Bioinformatics approaches of epitope based vaccine design against novel SARS-Coronavirus-2

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ABSTRACT

coronavirus disease (COVID-19), that has killed millions of lives within several months worldwide. In an attempt to find a covid-19 vaccine, we have performed research on possible epitope-based subunit vaccines design against the SARS-CoV-2 virus using the approaches of reverse vaccinology and immunoinformatics. Based on continual computational experimentation, three possible vaccine constructs have been designed; and based on molecular docking study, one vaccine construct was chosen to be the most suitable vaccine, which is supposed to be the most effective vaccine against the SARS-CoV-2. Subsequently, the molecular dynamics simulation and in silico codon adaptation experiments were conducted to check biological stability and find an effective mass production strategy for the selected vaccine. Our study aims to present the scientific community with a potential vaccine design using bioinformatics tools and to accelerate covid-19 vaccine researches against this highly infectious virus.

INTRODUCTION

Coronavirus disease (Covid-19) is caused by a deadly and highly infectious virus SARS coronavirus-2 (SARS-CoV-2), which has caused millions death upon infection and spreading within several months all around. In early 2020, World Health Organizations (WHO) has announced SARS Coronavirus-2 as a pandemic. Several protective measures have been taken from the beginning of this pandemic to reducing the spreading of the virus. Without vaccine its became impossible to eradicate this virus. Researchers are working hard to discover the covid-19 vaccine. During our research there was no vaccine to combat against this virus. However, there are now many vaccines at various stages to be used against SARS-CoV-2 [1]. For vaccine designing we have selected four viral proteins: Nucleocapsid phosphoprotein, surface glycoprotein, ORF3a protein, and membrane glycoprotein. These 4 proteins are very crucial for viral life cycle.

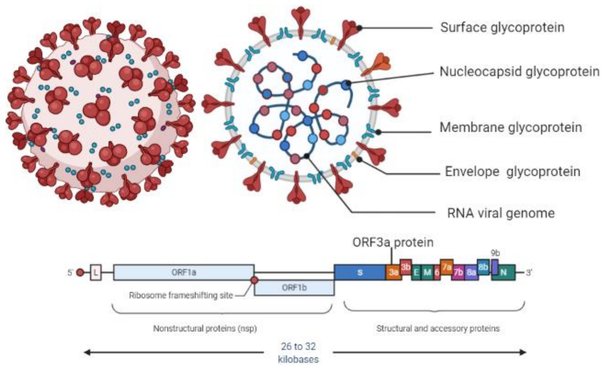

Fig 1. Severe Acute Respiratory Syndrome Coronavirus-2 (SARS-CoV-2)

MATERIALS AND METHODS

In an attempt to find a covid-19 vaccine, we have performed research on possible epitope-based subunit vaccines design against the SARS-CoV-2 virus using the approaches of reverse vaccinology and immunoinformatics. The method and materials were implemented previously in many studies [2,3,4].

