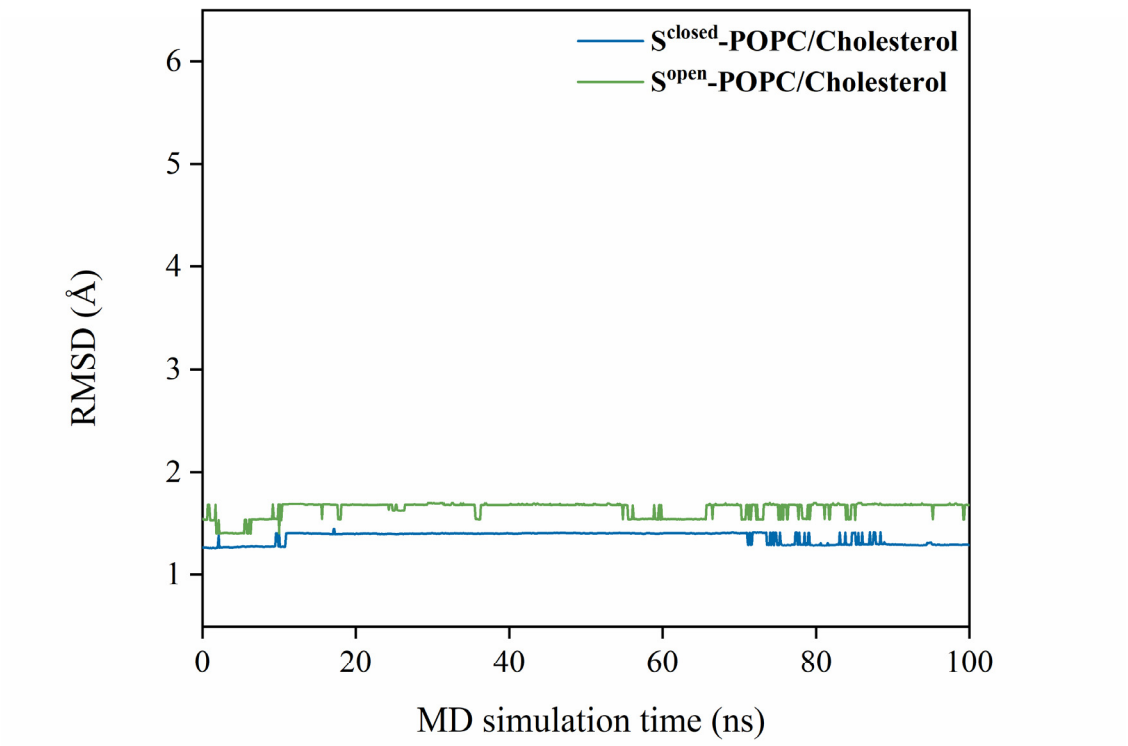

Figure S1. RMSD of S^{closed}-POPC/cholesterol and S^{open}-POPC/cholesterol systems.

