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Research article

In vitro and in silico evaluation of antiretrovirals against SARS-CoV-2: A drug repurposing approach

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Supplementary

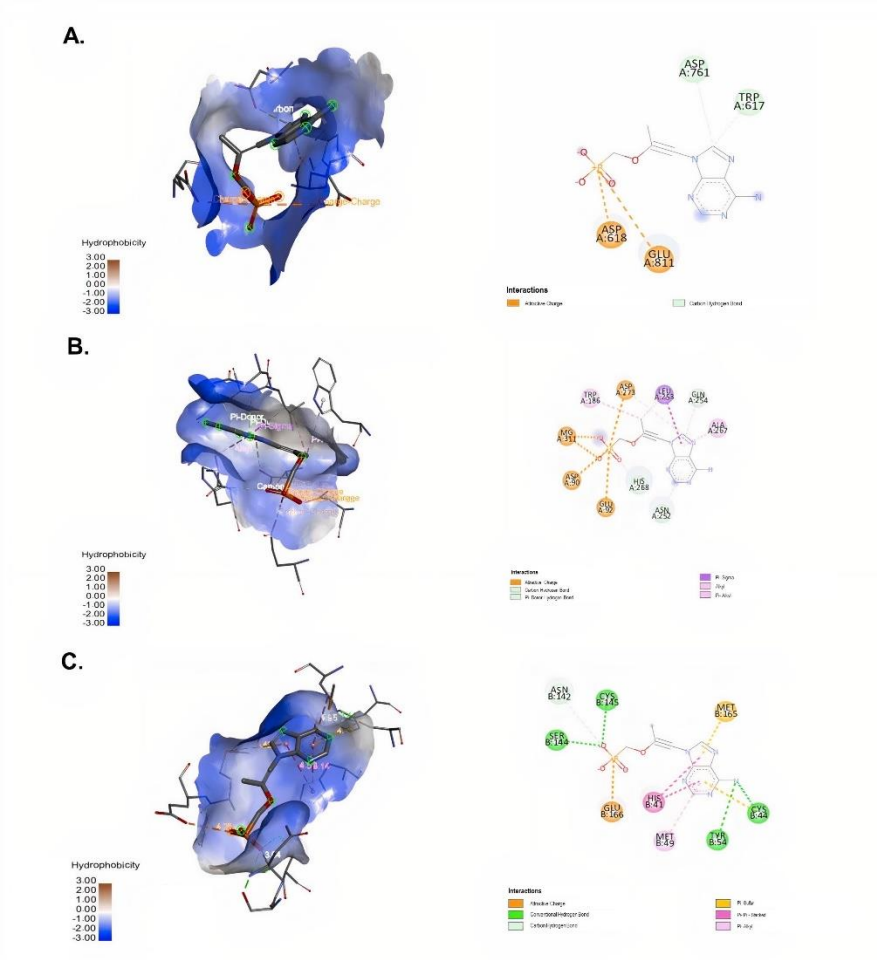

Figure S1. Interaction between tenofovir and SARS-CoV-2 non-structural proteins, using molecular docking. 3D (Figure left) and 2D (Figure right) representative images of the interaction of tenofovir with (A) RdRp (PDB ID:6M71), (B) ExoN-NSP10 (PDB ID:7MC6) and (C) 3CLpro (PDB ID:6M2N) by molecular docking. The types of interactions formed in the complexes are described in each Figure. The images were generated by using BIOVIA Discovery Studio Visualizer 16.1.

