# STUDI INTERAKSI ION $Na^+$ PADA PROTEIN p53 DENGAN KAJIAN SIMULASI DINAMIKA MOLEKUL

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## INTISARI

Simulasi dinamika molekul telah dilakukan untuk menentukan sifat struktur dan dinamika ion $Na^+$ pada permukaan protein p53. Medan gaya AMBER ff94 digunakan dalam mendeskripsikan interaksi potensial antar atom. Data struktur dalam bentuk grafik fungsi distribusi radial (RDF) lalu dapat digunakan untuk menentukan probabilitas tertinggi menemukan jarak $Na^+$-O dan bilangan koordinasi ion $Na^+$ pada kulit hidrasi pertama.

Waktu simulasi berjalan selama 500 ps, analisis grafik RDF menunjukkan bahwa probabilitas tertinggi menemukan jarak $Na^+$-O berada pada 2,35 Å, dengan bilangan integrasi sebesar 6. Di antara dua puncak RDF $Na^+$-O yang tidak melewati nol mengindikasikan adanya pergerakan molekul air di kulit hidrasi pertama. Grafik RDF hidrasi ini dibandingkan dengan hasil simulasi QM/MM. Jarak $Na^+$-O dari hasil simulasi ini memiliki nilai yang lebih tinggi, meskipun tidak terlalu signifikan. Energi ikat ion $Na^+$ pada permukaan protein p53 dihitung dengan metode MM-GBSA (*Molecular Mechanic - Generalized Born Surface* Area), menghasilkan nilai sebesar -0,4692 kkal/mol dan mengindikasikan interaksi yang terjadi relatif lemah.

Kata kunci: Simulasi dinamika molekul, AMBER, bilangan koordinasi, kulit hidrasi pertama, RDF, energi ikat

# THE STUDY OF INTERACTION OF $Na^+$ ION AT PROTEIN p53 BY MOLECULAR DYNAMIC SIMULATION

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## ABSTRACT

Molecular dynamic simulation has been performed to determine the structural and dynamical properties of the $Na^+$ ion at the protein p53 surface. The AMBER ff94 force field was used to describe interatomic potential interaction. The structural data in the form of radial distribution function (RDF) graph then can be used to determine the highest probability of finding $Na^+$-O distances and coordination numbers of $Na^+$ in the first hydration shell.

During 500 ps of simulation time, RDF graph analysis showed that the highest probability of finding the distance of $Na^+$-O from the complex was located at 2.35 Å and their integration number was 6. Between two peaks of the $Na^+$-O RDF which was not toward zero indicated the water moleculars in the first hydration shell. The RDF graph of this simulation was compared to QM/MM simulation result. The distance of $Na^+$-O from this simulation has a higher value, but not too significance. The binding energy of $Na^+$ ions at protein p53 surface was calculated by the MM-GBSA (*Molecular Mechanic - Genelarized Born Surface Area*) method, obtaining a value of -0.4692 kcal/mol and indicating relatively weak interaction.

Keywords: Molecular Dynamic Simulation, AMBER, coordination number, first hydration shell, RDF, binding energy