Review 2: "Binding Profile Assessment of N501Y: a More Infectious Mutation on the Receptor Binding Domain of SARS-CoV-2 Spike Protein"

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RR:C19 Evidence Scale rating by reviewer:

- **Strong.** The main study claims are very well-justified by the data and analytic methods used. There is little room for doubt that the study produced has very similar results and conclusions as compared with the hypothetical ideal study. The study's main claims should be considered conclusive and actionable without reservation.

Review:

The authors of this MS used molecular dynamics simulation to explain the change in the free binding energies between the receptor binding domain of the SARS-CoV-2 and the ACE2. The simulations show an enhanced binding affinities in the N501Y mutant. The results are consistent with a study published before in my lab. However, the author of this study have performed an enhanced sampling by running MD simulations for 200ns starting from different initial states. I found the results convincing and trustable.