

Supplementary material

The role of *Cannabis sativa* L as a Source of Cannabinoids against Coronavirus 2 (SARS-CoV-2): An *in Silico* Study to Evaluate their Activities and ADMET Properties

Figure S1 2D and 3D binding of cannabinolic acid (**A**) and cannabinol (**B**) within the active sites of SARS-CoV-2 M^{Pro}

Figure S2 2D and 3D binding of cannabinolic acid (**A**) and cannabicyclic acid (**B**) within the active sites of SARS-CoV-2 PL^{Pro}

Figure S3 2D and 3D binding of cannabinolic acid (**A**) and cannabinol (**B**) within the active sites of ACE-2

Figure S4 The presence cannabichromanon (**32**) inside the binding pockets of SARS-CoV-2 M^{Pro} (**A**), SARS-CoV-2 PL^{Pro} (**B**) and ACE-2 (**C**) displaying areas of aromaticity, hydrogen bond formation, hydrophobicity and solvent accessibility (SAS) of the receptor residues

Figure S5 2D binding modes of the respective co-crystalized ligands in SARS-CoV-2 M^{Pro} (**A**), SARS-CoV-2 PL^{Pro} (**B**) and ACE2 (**C**)

Figure S6 2D binding modes of remdesivir in SARS-CoV-2 M^{Pro} (**A**), SARS-CoV-2 PL^{Pro} (**B**) and ACE2 (**C**)

Figure S1 2D and 3D binding of cannabinolic acid **(A)** and cannabinol **(B)** within the active sites of SARS-CoV-2 M^{Pro}

