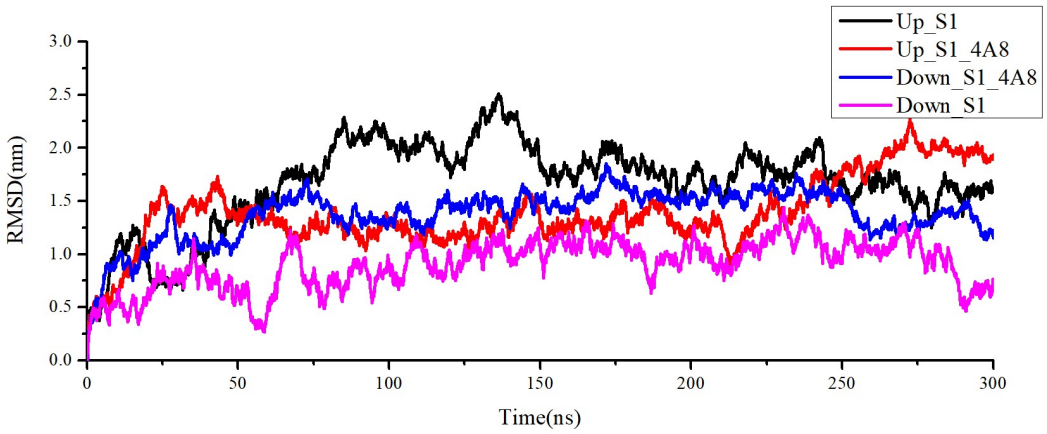

The Molecular Mechanism Study of Structural Regulation of the N-terminal Domain Binding Antibody on the Receptor Binding Domain of SARS-CoV-2

Received 00th January 20xx,
Accepted 00th January 20xx

DOI: 10.1039/x0xx00000x

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Supplementary Figures and Tables

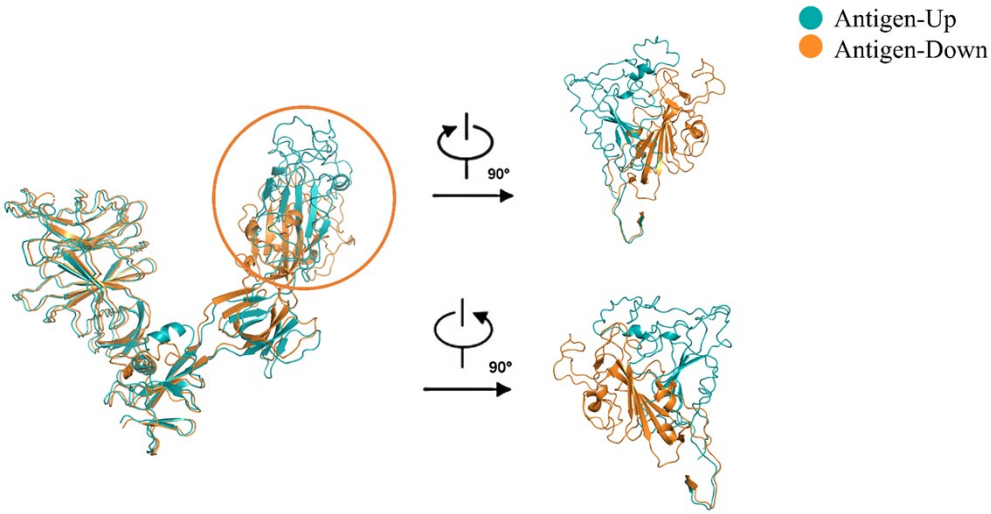

Fig. S1. Structure superposition comparison between Up and Down states of the S1 before simulation. (Where the dark green structure is the structure of the complex in the Up state and the orange structure is the structure of the complex in the Down state).

