

**In silico drug repurposing carvedilol and its metabolites against SARS-CoV-2 infection  
using molecular docking and molecular dynamic simulation approaches**

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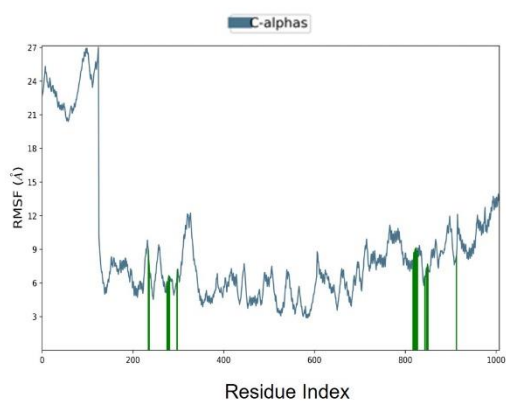
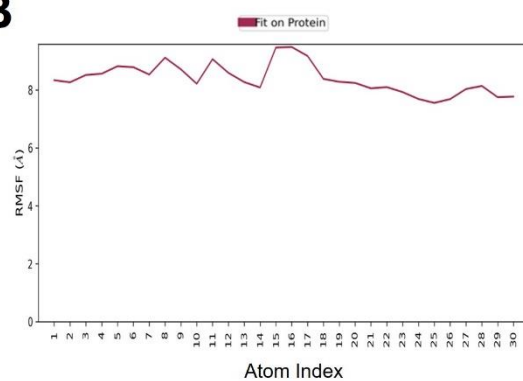
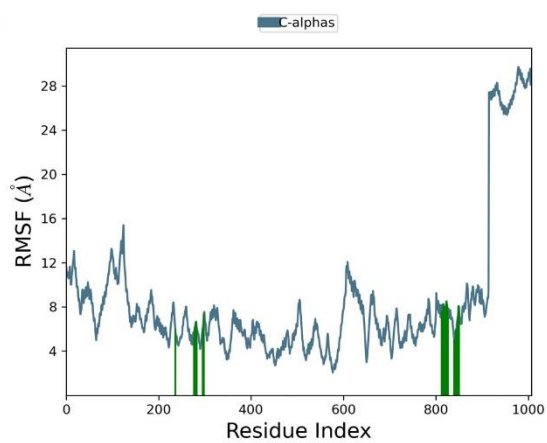
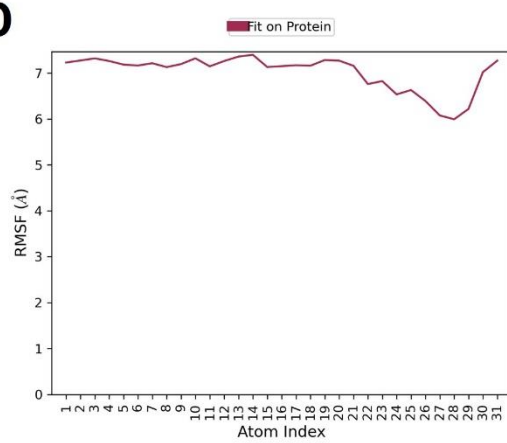
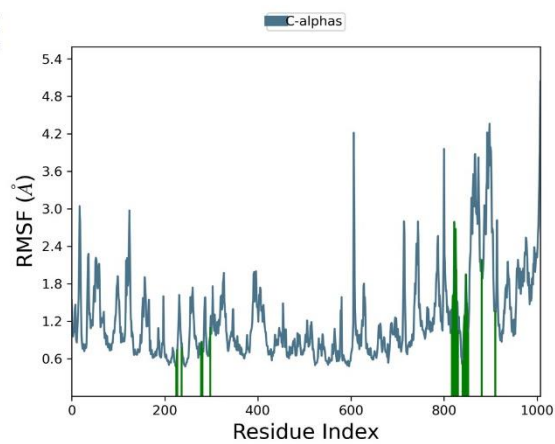
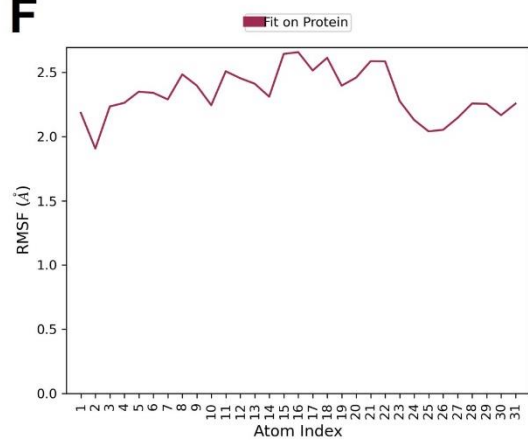
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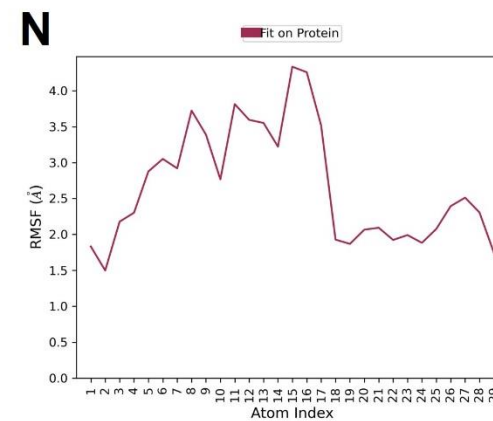