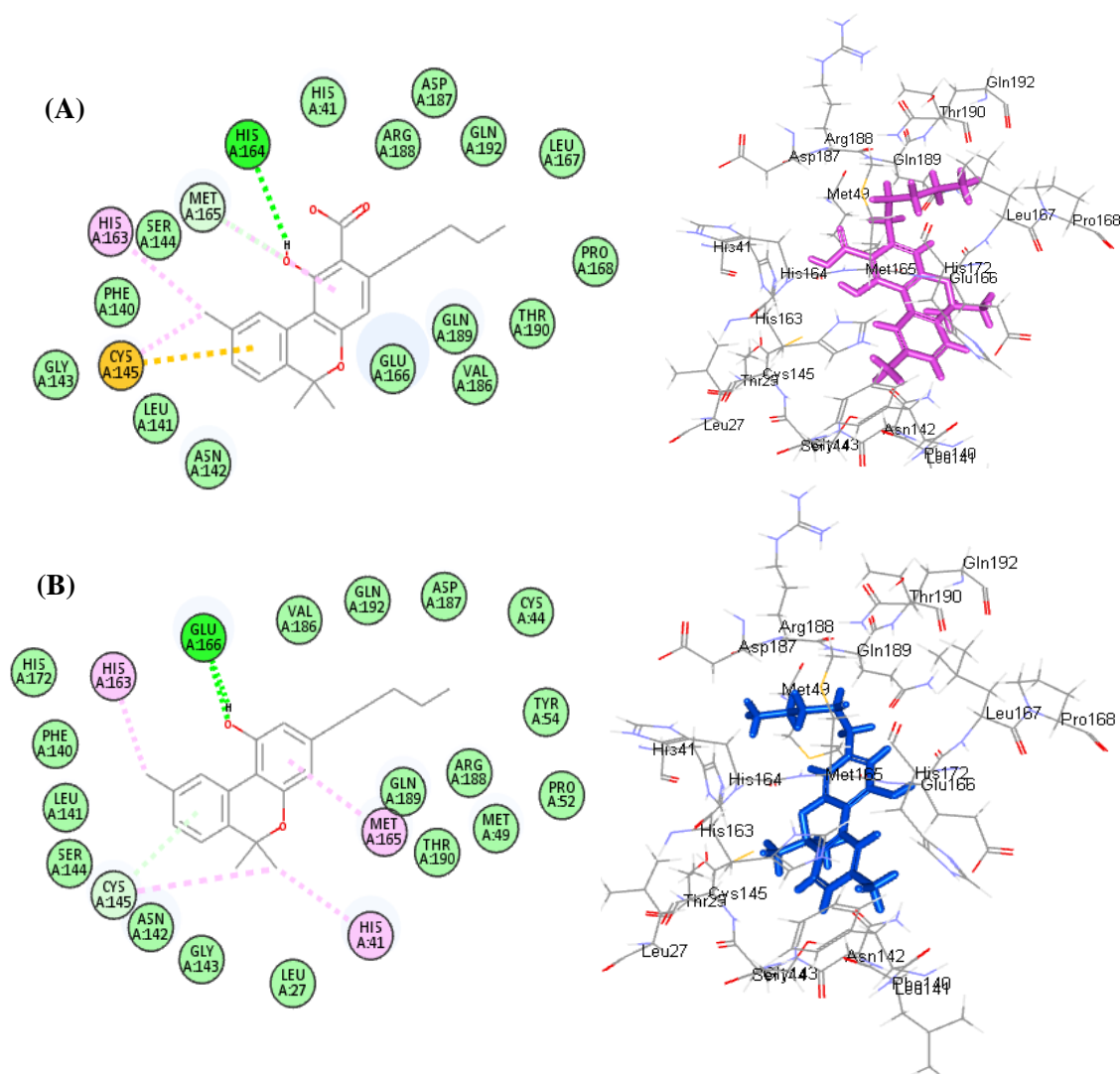


Figure S2 2D and 3D binding of cannabinolic acid **(A)** and cannabicyclic acid **(B)** within the active sites of , SARS-CoV- 2PL^{pro}

