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Immunoinformatics and molecular docking studies predicted potential multi epitope based peptide vaccine and novel compounds against novel sars-cov-2 through virtual screening

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Coronaviruses (CoVs) are enveloped positive-strand RNA viruses which have club-like spikes at the surface with a unique replication process. Coronaviruses are categorized as major pathogenic viruses causing a variety of diseases in birds and mammals including humans (lethal respiratory dysfunctions). Nowadays, a new strain of coronaviruses is identified and named SARS-CoV-2. Multiple cases of SARS-CoV-2 attacks are being reported all over the world. SARS-CoV-2 showed a high death rate; however, no specific treatment is available against SARS-CoV-2. In the current study, immunoinformatics approaches were employed to predict the antigenic epitopes against SARS-CoV-2 for the development of the coronavirus vaccine. Cytotoxic T-lymphocyte and B-cell epitopes were predicted for SARS-CoV-2 coronavirus protein. Multiple sequence alignment of three genomes (SARS-CoV, MERS-CoV, and SARS-CoV-2) was used for conserved binding domain analysis. The docking complexes of 4 CTL epitopes with antigenic sites were analyzed followed by binding affinity and binding interaction analyses of top-ranked predicted peptides with MHC-I HLA molecule. The molecular docking (Food and Drug Regulatory Authority library) was performed, and four compounds exhibiting the least binding energy were identified. The designed epitopes lead to molecular docking against MHC-I, and interactional analyses of the selected docked complexes were investigated. In conclusion, four CTL epitopes (GTDLEGNFY, TVNVLAWLY, GSVGFNIDY, and QTFSVLACY) and four FDA-scrutinized compounds exhibited potential targets as peptide vaccines and potential biomolecules against deadly SARSCoV-2, respectively. Multi epitope vaccine was also designed from different epitopes of coronavirus proteins joined by linkers and led by an adjuvant. Our investigations predicted epitopes and the reported molecules that may have the potential to inhibit the SARS-CoV-2 virus. These findings can be a step towards the development of a peptide-based vaccine or natural compound drug target against SARS-CoV-2.

Biography

Sheikh Arslan Sehgal current study is aimed at exploring and identifying potential B and T-cell epitopes through immunoinformatics approaches which help to design an effective vaccine against deadly SARS-CoV-2. In addition, the study is aimed at pointing out specific peptides from the corona viral proteome, which have the ability to bind with Major Histocompatibility Complex (MHC), one of the most crucial steps in vaccine designing. A multi epitope vaccine was also designed from different epitopes of coronavirus proteins joined by linkers and led by an adjuvant. Our investigations predicted epitopes and the reported molecules that may have the potential to inhibit the SARS-CoV-2 virus. These findings can be a step towards the development of a peptide-based vaccine or natural compound drug target against SARS-CoV-2.

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