

STUDI INTERAKSI ION Ca²⁺ TERHADAP PROTEIN p53 MENGGUNAKAN SIMULASI DINAMIKA MOLEKULAR

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INTISARI

Simulasi dinamika molekular ion Ca²⁺ dengan protein p53 pada pelarut air telah dilakukan untuk menentukan sifat struktur dan dinamika interaksi yang terjadi di antara keduanya. Interaksi potensial antar atom dideskripsikan menggunakan medan gaya AMBER ff94 selama 0,5 ns pada kotak simulasi berbentuk kubus dengan tipe air TIP3P. Analisis dilakukan dari data trayektori hasil *output* berupa grafik RMSD (*Root Mean Square Deviation*), RMSF (*Root Mean Square Fluctuation*), RDF (*Radial Distribution Function*), CND (*Coordination Distribution Number*) dan ikatan hidrogen.

Hasil penelitian menunjukkan bahwa terdapat interaksi antara ion Ca²⁺ dengan 6 atom oksigen dari molekul air juga 2 atom oksigen dari residu asam amino Asp169, yaitu OD1 dan OD2 yang masing-masing berjarak 2,42 dan 2,53 Å. Terbentuk satu ikatan hidrogen yang cukup kuat pada situs ikat kompleks selama simulasi antara OD1 dan atom H molekul air. Interaksi ion Ca²⁺ terhadap protein p53 yang terjadi relatif lemah dengan energi bebas ikatan sebesar -2,529 kJ/mol.

Kata Kunci: AMBER, ion Ca²⁺, protein p53, simulasi dinamika molekular

STUDY OF INTERACTION BETWEEN Ca²⁺ ION INTO p53 PROTEIN USING MOLECULAR DYNAMIC SIMULATION

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ABSTRACT

Molecular dynamic simulations of Ca²⁺ ions with p53 protein in water have been carried out to determine the structure and the dynamics of interactions that occur between the two. Potential interactions among the atoms are described using AMBER ff94 force field for 0.5 ns in a cube-shaped simulation box with the water type of TIP3P. The analysis was performed from the trajectory data of output results in the form of RMSD (Root Mean Square Deviation) graphs, RMSF (Root Mean Square Fluctuation), RDF (Radial Distribution Function), CND (Coordination Distribution Number) and hydrogen bonds.

The results showed that there were interactions between Ca²⁺ ions and 6 oxygen atoms from water molecules as well as 2 oxygen atoms from Asp169 amino acid residues, called OD1 and OD2, which have distance of 2.42 and 2.53 Å respectively. During simulation, one hydrogen bond that is strong enough located at binding sites complex between OD1 and H atom of water molecules. Interaction of Ca²⁺ ions into p53 protein is relatively weak with the binding free energy -2.529 kJ/mol.

Keyword: AMBER, Ca²⁺ ions, p53 protein, molecular dynamics simulation