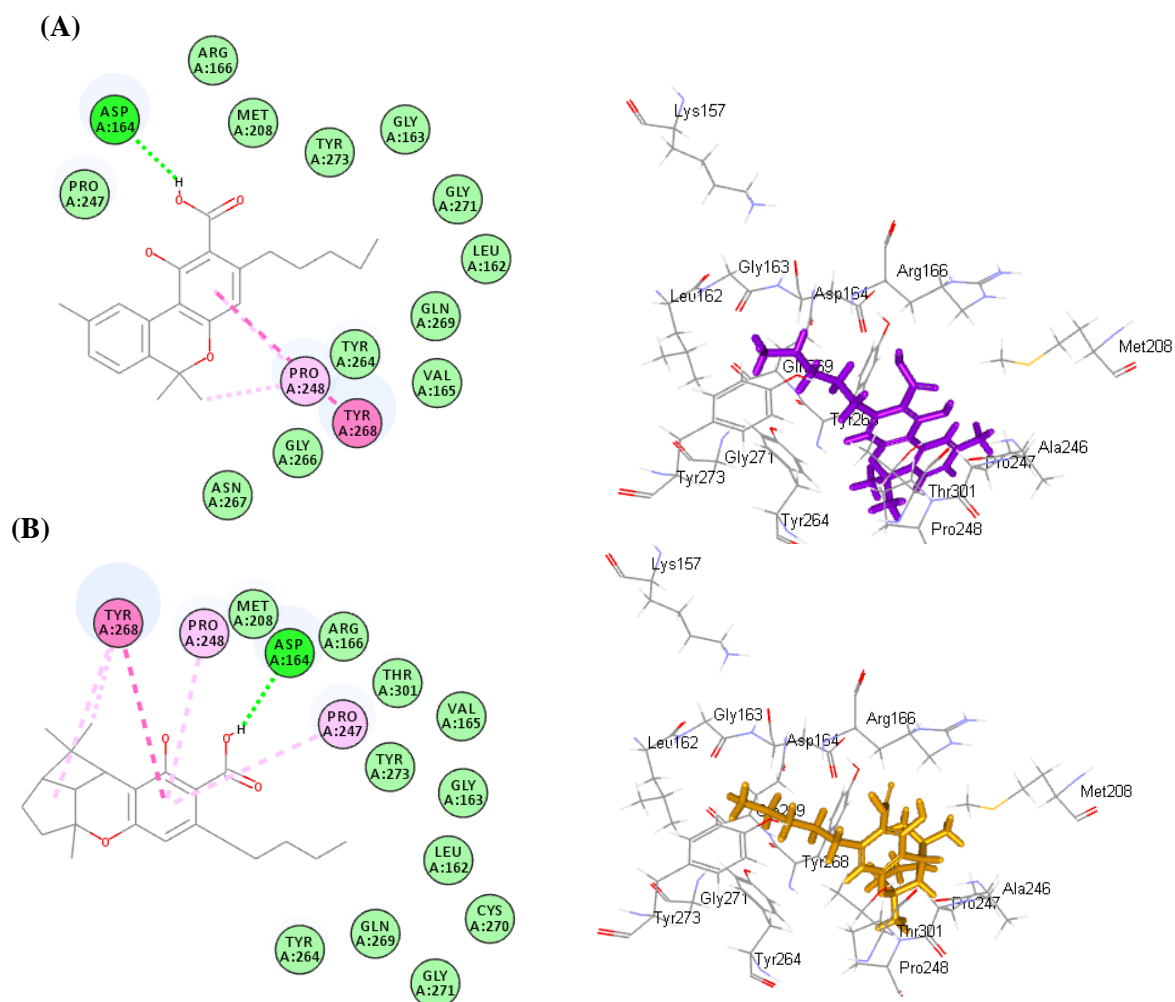


Figure S3 2D and 3D binding of cannabinolic acid **(A)** and cannabinol **(B)** within the active sites of ACE-2

