Supplementary Information (SI) for Physical Chemistry Chemical Physics.
This journal is © the Owner Societies 2025

Supporting Information

Unraveling the impact of binary vs ternary alcohol solutions on the conformation and solvation of the SARS-CoV-2 receptor-binding domain

Rabiul Gazi and Madhurima Jana*

Molecular Simulation Laboratory, Department of Chemistry, National Institute of Technology, Rourkela - 769008, India

*Email: janam@nitrkl.ac.in

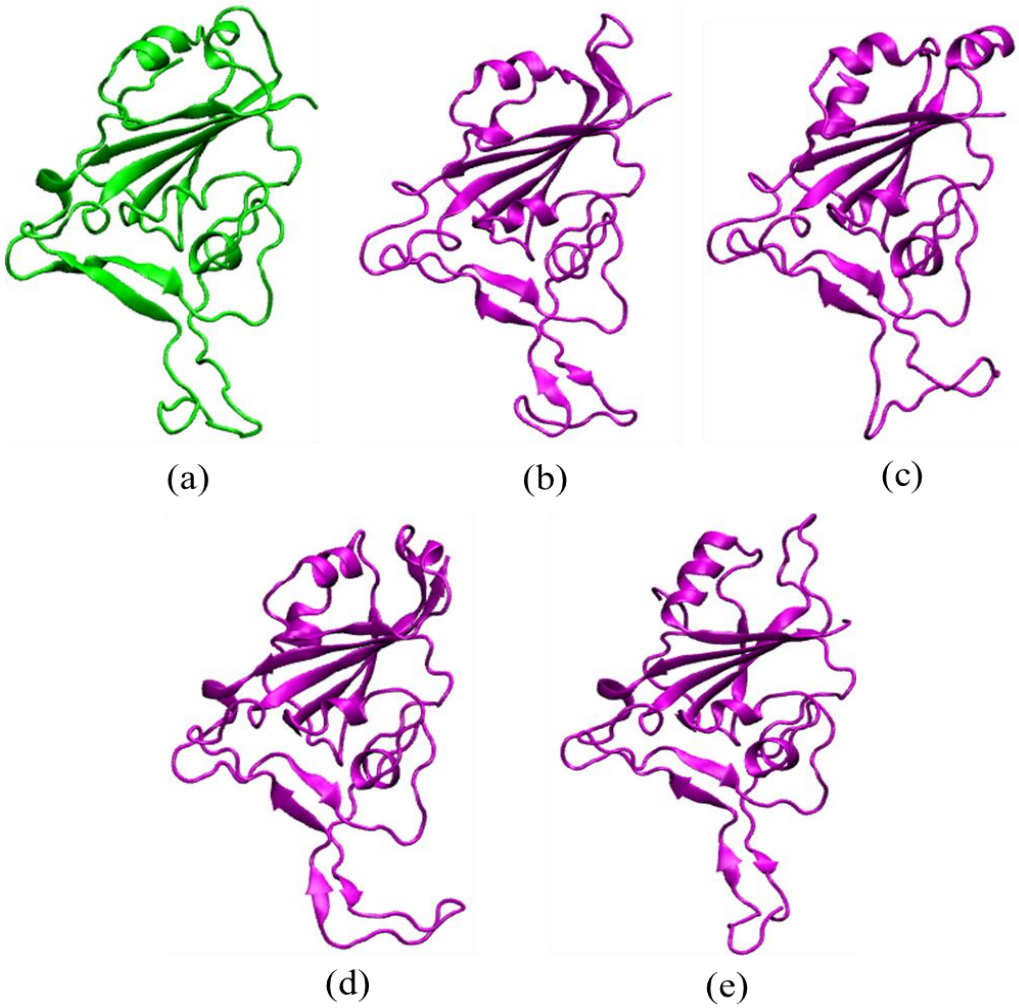

Figure S1. The representative snapshot of (a) native protein (in green) and the snapshots of the protein in each solution at end of the simulations (magenta) is shown (b) in pure water, (c) in etoh, (d) in *iso*-pr and (e) in *n*-pr at 300 K.

We quantified RMSD to understand the conformational features of RBD from the new simulations. The results are compared with that in pure water at 300 K and mix-1 in two different temperatures. The Figure S2 depicts the time evolution of the root-mean-square deviation (RMSD). For comparison, we have shown that the results only for 500 ns to 600 ns. A conformational jump of RBD was noted at 350 K in pure water after ~65 ns (in the timescale of 100 ns) of the simulation compared to 300 K in pure water. However, such a change is minor compared to the significant changes in the RBD conformations in mix-1, at both 300 K and 350 K, as noted from the RMSD plot. Notably, the changes were significantly small when the RBD was simulated at 350 K in the presence of alcohols. Such preliminary results infer that apart from the temperature, alcohols affect the RBD dynamics and can rupture the RBD conformation. Details of such comparison can be addressed in our future studies.

