عنوان مقاله:

Multi-epitope Based Peptide Vaccine Design Using Three Structural Proteins (S, E, and M) of SARS-CoV-۲: An In Silico Approach

محل انتشار:

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نویسندگان:

Arpita Singha Roy - *Department of Biotechnology and Genetic Engineering, Noakhali Science and Technology University, Sonapur, ۳۸۱۴, Noakhali, Bangladesh*

Mahafujul Islam Quadery Tonmoy - *Department of Biotechnology and Genetic Engineering, Noakhali Science and Technology University, Sonapur, ۳۸۱۴, Noakhali, Bangladesh*

Atqiya Fariha - *Department of Biotechnology and Genetic Engineering, Noakhali Science and Technology University, Sonapur, ۳۸۱۴, Noakhali, Bangladesh*

Ithmam Hami - *Department of Biotechnology and Genetic Engineering, Noakhali Science and Technology University, Sonapur, ۳۸۱۴, Noakhali, Bangladesh*

Ibrahim Khalil Afif - *Department of Biotechnology and Genetic Engineering, Noakhali Science and Technology University, Sonapur, ۳۸۱۴, Noakhali, Bangladesh*

Md. Adnan Munim - *Department of Biotechnology and Genetic Engineering, Noakhali Science and Technology University, Sonapur, ۳۸۱۴, Noakhali, Bangladesh*

Mohammad Rahanur Alam - *Department of Food Technology and Nutrition Science, Noakhali Science and Technology University, Sonapur ۳۸۱۴, Noakhali, Bangladesh*

Md. Shahadat Hossain - *Department of Biotechnology and Genetic Engineering, Noakhali Science and Technology University, Sonapur, ۳۸۱۴, Noakhali, Bangladesh*

خلاصه مقاله:

Introduction: The ongoing global pandemic of coronavirus disease (COVID-۱۹) caused by Severe Acute Respiratory Syndrome Coronavirus- ۲ (SARS CoV-۲) has jeopardized our health system and leaving everyone in disarray. Despite the diligent cumulative effort of academia, there is hardly any light in the end tunnel so far in developing efficient and sustainable treatment options to tackle this public health threat. Therefore, designing a suitable vaccine to overcome this hurdle calls for immediate attention. The current study aimed to design a multi-epitope based vaccine using immunoinformatics tools. Materials and Methods: We approached the structural proteins: S, E, and M proteins of SARS CoV-۲ since they facilitate the infection of the virus into a host cell. By using different bioinformatics tools and servers, the multiple B-cell and T-cell epitopes were predicted potential for the required vaccine design. The phylogenetic analysis provides in-depth knowledge on ancestral molecular changes and the molecular evolutionary

relationship of S, E, and M proteins. Results: Based on the antigenicity and surface accessibility of the spike (S), envelope (E), and membrane (M) proteins, eight epitopes were selected by various B cell and T cell epitope prediction tools. Molecular docking was executed to interpret the binding interactions of these epitopes from where three potential epitopes WTAGAAAYY, YVYSRVKNL, and GTITVEELK were finalized with their noticeable higher binding affinity scores -۹.۱,-۷.۴, and -۷.۰ kcal/mol, respectively. It is noteworthy to mention that the targeted epitopes are believed to cover ۹۱.۰۹% of the population coverage worldwide. Conclusions: In sum, we identified the three most potential epitopes at length, which might be turned to our purpose of designing the peptide-based vaccine against SARS CoV-۲.

کلمات کلیدی:

SARS-CoV-۲, Structural Protein, Epitope, antigenicity, Molecular docking