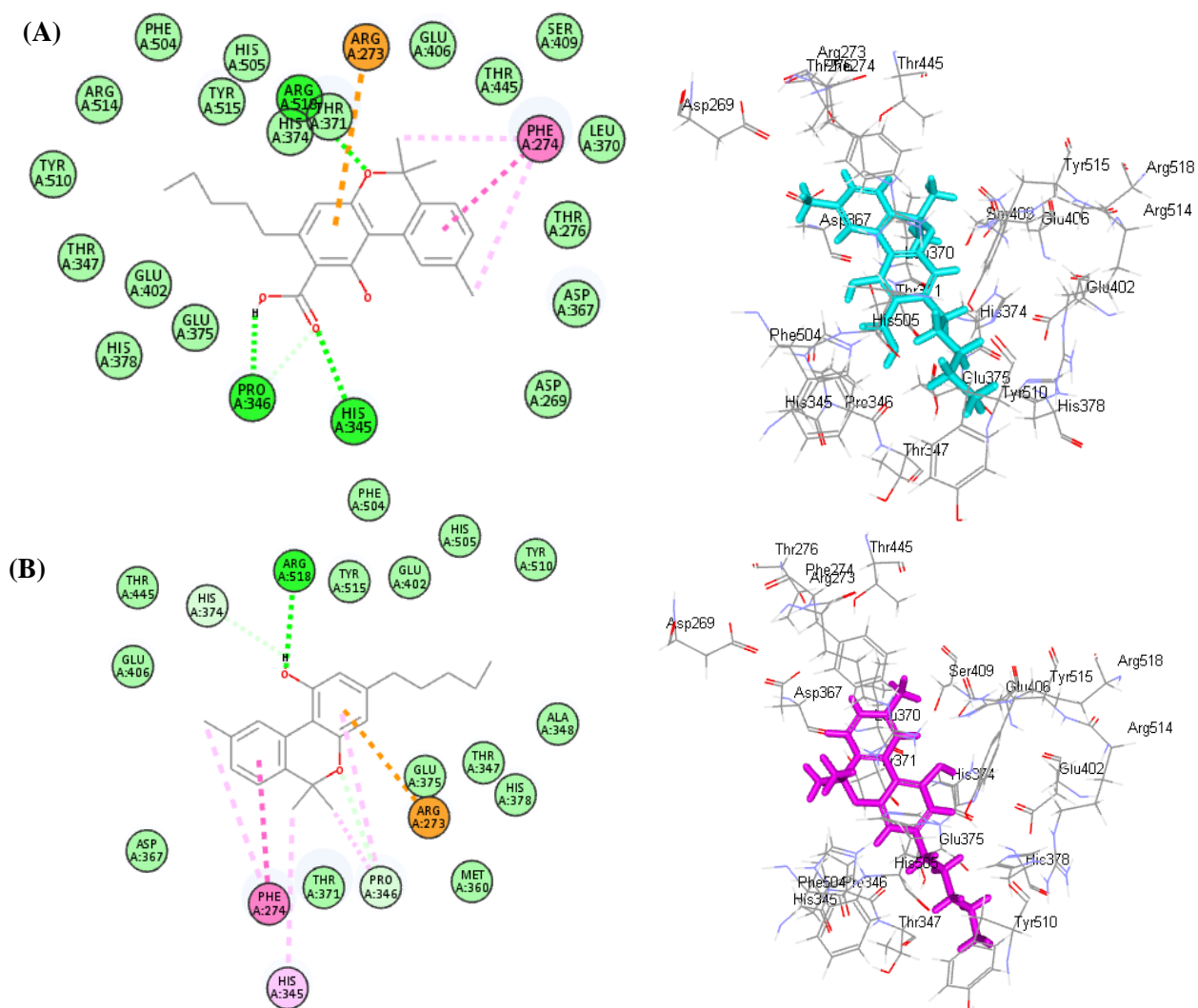


Figure S4 The presence cannabichromanon (**32**) inside the binding pockets of SARS-CoV-2 M^{Pro} (A), SARS-CoV-2 PL^{Pro} (B) and ACE-2 (C) displaying areas of aromaticity, hydrogen bond formation, hydrophobicity and solvent accessibility (SAS) of the receptor residues