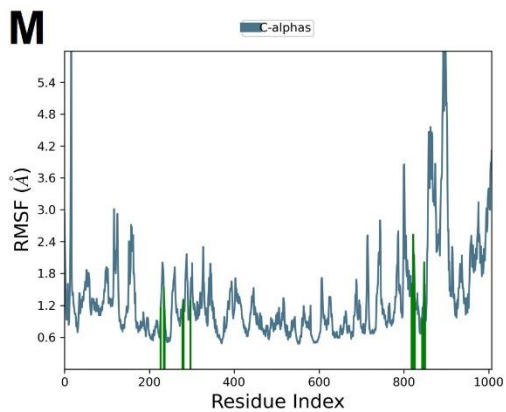
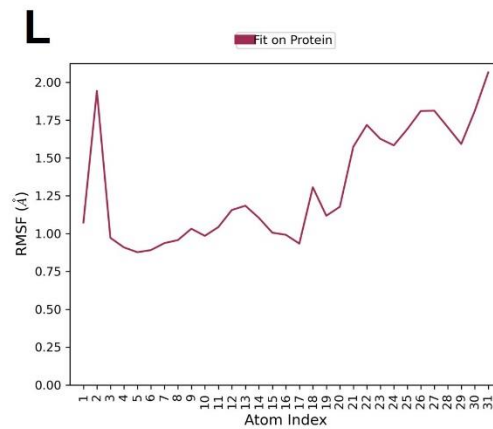
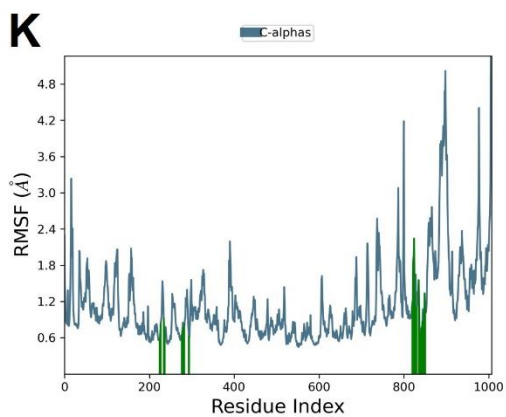
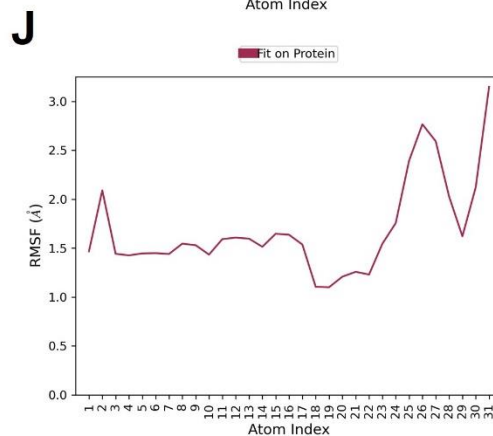
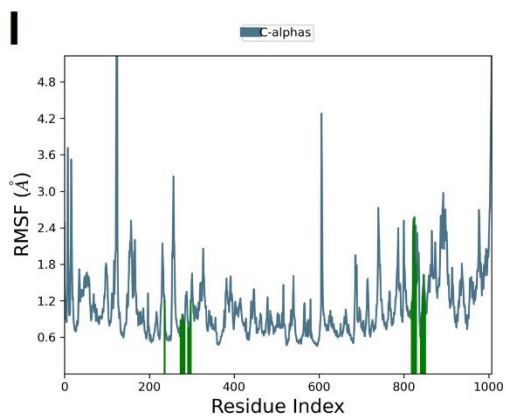
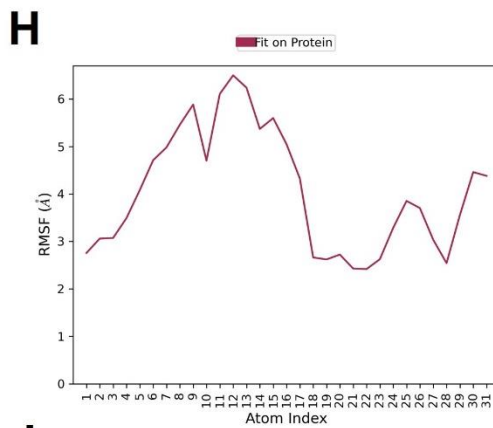
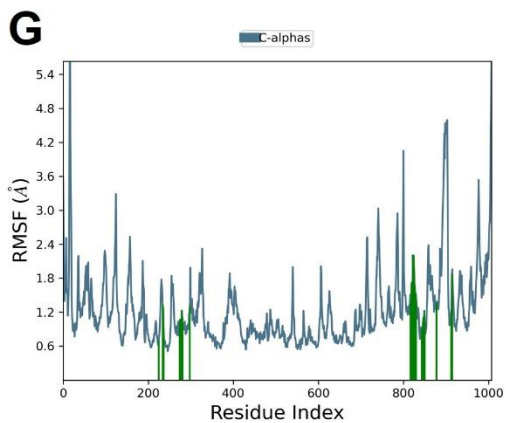
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**Supplementary Figure 1 and legend:**

**A****B****C****D****E****F**



**Supplementary Figure 1.** The Root Mean Square Fluctuation (RMSF) of protein and ligands. (A) RMSF of RdRp protein of SARS-CoV-2 with (B) RMSF of ligand Carvedilol. (C) RMSF of RdRp protein with (D) RMSF of ligand 1-hydroxyl carvedilol. (E) RMSF of RdRp protein with (F) RMSF of ligand 3-hydroxyl carvedilol. (G) RMSF of RdRp protein with (H) RMSF of ligand 4-hydroxyl carvedilol. (I) RMSF of RdRp protein with (J) RMSF of ligand 5-hydroxyl carvedilol. (K) RMSF of RdRp protein with (L) RMSF of ligand 8-hydroxyl carvedilol. (M) RMSF of RdRp protein with (N) RMSF of ligand O-desmethyl carvedilol. Ligand contacts are colored with green vertical bars indicating protein residues that interact with the ligands.