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Review of: "Evaluation of Xa inhibitors as potential inhibitors of the SARS-CoV-2 Mpro protease"

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Potential competing interests: The author(s) declared that no potential competing interests exist.

The authors have evaluated the binding potential of Xa inhibitors, apixaban, betrixaban and rivaroxaban to the Mpro protein of SARS-CoV-2 using experimental and computational methods. The methods used are robust and the results are thoroughly validated. However, there are a few minor issues and queries.

1. While the RMSD between the crystal pose and docked pose generated by Glide have been reported to be ≤ 2.0 Å, the authors have used an RMSD threshold of 2.5 Å. Is there any particular reason behind considering a higher threshold value?
2. Table S1: What the asterisks beside the PDB IDs indicate?
3. Were the ligand-protein complexes stable throughout the simulation trajectory or did any compound dissociate from the protein during simulation?