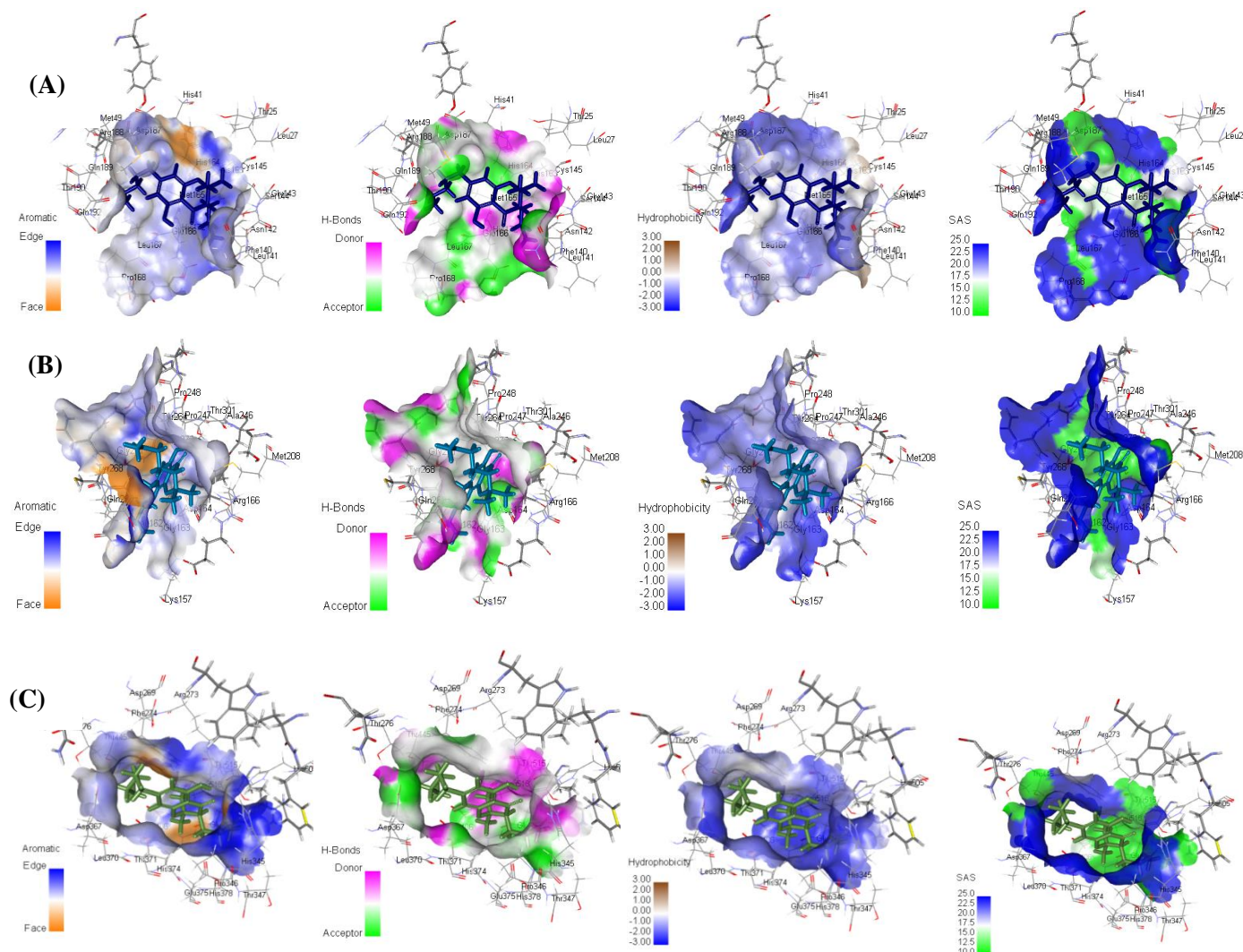
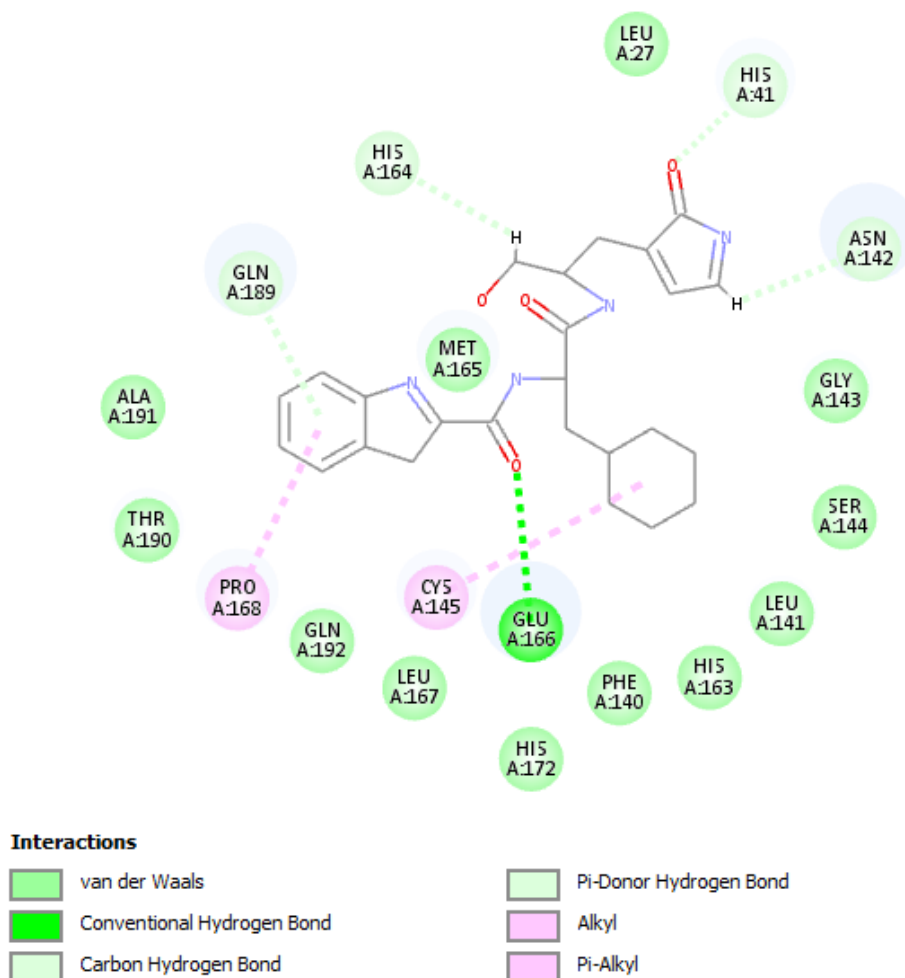