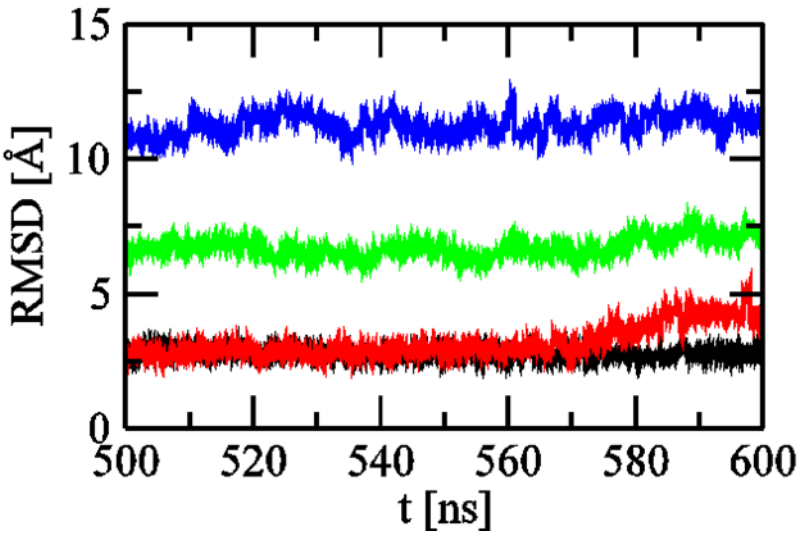

Figure S2. The time dependent root-mean-square deviation (RMSD), of the RBD in pure water and mix-1 at 300 K and 350 K.

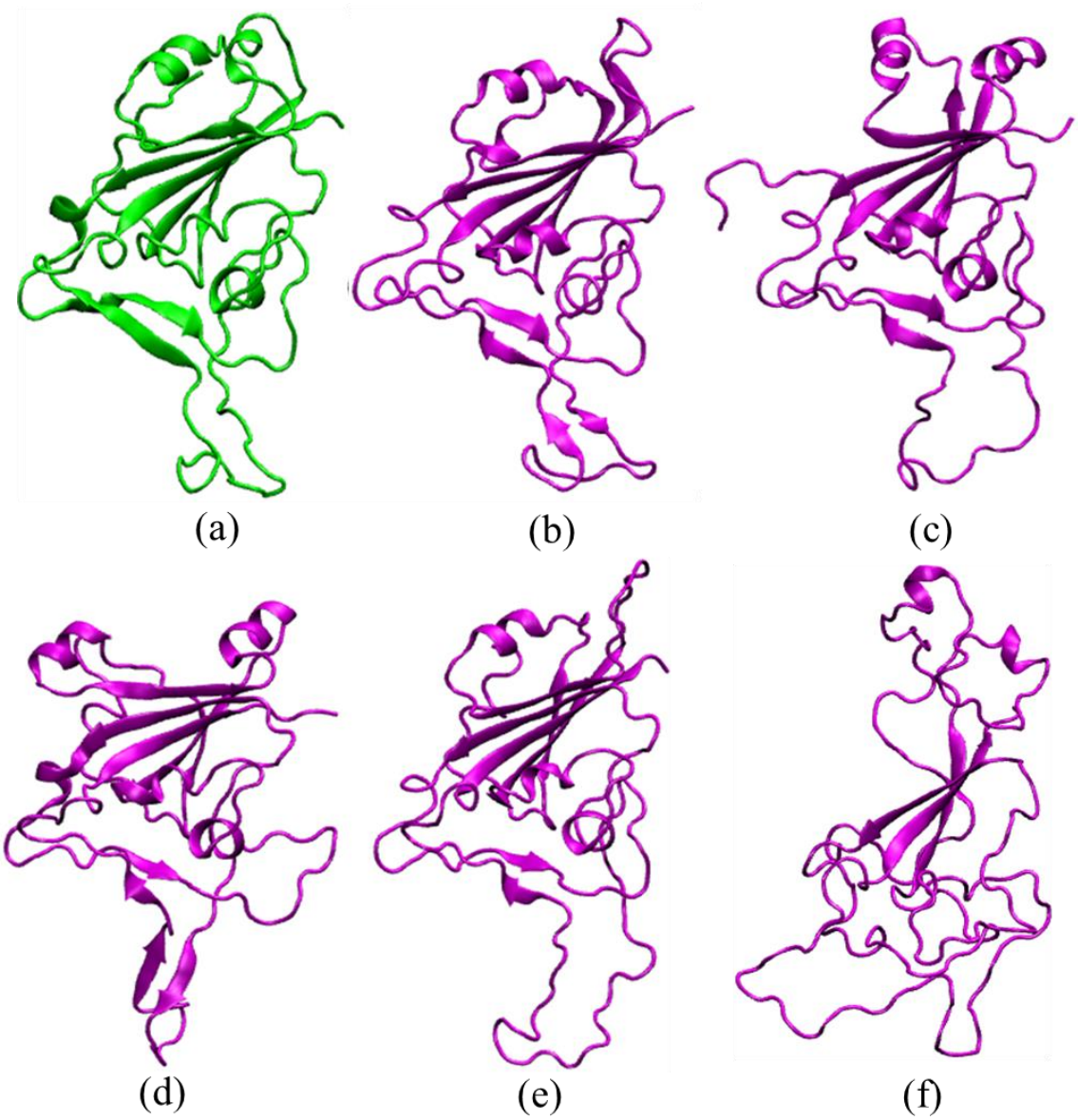

Figure S3. The representative snapshot of (a) native protein (in green) and the snapshots of the protein in each solution at end of the simulations (magenta) is shown (b) in pure water, (c) in mix-1, (d) in mix-2 and (e) in mix-3 at 300 K and (f) in mix-1 at 350 K.