

## ABSTRAK

Pandemi Corona Virus Disease 19 (COVID-19) telah menyerang seluruh negara di dunia termasuk Indonesia dan menjadi isu Kesehatan global, setelah 2 tahun lamanya telah bermunculan berbagai jenis vaksin untuk mengurangi penyebaran COVID-19. Namun virus dari COVID-19 yaitu *Severe Acute Respiratory Syndrome Coronavirus 2* atau SARS-CoV-2 terus mengalami mutasi terutama pada protein Spike yang berperan dalam masuknya virus kedalam hostnya. SARS-CoV-2 terus mengalami mutasi hingga memunculkan berbagai *Varian of Concern* seperti varian Delta dan varian Omicron yang paling terbaru. Penelitian ini bertujuan untuk memetakan mutasi yang ada di Indonesia, mengetahui efek mutasi terutama pada varian Delta dan Omicron terhadap transmibilitas dan antibodi netralisasi. Langkah pertama dari penelitian ini ialah memodelkan protein Spike natif, varian delta dan varian omicron kemudian simulasi dinamika molekul *Coarse Grained* protein spike beserta simulasi RBD dan reseptor ACE2 dan antibodi netralisasi dari vaksin astrazeneka. Hasil simulasi menunjukkan jika terdapat fluktuasi yang tinggi pada RBD varian Omicron akibat adanya mutasi pada daerah tersebut yang menyebabkan meningkatnya interaksi dengan reseptor ACE2 namun mengurangi interaksi dengan antibodi netralisasi. Hasil penelitian ini dapat memberikan informasi terkait efek mutasi yang terjadi sehingga dapat membantu dalam pengembangan desain vaksin yang baru.

**Kata Kunci:** SARS-CoV-2, *Varian of Concern*, energi Interaksi, ACE 2, Antibodi Netralisasi, *Coarse Grained Molecular Dynamics*.

## ABSTRACT

The Corona Virus Disease 19 (COVID-19) pandemic has attacked all countries in the world including Indonesia and has become a global health issue, after 2 years various types of vaccines have emerged to reduce the spread of COVID-19. However, the virus from COVID-19, namely Severe Acute Respiratory Syndrome Coronavirus 2 or SARS-CoV-2, continues to experience mutations, especially in the Spike protein which plays a role in the entry of the virus into its host. SARS-CoV-2 continues to mutate to give rise to various Variants of Concern such as the Delta variant and the most recent Omicron variant. This study aims to map mutations that exist in Indonesia, to determine the effect of mutations, especially the Delta and Omicron variants on transmissibility and neutralizing antibodies. The first step of this research is to model the native Spike protein, delta variant and omicron variant and then simulate the molecular dynamics of Coarse Grained spike protein along with simulation of RBD and ACE2 receptors and neutralizing antibodies from the astrazeneka vaccine. The simulation results show that there is a high fluctuation in the RBD of the Omicron variant due to a mutation in that area which causes increased interaction with the ACE2 receptor but reduces the interaction with neutralizing antibody. The results of this study can provide information regarding the effects of mutations that occur so that they can assist in the development of new vaccine designs.

**Keyword:** SARS-CoV-2, *Variant of Concern*, Energy Interaction, ACE 2, Antibody Neutralizing, *Coarse Grained Molecular Dynamics*