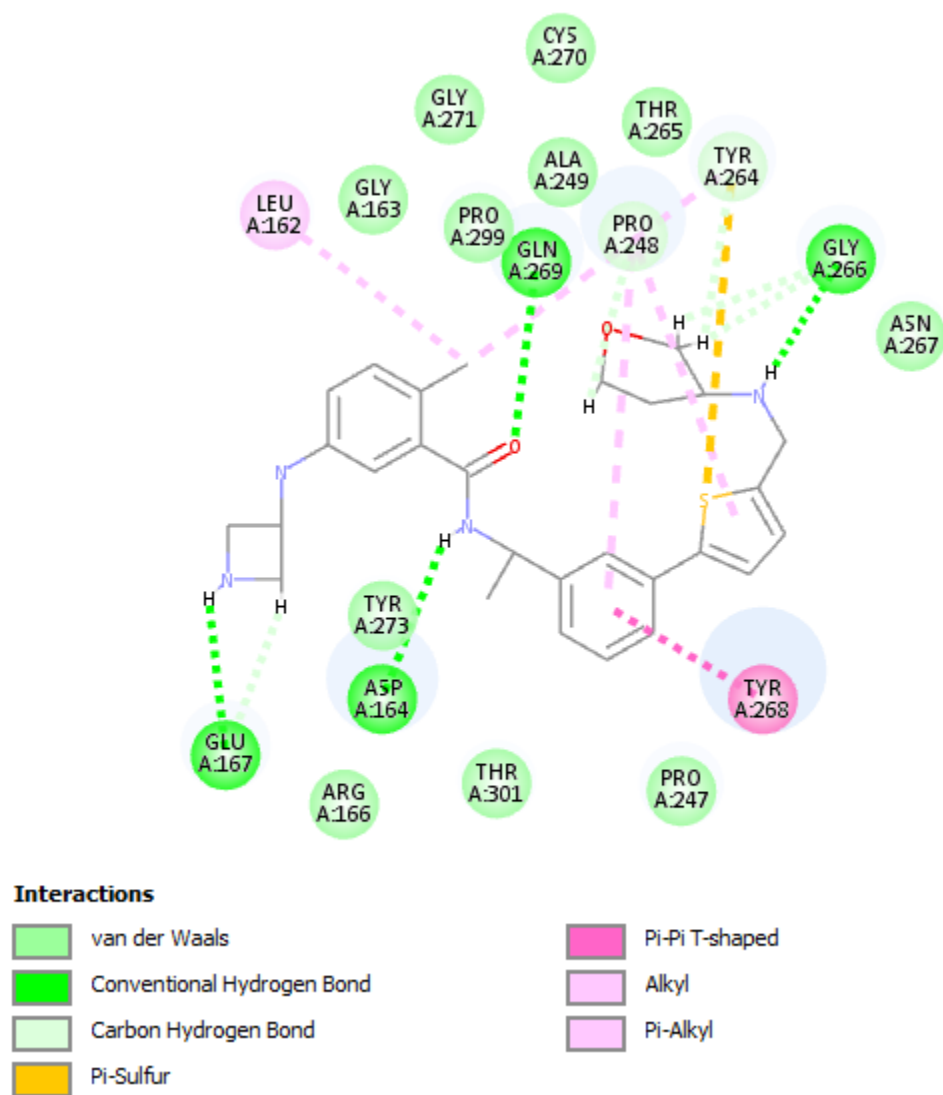


