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The effect of initial temperature on the mechanical interaction of 3DN5/5OTF protein-based structures using molecular dynamics simulation

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Abstract

Nowadays, advances in science and technology in biological macromolecules have led to the early detection and treatment of cancer-based cells. In this study, molecular dynamics (MD) simulation examines atomic interactions between 3DN5 and 5OTF structures. Technically, the effect of the initial temperature on the atomic behavior (AB) of the simulated samples is investigated. The stability of simulated structures is examined with changes in temperature and kinetic energy (KE) quantities. The biomechanical interaction is examined by the radius of gyration (RoG), interaction energy (IE), and interaction force (IF). The results show that the RoG changes from a numerical value of 40.25 to 41.33 Å, and the IE and IF converge to −552.38 kcal/mol and −207.10 kcal/mol.Å after 10 ns, respectively. Due to the temperature effect on the AB of the structures, the RoG increases by increasing the initial temperature from 41.33 to 58.91 Å. By increasing the initial temperature to 350 K, the IE increases from −551.38 to −500.11 kcal/mol, and the IF increases from −207.10 to −183.39 kcal/mol.Å. Finally, the results of these studies are expected to lead to early detection and treatment of cancer cells.