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Interaction of human glyceraldehyde-3-phosphate dehydrogenase with cofactor based on molecular docking data

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Abstract

The analysis of the interaction of tetrameric glyceraldehyde-3-phosphate dehydrogenase with cofactor NAD was performed by computational methods. Method of molecular docking was used for calculation of interaction energy between molecules of cofactor and the protein. Gaussian network model was used to evaluate the changes in the protein backbone dynamics that took place as a result of the cofactor binding. It has been shown that the cofactor molecules form strong complexes with protein tetramer, wherein the energy of interaction of individual cofactor molecule with different subunits of the protein apo-forms differ insignificantly. At the same time the presence of other NAD molecules in the complex systematically decreased the interaction energy of protein – cofactor complex, this could contribute to negative cooperativity of the cofactor molecule binding to glyceraldehyde-3-phosphate dehydrogenase tetramer.