Figure S52D binding modes of the respective co-crystallized ligands in SARS-CoV-2 M^{Pro} **(A)**, SARS-CoV-2 PL^{pro} **(B)** and ACE2 **(C)**

(A)



(B)



(C)

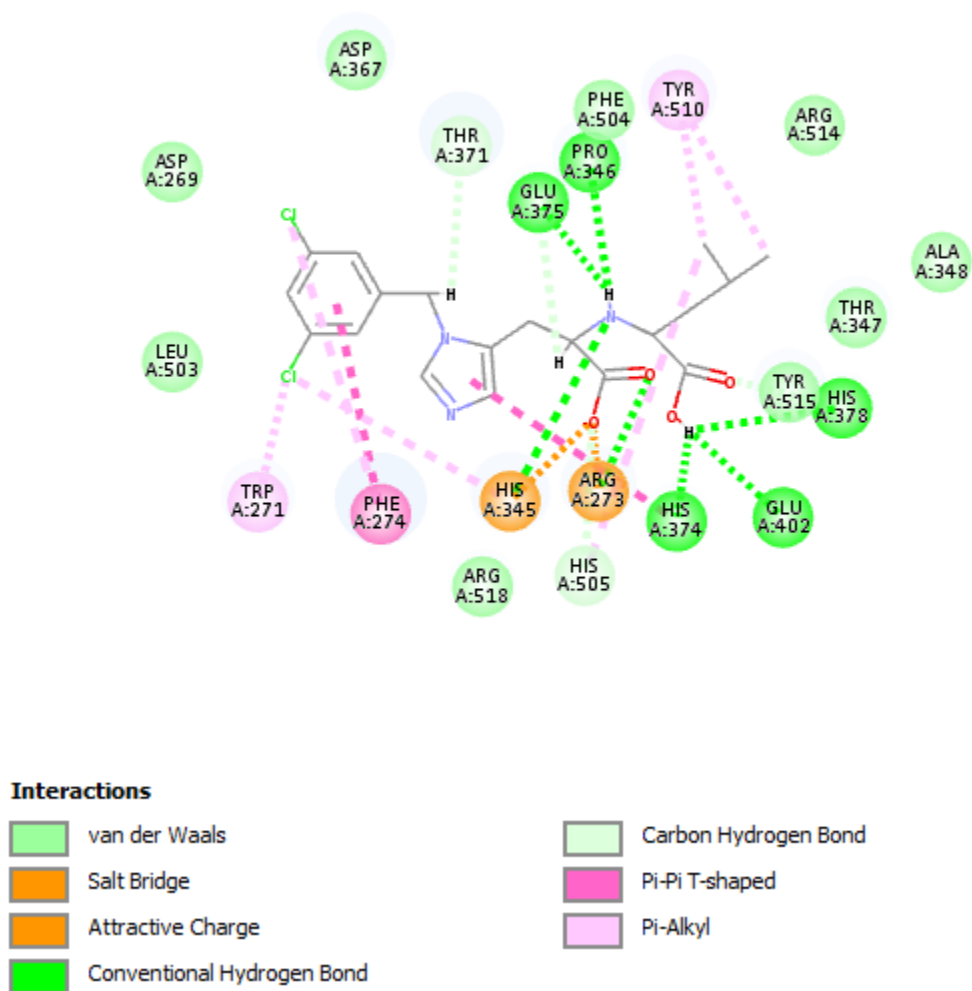