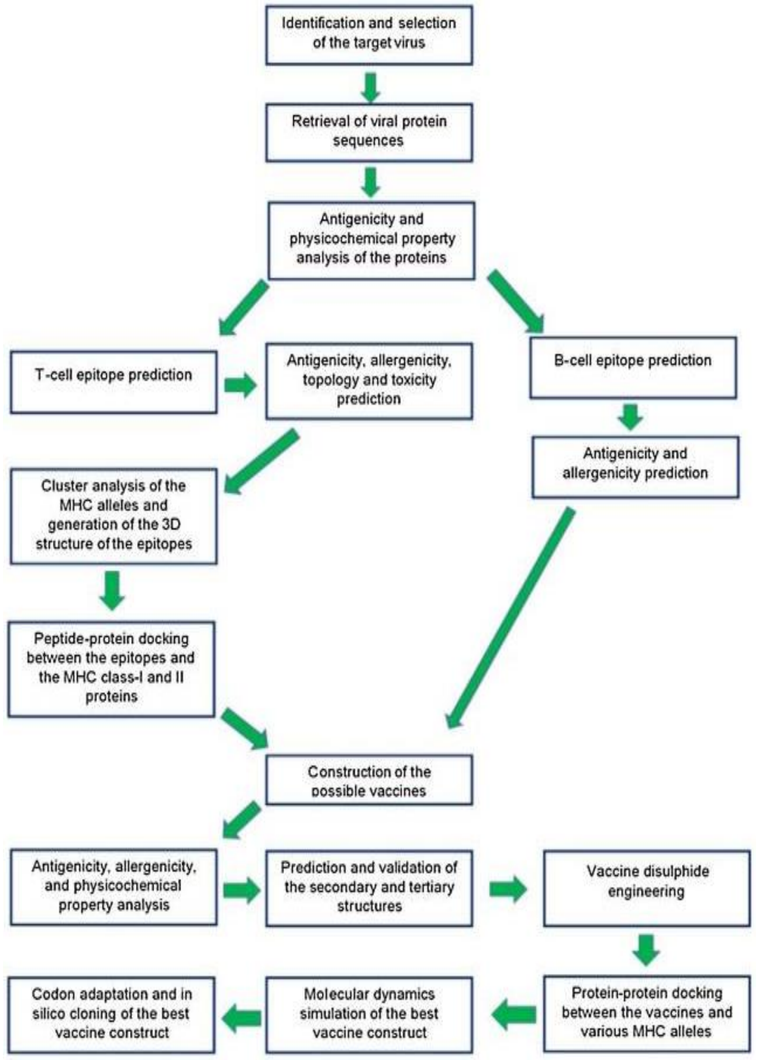

Fig 2. Step-by-step strategies employed in the overall vaccine designing study [4]

RESULTS AND DISCUSSIONS

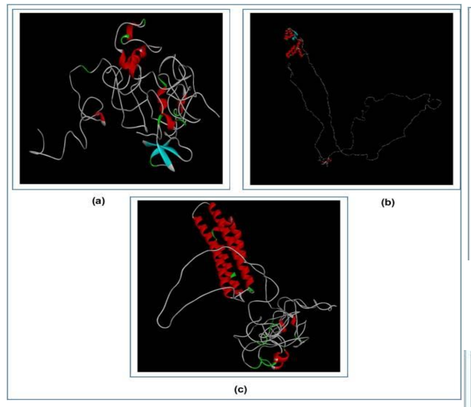

Fig.3.3D structures of three predicted vaccine constructs. (a) CV-1, (b), (c) CV-3 [4]

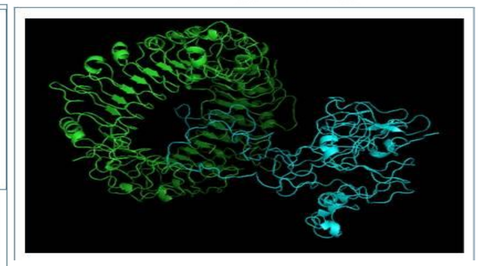

Fig 4. The interaction between TLR-8 (in green color) and CV-1 vaccine construct (in light blue color). The interaction was visualized with PyMol [4]

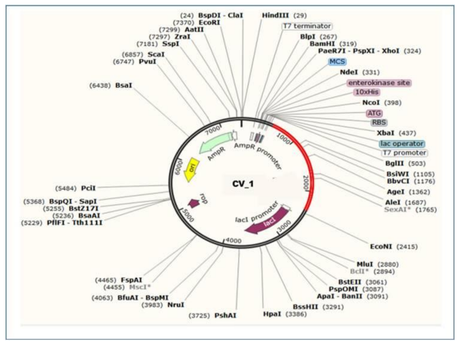

Fig.6. In silico restriction cloning of CV-1 vaccine sequences in the pET-19b plasmid [4]

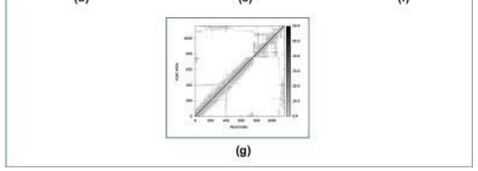

Fig.5. The results of molecular dynamics simulation study of CV-1 and TLR-8 docked complex [4]

CONCLUSION

According to the results of all the experiments conducted throughout our research, suggested vaccine constructs especially CV-1, revealed that these vaccines might confer good immunogenic response, possibly block the viral entry and destroy the viral life cycle [6]. If satisfactory results are achieved in numerous vivo and in vitro tests and trials, these vaccine constructs can be used effectively against the SARS-CoV-2.

REFERENCES

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