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Development of a Novel Chimeric Poly-Epitope Vaccine against COVID-19: A Computer-Aided Study

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Today, the outbreak of COVID-19 pandemic in December 2019 affected the economy and health around the world then the concern of vaccination against COVID-19 disease is at the top of all country's plans. Objectives: This study was performed to design a safe multi-epitope vaccine based on spike (S), envelope (E), nucleocapsid (N) and membrane (M) proteins of SARS-COV-2 virus. Methods: In this regard, the most reliable and accurate online tools were used to predict the best B cell, T cell and IFN- γ epitopes of N, S, M and E proteins. Then the best predicted epitopes along with HBHA protein were applied to assemble a novel multi-epitope vaccine using peptide linkers. The physicochemical properties and protein structures of this recombinant vaccine were evaluated using the on line tools. Finally, interaction of the vaccine and TLR/MD2 receptor was assessed using molecular docking strategy. In silico prediction of epitopes was successfully performed based on tracking the epitopes with the highest scores and the highest repetition rate among the results obtained from the online tools. The final developed chimeric poly-epitope structure had -0.210 GRAVY and 36.39 instability index which implies the stability of the protein. The estimated half-life of the final structure was calculated 30 hours in mammalian reticulocytes and >10 hours in *Escherichia coli*. In final tertiary structure 93% of residues were in the core region and had a score of 52.73 for 3D verification and -5.55 for Z-score. Results of protein-protein docking have demonstrated that HBHA and TLR/MD2 receptor successfully docked with the lowest energy of -1310.6. Based on the acceptable characterization of developed structure consisting of immunogenic epitopes, it seems this structure can be considered as a reliable subunit vaccine against the coronavirus.

Biography

Nemat Shams received Ph.D in Microbiology in 2007 at University of Tehran. He has been teaching immunology for 25 years. His research interest is Diagnosis of Zoonotic and Infectious diseases, Molecular Biology and Vaccine Designing. He has completed his PhD at the age of 25 years from Andhra University and postdoctoral studies from Stanford University School of Medicine. He is the director of XXXX, a premier Bio-Soft service organization. He has published more than 25 papers in reputed journals and has been serving as an editorial board member of repute.

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