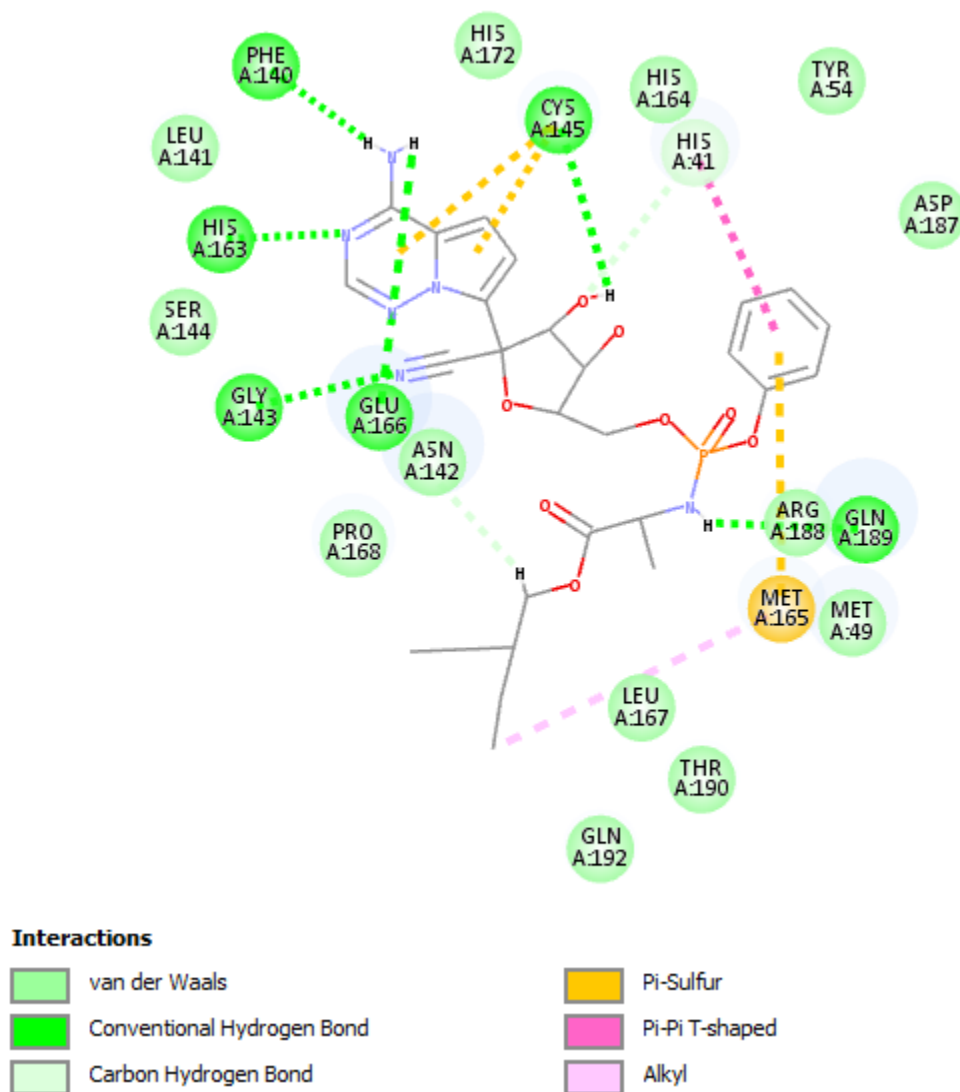
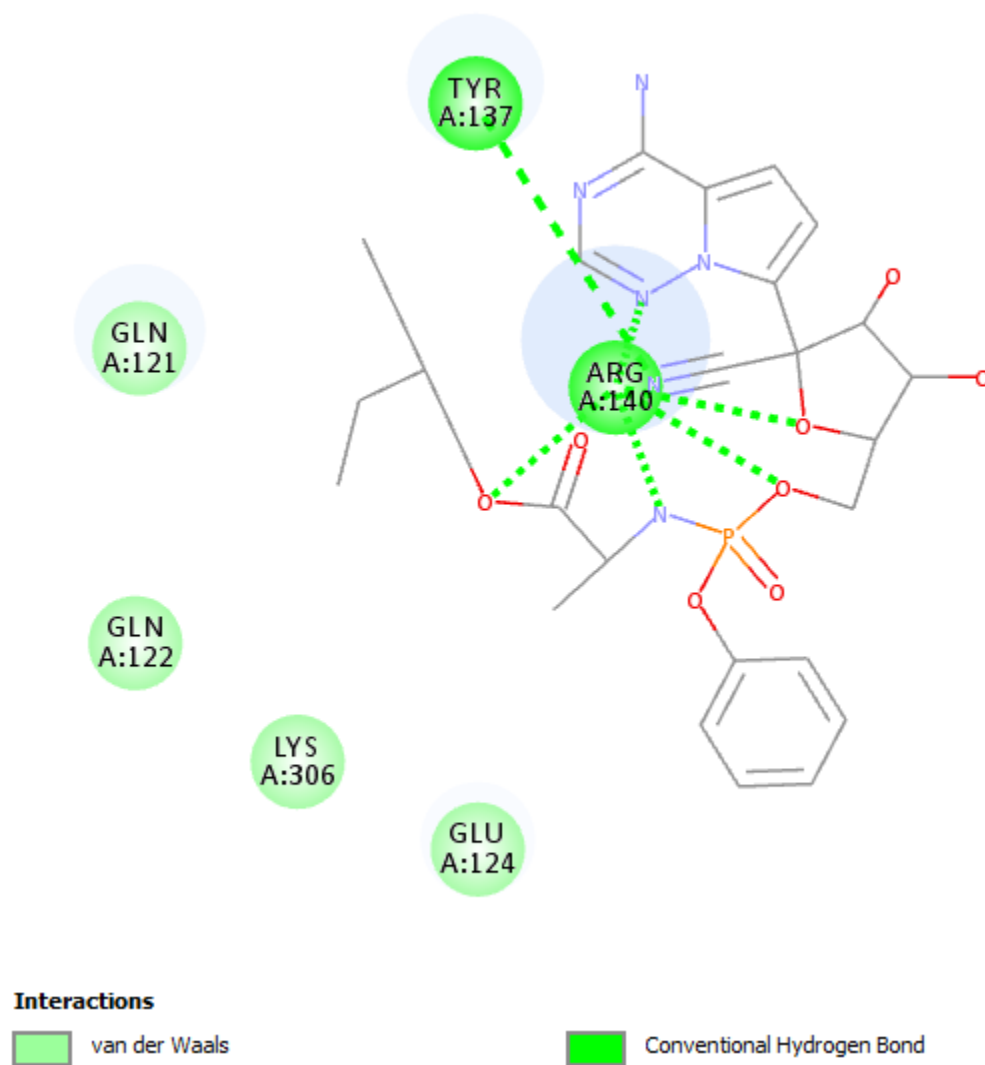


Figure S62D binding modes of remdesivir in SARS-CoV-2 M^{Pro} **(A)**, SARS-CoV-2 PL^{Pro} **(B)** and ACE2 **(C)**

(A)



(B)



(C)

