

Supplemental Material

Supplemental Figure S1. The root mean square deviation (RMSD) analyses of MD simulations for mutant structure of SARS-CoV-2 spike complexed with ACE2.

RMSD plots of protein backbone Ca carbon in (A) wild-type, (B) D614G, (C) N501Y:D641G, (D) K417N:N501Y:D641G, and (E) E484K:N501Y:D641G during the 100 ns of the MD simulations are depicted.

