

Investigation of Interaction between Interferons and Polyethylene Glycol Using Molecular Dynamics Simulation

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Abstract : Chemical bonding between polyethylene glycol (PEG) with pharmaceutical proteins called pegylation is one of the most effective methods of improving the pharmacological properties. The covalent attachment of polyethylene glycol (PEG) to proteins will increase their pharmacologic properties. For the formation of a combination of pegylated protein should first be activated PEG and connected to the protein. Interferons (IFNs) are a family of cytokines which show antiviral effects in front of the biological and are responsible for setting safety system. In this study, the nature and properties of the interaction between active positions of IFNs and polyethylene glycol have been investigated using molecular dynamics simulation. The main aspect of this theoretical work focuses on the achievement of valuable data on the reaction pathways of PEG-IFNs and the transition state energy. Our results provide a new perspective on the interactions, chemical properties and reaction pathways between IFNs and PEG.

Keywords : interaction, interferons, molecular dynamics simulation, polyethylene glycol

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