In Silico Study of SARS-CoV-2 Vaccine Candidate: Spike Glycoprotein

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Abstract

This study aimed to perform the analysis of toxicity prediction, allergenicity prediction, and *in silico* cloning of peptides originated from SARS-CoV-2 spike glycoprotein in the previous study. Allergenicity prediction employed AllerPred to predict the non-allergen peptides and toxicity prediction performed using ToxinPred. Then, this study designed the *in silico* cloning of SARS-CoV-2 spike glycoprotein with pET-28a(+) using SnapGene software. Therefore, this study successfully constructed the SARS-CoV-2 vaccine candidate via *in silico* method. Therefore, these data could be used to design a peptide-based vaccine against SARS-CoV-2. However, the advanced study is recommended confirmation, such as *in vitro* and *in vivo* study.

Keywords: *Allergenicity Prediction, COVID-19, In Silico Cloning, Toxicity Prediction, Vaccine.*

Introduction

SARS-CoV-2 is the seventh coronavirus that has crossed the species barrier to infect human. The virus was first declared in China in 2019 and appeared sporadically all over China and many other nations worldwide[1]. In March 2020, the WHO declared that the infection was a pandemic. The sudden outbreak and quick deployment of COVID-19 have endangered the global health and economy[2,3]. At present, the virus has infected more than 60 million people globally with more than 1.5 million global deaths[4].

Taxonomically, coronaviruses belong to the *Coronaviridae* family in the order Nidovirales, with examples in four distinct genera: *Alphacoronavirus*, *Betacoronavirus*, *Deltacoronavirus*, and *Gammacoronavirus*[5,6]. The structural proteins are encoded by four genes, specifically the envelope (E), nucleocapsid (N), membrane (M), and spikeglycoprotein (S)[7,8]. Previous studies have shown that the spike glycoprotein plays a crucial role in binding to receptors on the host cell[9,10]. Therefore, this protein is a key target for a number of antiviral therapies and a promising antigen for generating vaccines formulated against many coronaviruses[11].

Scientists have shown that vaccines are being developed against SARS-CoV-2 by various research groups worldwide[12,13,14]. Despite these promising treatment options, COVID-19 remains a serious disease with no proven effective medication. Therefore, there is an urgent need to investigate the genome of SARS-CoV-2. This study performs the analysis of toxicity prediction, allergenicity prediction, and *in silico* cloning of peptides originated from SARS-CoV-2 spike glycoprotein in the previous study to design a peptide-based vaccine against SARS-CoV-2.

Materials and Methods

Allergenicity Prediction of the Predicted Peptides

The predicted peptides revealed from our previous study[9]. In this study, an extensive analysis of the allergenicity prediction of the predicted peptides was conducted using AllerTOP with default settings. Then, the predicted peptides submitted to this web server as demonstrated by Peele *et al*.[15].

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Toxicity Prediction of the Predicted Peptides

This study predicted protective non-toxic antigens performing ToxinPred. The standard thresholds as reported by Gupta *et al*.[16].

In Silico Cloning

Here, the pET28a(+) expression vector selected for cloning, and its nucleotides sequences were collected from the Addgene vector database[17]. Then, SnapGene software was used for pursuing the *in silico* cloning of peptide-based vaccine component against SARS-CoV-2[18].

Results and Discussion

In this study, the *in silico* analysis of allergenicity prediction and toxicity prediction of the predicted peptides presented in Table 1. The pET28a(+) vector was used to clone the vaccine construct DNA sequence (5485 bp) using SnapGene software (Figure 1). The *in silico* electrophoresis of the spike glycoprotein, plasmid, and the insert gene showed in Figure 2.

Table 1. The results of allergenicity and toxicity predictions of the predicted peptides.

Predicted Peptides	Allergenicity Prediction	Toxicity Prediction
KNHTSPDVDLG	Non-Allergen	Non-Toxin
VRQIAPGQTGKIAD	Non-Allergen	Non-Toxin
RTQLPPAYTNS	Probable Allergen	Non-Toxin
YGFQPTNGVGYQ	Probable Allergen	Non-Toxin
SGTNGTKRFDN	Probable Allergen	Non-Toxin
ILPDPSKPSKRS	Non-Allergen	Non-Toxin
LTPGDSSSGWTAG	Non-Allergen	Non-Toxin
RDIADTTDAVRDPQ	Non-Allergen	Non-Toxin

*Note: The results based on Ansori *et al*.[9]

