PERANCANGAN VAKSIN BERBASIS EPITOP VIRUS *MONKEYPOX* SECARA *IN SILICO*

SKRIPSI

diajukan untuk memenuhi sebagian syarat untuk memperoleh gelar Sarjana Sains
Program Studi Biologi

Oleh

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PROGRAM STUDI BIOLOGI
FAKULTAS PENDIDIKAN MATEMATIKA DAN ILMU PENGETAHUAN ALAM
UNIVERSITAS PENDIDIKAN INDONESIA
BANDUNG

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Sebuah skripsi yang diajukan untuk memenuhi salah satu syarat memperoleh gelar Sarjana Sains pada Program Studi Biologi,
Fakultas Pendidikan Matematika dan Ilmu Pengetahuan Alam

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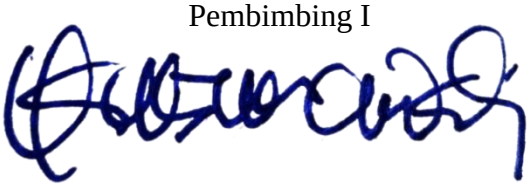
PERANCANGAN VAKSIN BERBASIS EPITOP VIRUS *MONKEYPOX* SECARA *IN SILICO*

Disetujui dan disahkan oleh pembimbing

Pembimbing I



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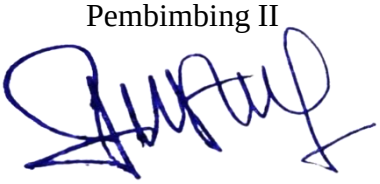
Pembimbing II



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LEMBAR PERNYATAAN

Dengan ini saya menyatakan bahwa skripsi dengan judul "Perancangan Vaksin Berbasis Epitop Virus *Monkeypox* secara *In Silico*" ini beserta seluruh isinya adalah benar-benar karya saya sendiri. Saya tidak melakukan penjiplakan atau pengutipan dengan cara-cara yang tidak sesuai dengan etika ilmu yang berlaku dalam masyarakat keilmuan. Atas pernyataan ini, saya siap menanggung sanksi apabila di kemudian hari ditemukan adanya pelanggaran etika keilmuan atau ada klaim dari pihak lain terhadap keaslian karya saya ini.

Bandung, Agustus 2023

Yang membuat pernyataan,

Dwi Nur Triharsiwi

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Penulis

ABSTRAK

Perancangan Vaksin Berbasis Epitop Virus *Monkeypox* secara *In Silico*

Wabah penyakit monekypox atau cacar monyet telah dilaporkan terjadi di berbagai negara, tetapi vaksin spesifik untuk monkeypox belum ditemukan. Penelitian ini bertujuan untuk menganalisis epitop dengan pendekatan *in silico* dari virus *monkeypox* yang memiliki potensi untuk dikembangkan menjadi vaksin spesifik. Serangkaian analisis *in silico* dilakukan, seperti prediksi epitop, analisis karakter imunologis, penambatan molekuler, simulasi dinamika molekuler, prediksi interaksi epitop dengan sistem imun, dan prediksi cakupan populasi. Penelitian menunjukkan bahwa terdapat 4 kandidat epitop untuk MHC I dan 3 kandidat epitop untuk MHC II yang memiliki kemampuan afinitas tinggi. Hasil akhir penelitian ini adalah dua rekomendasi epitop yang dapat dikembangkan menjadi vaksin yang menargetkan respon MHC I dan II. Setiap kandidat epitop memiliki karakter imunologis, seperti antigen, tidak alergen, tidak toksik, terkonservasi, dan tidak homolog dengan protein dalam tubuh manusia. Analisis penambatan molekuler menunjukkan bahwa epitop terbaik yang memiliki nilai *binding free energy* terendah, yaitu epitop KQKWRCVVY dengan MHC I -867,7 kkal/mol dan epitop AVCLLFIQSYSIYEN dengan MHC II -833.5 kkal/mol. Simulasi dinamika molekuler menunjukkan dua epitop terbaik dapat berinteraksi dengan protein MHC dengan stabil. Kedua epitop terbaik menunjukkan kemampuan untuk menginduksi respon imun seluler dan dapat memiliki cakupan sebesar 94,9% dari populasi dunia.

Kata kunci: epitop, *in silico*, MHC, *monkeypox*, vaksin

ABSTRACT

An *In silico* Approach to Epitope-Based Vaccine Design Against Monkeypox Virus

Outbreaks of monekypox have been reported in various countries, but there is no clinically validated specific vaccine for monkeypox. This study aimed to analyzed epitopes with an *in silico* approach from monkeypox viruses which has the potential to be developed into vaccines. A series of *in silico* analyzes were performed, such as prediction of epitopes, analysis of immunological characters, molecular docking, molecular dynamics simulations, prediction of epitope interactions with the immune system, and prediction of population coverage. The research showed that there were 4 MHC I epitope candidates and 3 MHC II epitope candidates that had high affinity abilities. The result of this research were two recommendations of epitope which has potential to be developed into vaccine that targeted MHC I and II responses. Each candidate epitope had immunological characteristics, such as antigen, non-allergenic, non-toxic, durable, and not homologous to proteins in the human body. The molecular docking simulation revealed that the best epitope with the lowest bond free energy value was KQKWRCVVY epitope with MHC I -867.7 kcal/mol and AVCLLFIQSYSIYEN epitope with MHC II -833.5 kcal/mol. The molecular dynamics simulations demonstrated that the best two epitopes could stably interacted with MHC proteins. The two best epitopes exhibited the ability to induce cellular immune responses and 94.9% of the world's population would be covered.

Keywords: epitope, *in silico*, MHC, monkeypox, vaccine

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DAFTAR GAMBAR

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