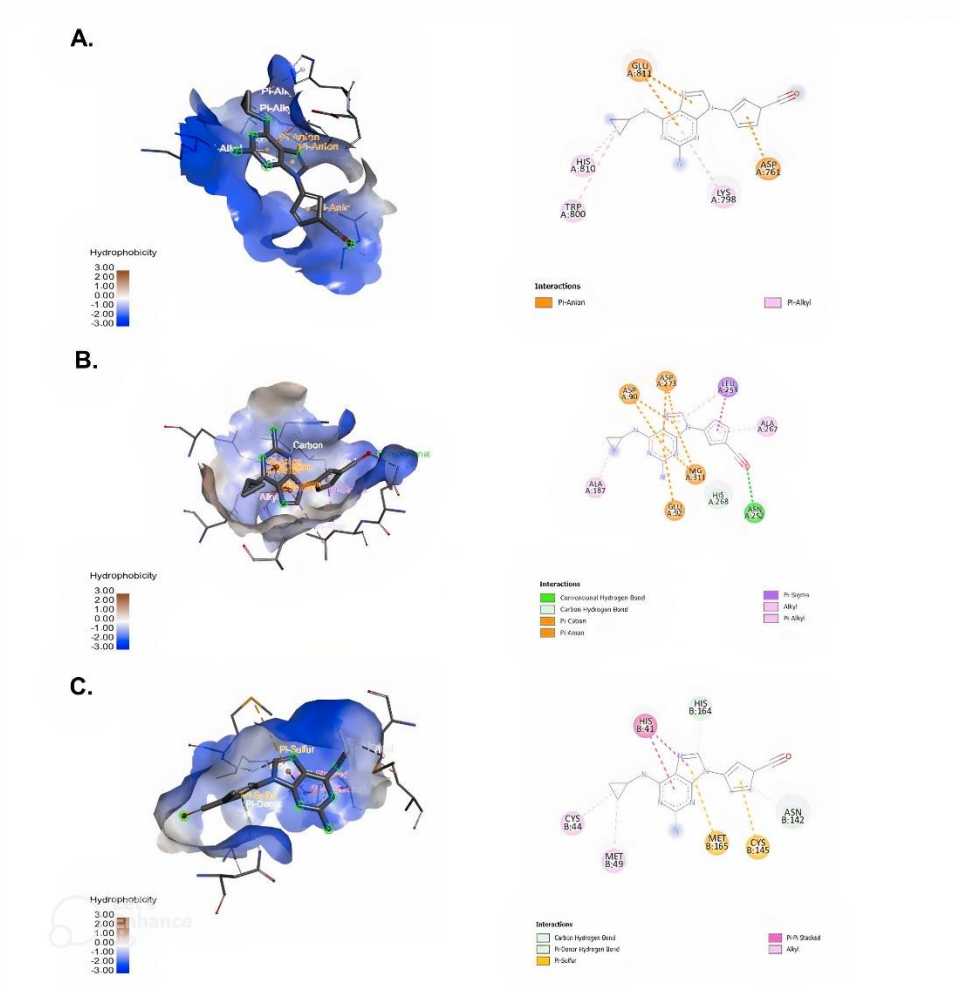

Figure S2. Interaction between abacavir and SARS-CoV-2 non-structural proteins, using molecular docking. 3D (Figure left) and 2D (Figure right) representative images of the interaction of abacavir with (A) RdRp (PDB ID:6M71), (B) ExoN-NSP10 (PDB ID:7MC6) and (C) 3CLpro (PDB ID:6M2N) by molecular docking. The types of interactions formed in the complexes are described in each Figure. The images were generated by using BIOVIA Discovery Studio Visualizer 16.1.

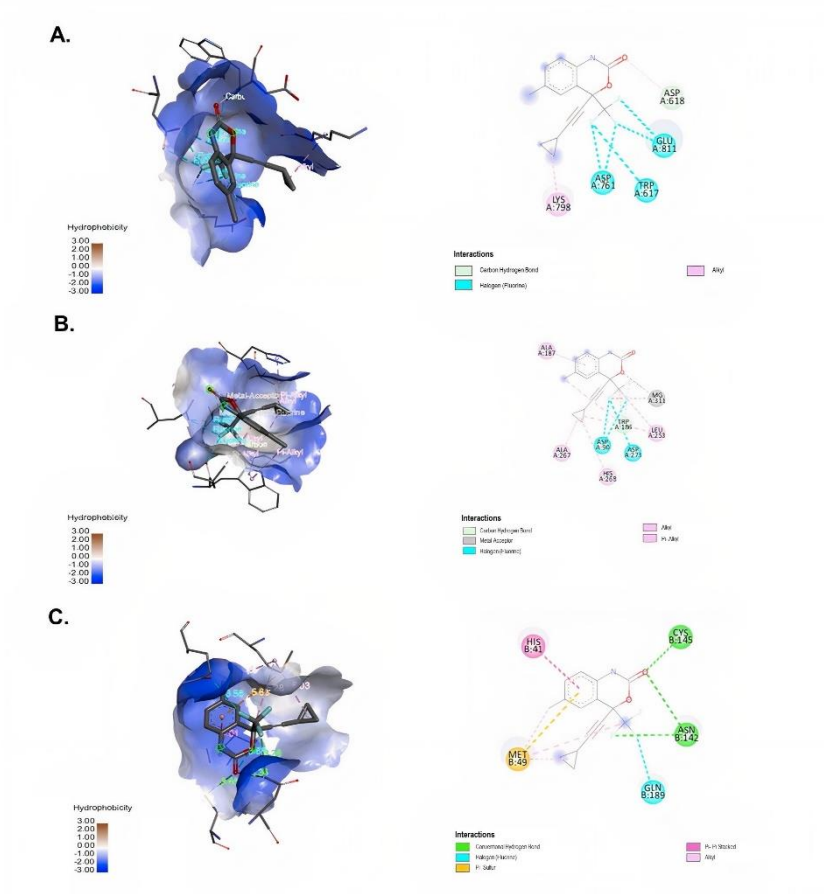

Figure S3. Interaction between efavirenz and SARS-CoV-2 non-structural proteins, using molecular docking. 3D (Figure left) and 2D (Figure right) representative images of the interaction of efavirenz with (A) RdRp (PDB ID:6M71), (B) ExoN-NSP10 (PDB ID:7MC6) and (C) 3CLpro (PDB ID:6M2N) by molecular docking. The types of interactions formed in the complexes are described in each Figure. The images were generated by using BIOVIA Discovery Studio Visualizer 16.1.