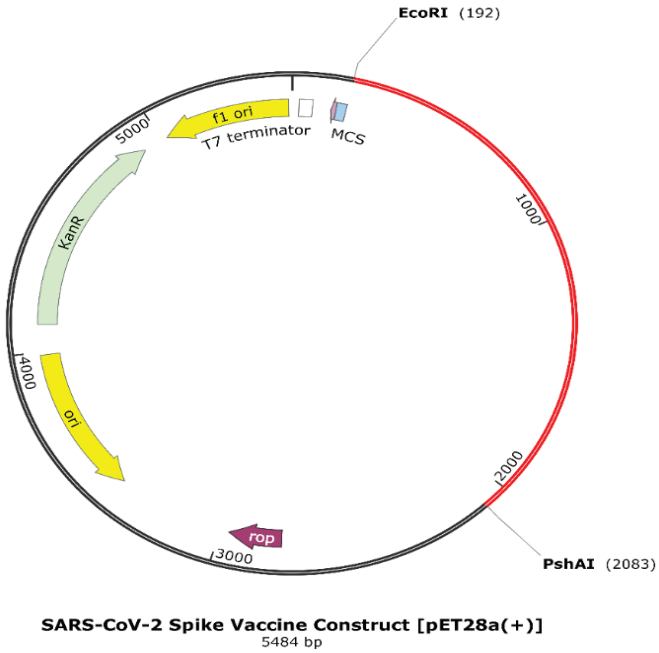

Figure 1. Schematic representation of *in silico* cloning of vaccine candidate within pET28a(+) expression vector.

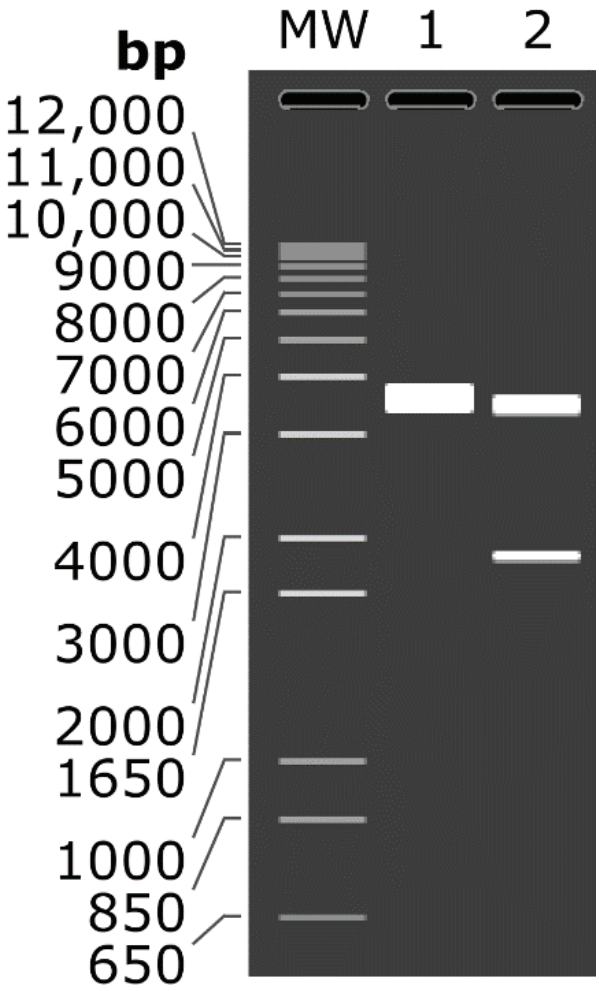

Figure 2. Schematic representation of *in silico* electrophoresis of the spike glycoprotein, plasmid, and the insert gene. 1: Spike glycoprotein of SARS-CoV-2; 2: pET28a(+) expression vector and the insert gene.

In addition, COVID-19 vaccine development has started in many research centers and pharmaceutical industries following the announcement of SARS-CoV-2 agent and its full genome recognized. Recently, the available assemble data stated that COVID-19 vaccine candidates were grouped into the following types: protein-based, epitope, inactivated or live-attenuated virus, virus-like particle, nucleic acid-based, and viral vectors[19,20]. Today, more than one year after the prevalence of novel coronavirus, vaccine and antiviral products are still in progress due to the pandemic paradigm development with several medication options and vaccines are in clinical trials globally[19,21,22]. Furthermore, scientists considered traversing the new concepts and latest cultivation in each type of vaccine to formularize a potent vaccine against COVID-19.

Previous research stated that *in silico* study is promoted as a useful method to generate vaccine against various diseases, such as dengue, zika, cancer, and HIV[23]. This method is employed by identifying MHC 1 and 2, B-cell and T-cell epitopes correlated with antigen presentation[24,25]. This type of vaccine consists of antibodies associated with the regions of foreign particles. These antibodies are straightforward and considered as the effective control. Based on the available data, the epitope-based virus might be a significant alternative vaccine formulation to fight SARS-CoV-2. Recently, there are various programs on vaccine developments[23]. Nevertheless, both *in vitro* and *in vivo* researches are further required for the advanced explanation of epitopes for the invention of SARS-CoV-2 vaccine.

Conclusion

In summary, the data of this study could be used to design an epitope-vaccine against SARS-CoV-2. However, the advanced study is recommended confirmation, such as *in vitro* and *in vivo* study.

Conflict of Interest : The author declare that they have no conflict of interest.

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Ethical Approval : This study does not require ethical approval.

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