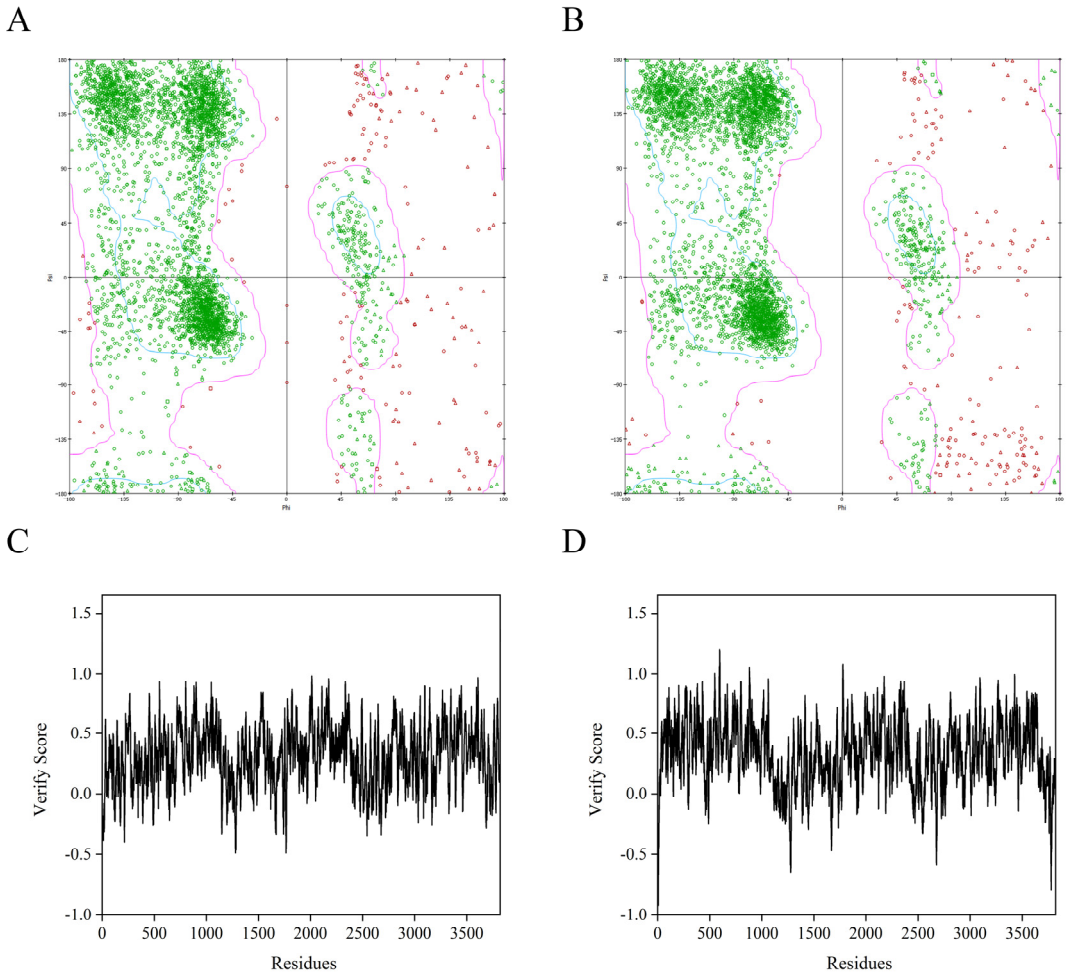

Figure S2. The Ramachandran plots of (**A**) S^{closed} and (**B**) S^{open}. The Profile-3D plots of (**C**) S^{closed} and (**D**) S^{open}. The homology modeling structures of S^{closed} and S^{open} are associated with 90% residues being in allowed region of Ramachandran plot (Procheck program) and 90% residues exhibiting reasonable folding (Profile-3D program).

