Supporting Information

Structure-Based Virtual Screening and Biochemical Validation to Discover Potential Inhibitor of SARS-CoV-2 Main Protease

Akshita Gupta[1#], Chitra Rani[1#], Pradeep Pant[2,4], Viswanathan Vijayan[1], Naval Vikram[3], Punit Kaur[1], Tej Pal Singh[1], Sujata Sharma[1]*, Pradeep Sharma[1]*

[1]Department of Biophysics, All India Institute of Medical Sciences, New Delhi-110029

[2]Department of Chemistry, Indian Institute of Technology Delhi, India

[3]Department of Medicine, All India Institute of Medical Sciences, New Delhi-110029

[4]Computational Biochemistry, University of Duisburg Essen, Germany

[#] **Authors contributed equally**

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***Corresponding author**

Dr. Pradeep Sharma*	**Prof. Sujata Sharma***
Department of Biophysics	Department of Biophysics
All India Institute of Medical Sciences	All India Institute of Medical Sciences
Ansari Nagar, New Delhi - 110 029	Ansari Nagar, New Delhi - 110 029
India	India
Tel: 011-26564608	Tel: 011-26564608
E-mail: pradeepbdk@gmail.com	E-mail: sujatasharma.aiims@gmail.com

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We used SwissDock (webserver) and PatchDock (downloadable code) to dock the four ligands considered for the study. The PatchDock results were further optimized using FireDock. It was observed that the active site of the protein (as in the co-crystal structure) was present in cluster1 in almost all cases, or in cluster 2/3 in the rest of the cases. The overlay of the docked complexes suggested that the binding of these ligands are reasonably similar for Glide docking and FireDock, and a slightly different binding mode was observed via SwissDock. The difference in the overall binding mode is anticipated due to the several rotatable bonds in the ligands. Overall, we observed that the Glide dock and FireDock results are similar.

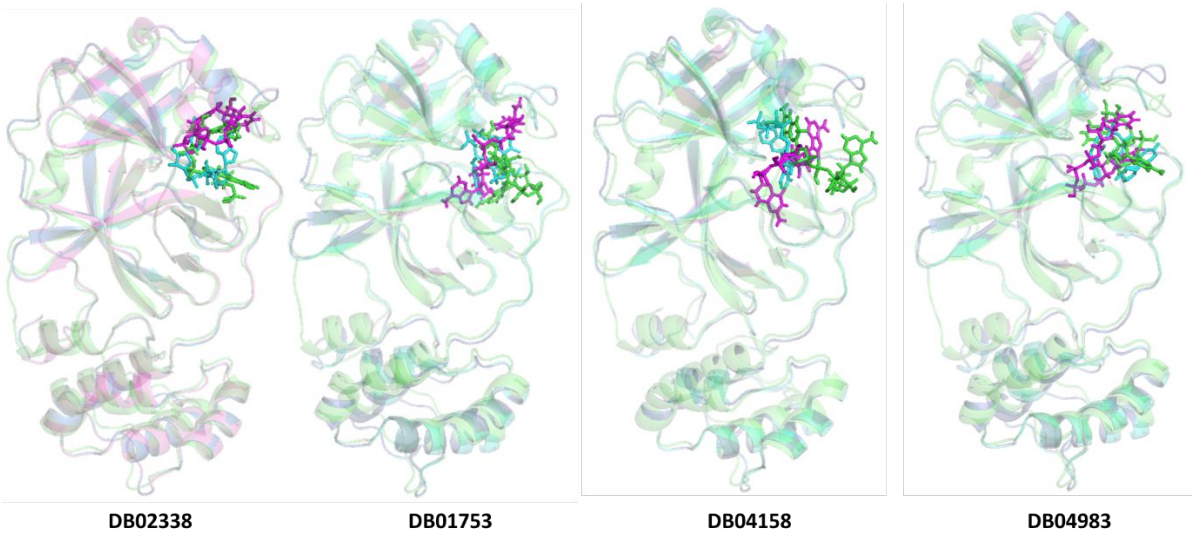

Figure S1. Binding of the ligands considered for the study using Glide (green), SwissDock (magenta), and FireDock optimization (cyan)