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## Choosing the correct antiviral for triple epidemic: An in silico approach

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Globally, influenza viruses, Respiratory Syncytial Virus (RSV) and SARS-CoV-2 have combined to cause a triple epidemic. Choosing the right antiviral agent to be used in against all three different viruses is very important for reducing overuse of antivirals in patients. Based on the clinical investigations, ten distinct antiviral medications and/or therapeutic candidates that have been employed in COVID-19, RSV and influenza infections were chosen for this study. All 10 different antiviral agents were analyzed to calculate the binding affinities and interactions of ligands with their target viral proteins by using molecular docking approach. The RNA-dependent RNA polymerase (RdRp) of the SARS-CoV-2, the PB1-PB2 protein complex of the influenza A virus and the RSV F glycoprotein were chosen as potential viral targets of the molecular docking analysis, respectively. The drug-binding pockets and inhibitory sites were studied, along with the interactions and binding affinities of the ligands. As a result, three of the ten ligands examined had the highest affinity for three viral infections at the docking site of interest. The antiviral drugs with the highest affinities for their targets were AVG-388, Remdesivir and Nirmatrelvir. Investigations employing molecular dynamics simulations were also conducted and the results were illustrated via graphs of Root-Mean-Square Deviation (RMSD). The results of the simulation revealed that the affinity remained constant, suggesting that the chosen ligands may function as potent therapeutic agents. In conclusion, in comparison to other ligands, AVG-388, Remdesivir and Nirmatrelvir might be suggested as potent antiviral molecules against the triple epidemic.

### Biography

Emine Erdag graduated from Near East University Faculty of Pharmacy in 2016 and completed her PhD programme at the Department of Pharmaceutical Chemistry in 2020. Her doctoral thesis is entitled "Synthesis and Characterization of New 3-Substituted-2(3H) Benzoxazolone Derivatives as Cytotoxic and Antimicrobial Agents". She has been working as a faculty member in the Department of Pharmaceutical Chemistry since October 2020. Her research interests include medicinal chemistry, pharmacology, organic synthesis, drug design and in silico molecular docking.

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