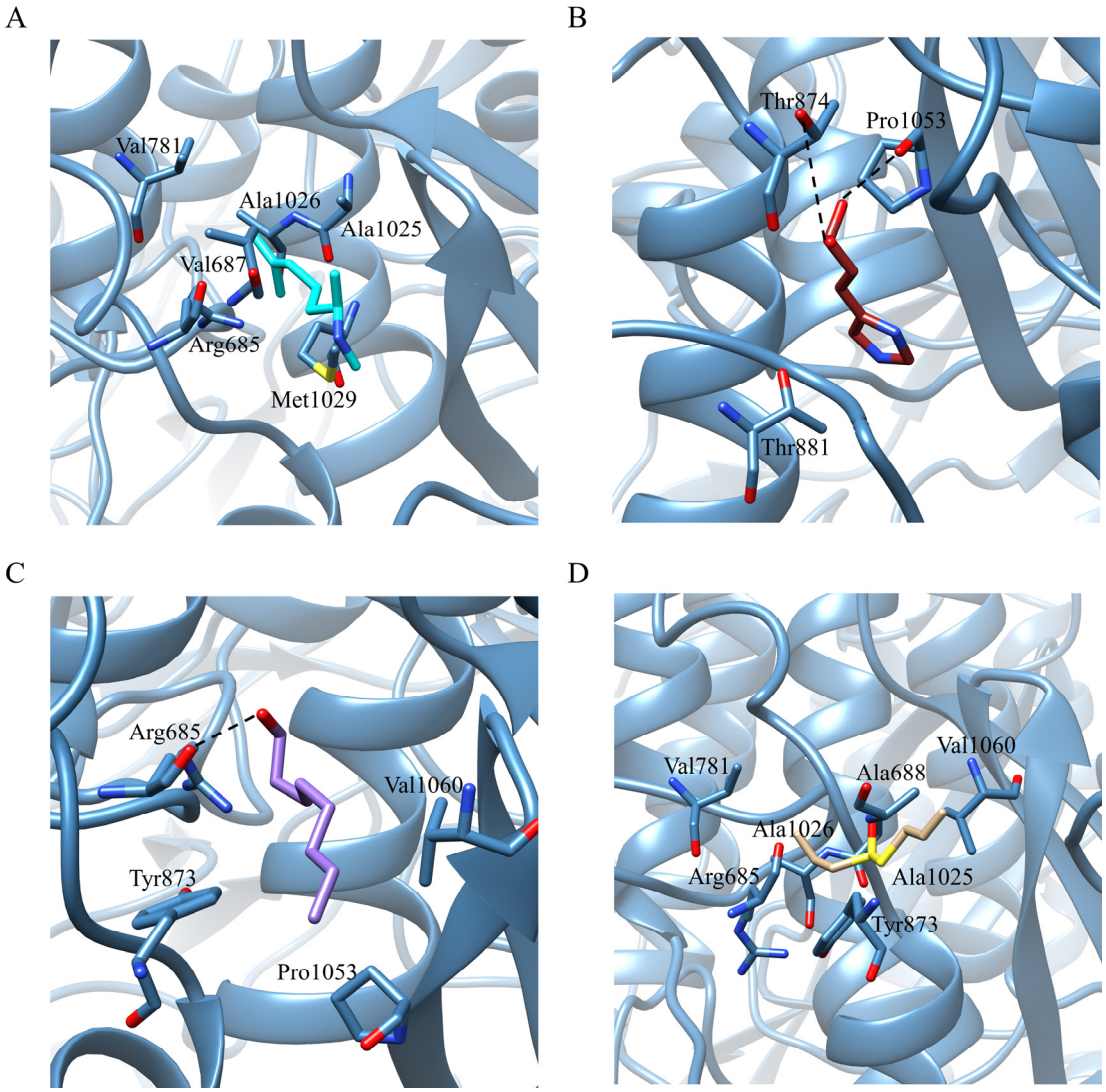

Figure S3. The binding interface of S^{closed} structure and (**A**) isometheptene, (**B**) urocanic acid, (**C**) 1-octanol and (**D**) allicin. The key residues are represented by stick models, and the important H-bonding interactions are labeled in the black lines.

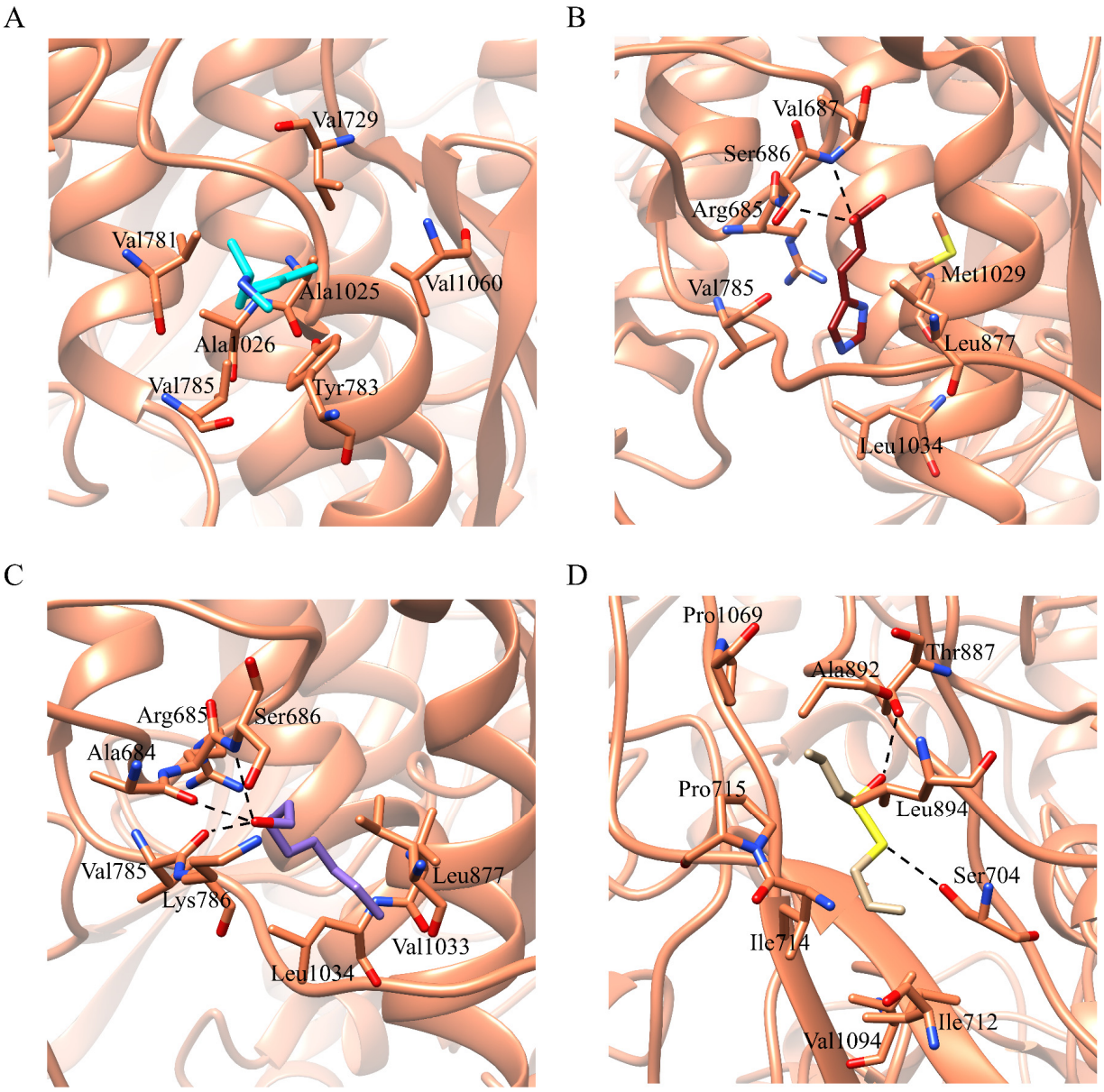

Figure S4. The binding interface of S^{open} structure and (**A**) isometheptene, (**B**) urocanic acid, (**C**) 1-octanol and (**D**) allicin. The key residues are represented by stick models, and the important H-bonding interactions are labeled in the black lines.