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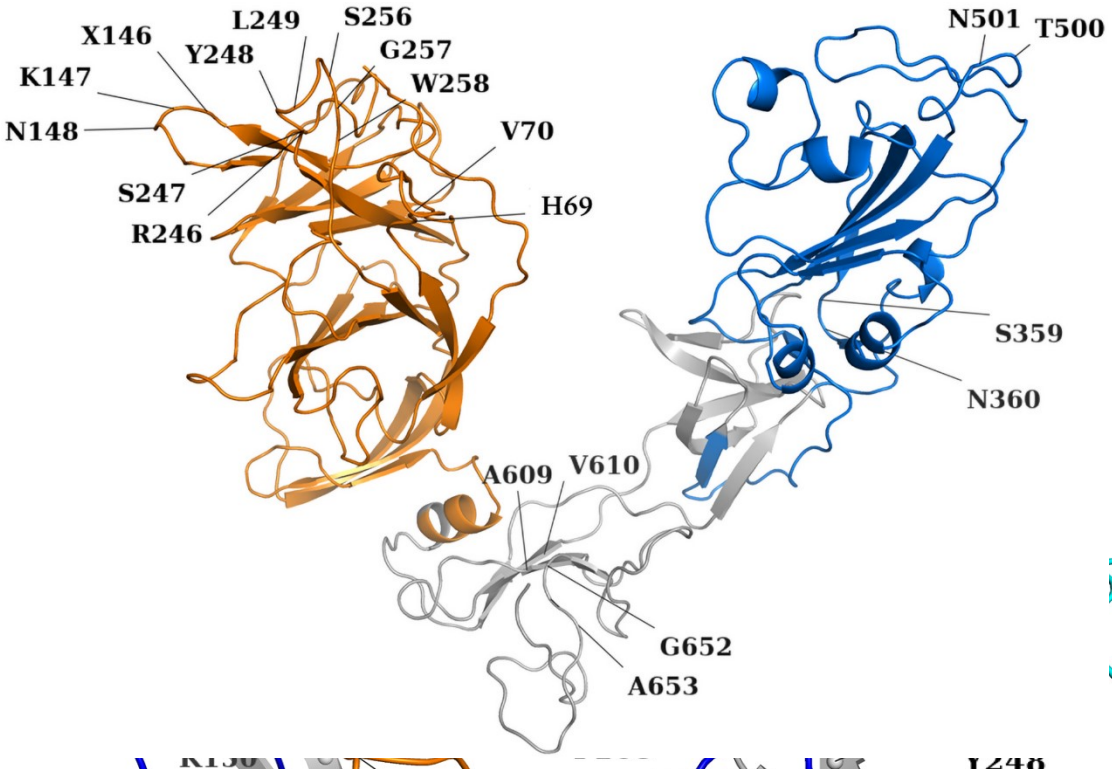

Fig. S5. Distribution of important contiguous residues on S1. (The orange part is NTD, the blue part is RBD, and the gray part is SD1 and SD2).

Fig. S3. Structure comparison of 4A8 antibody and NTD binding site. (Left panel is Up state, right panel is Down state, blue part is 4A8 antibody, green part is NTD, the rest key structures have been marked with different colors in the figure).

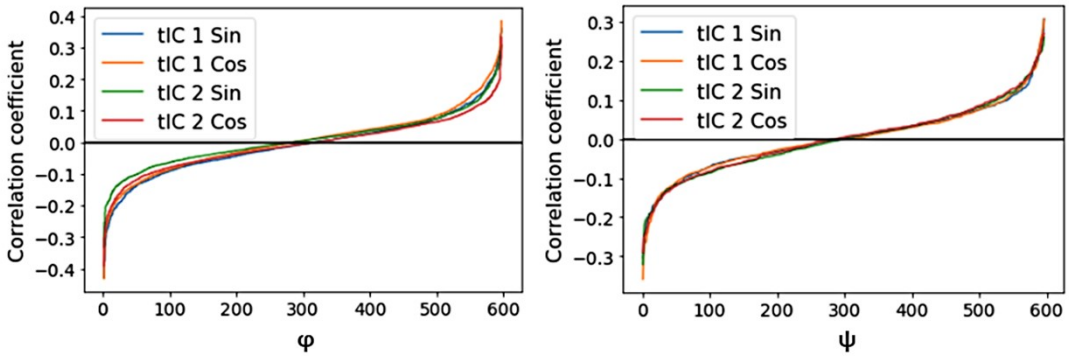

Fig. S4. Correlation coefficients of φ (left) and ψ angles (right) in ascending order.

Table S1. Analysis of H-bonds occupancy between S1 and 4A8 in the Up state, "L" represents ligand 4A8 and "R" represents receptor S1.

Acceptor	Donor	Occupancy(%)
L E31	R R246	49.90
L E72	R K147	43.51
L E72	R K134	36.73
L E31	R R246	36.53
L D52	R K137	23.95
L L32	R K134	22.56
L E54	R K137	21.76
L E31	R Y235	18.16
R N135	L T74	17.96
L D52	R K137	17.76
L E29	R K134	16.57
L D52	R K137	15.17

Table S2. Analysis of H-bonds occupancy between S1 and 4A8 in the Down state, "L" represents ligand 4A8 and "R" represents receptor S1.

Acceptor	Donor	Occupancy(%)
L E31	R R246	50.70
R Y132	L Y111	35.53
L L32	R K147	23.15
L E31	R Y132	22.16
L L32	R K134	20.76
L D55	R K137	18.56
L E31	R233	15.57