عنوان مقاله:

Vaccine design, adaptation, and cloning design for multiple epitope-based vaccine derived from SARS-CoV-۲ surface glycoprotein (S), membrane protein (M) and envelope protein (E): In silico approach

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خلاصه مقاله:

Introduction: The SARS Coronavirus-۲ (SARS-CoV-۲) pandemic has become a global epidemic that has increased the scientific community's concern about developing and finding a counteraction against this lethal virus. So far, hundreds of thousands of people have been infected by the pandemic due to contamination and spread. This research was therefore carried out to develop potential epitope-based vaccines against the SARS-CoV-۲ virus using reverse vaccinology and immunoinformatics approaches.Material and Methods: The material of SARS-COV۲ Surface Glycoprotein (S), Membrane Protein (M), and Envelope Protein (E) were downloaded from the NCBI protein database. Each protein has undergone epitopes prediction for MHC class I epitopes, MHC class II epitopes, and Antibody of B-cell epitopes. Selected epitopes according to their antigenicity score was tested for allergenicity and toxicity. Finally, filtered epitopes were used in vaccine construction. Vaccines were constructed, docked against Toll-like receptor ۳, and undergone Molecular Dynamic simulation. The vaccine with the best scores, subjected to immune stimulation and cloning design.Results: Three vaccines were constructed, COVac-۱, COVac-۲, and COVac-۳. Each vaccine was submitted into a deep investigation. The molecular dynamic simulation determines the stability and physical movement of protein atoms and molecules. After Molecular dynamics simulation, COVac-۱ was having the best scores. COVac-۱ was then subjected to immune simulation analysis to insure the stimulation of innate and adaptive immunity. After passing the immune simulation, COVac-۱ was integrated into E.coli pET-۳۰b plasmid using in silico cloning design.Conclusion: Viral pandemics are threatened to face humanity today. The best scenario to fight against any pandemic is utilizing the full power of computational biology, especially immune-informatics, to design and discover in silico new vaccines or molecules that may stimulate the immune system against the invader pathogens or inhibit the .pathogen life cycle

کلمات کلیدی:

In Silico Vaccine Design, SARS-CoV-۲, Reverse Vaccinology, Immunoinformatics