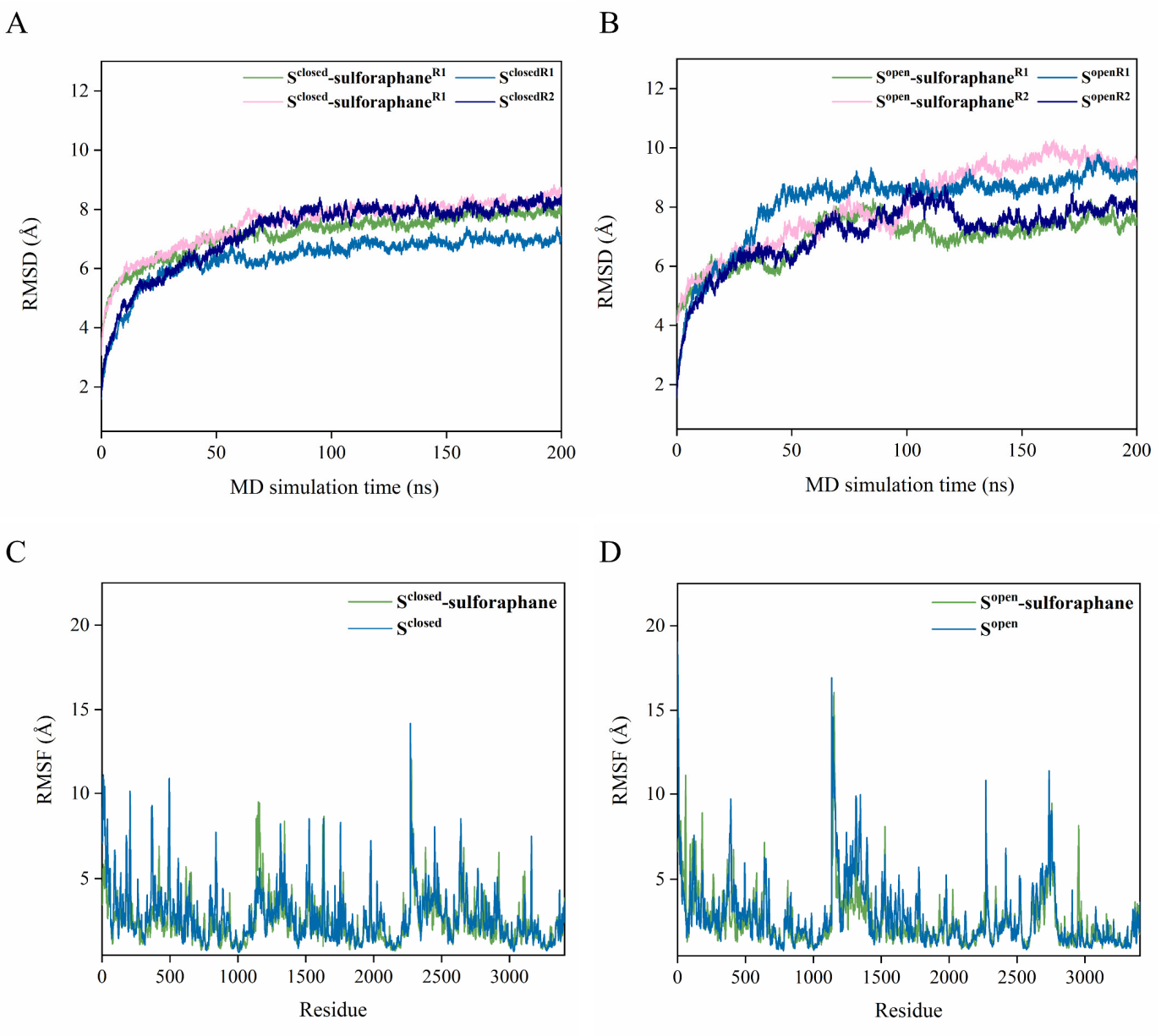

Figure S5. RMSD of various systems: (**A**) S^{closed} and (**B**) S^{open}. RMSF per residue for various systems: (**C**) S^{closed} and (**D**) S^{open}.