MOLECULAR DYNAMICS SIMULATION OXIDIZED AND REDUCED STATES OF PROTEINS, CONTAINING Fe_4S_4 CLUSTERS IN WATER ENVIRONMENT

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The effect of solvent on the protein conformation is studied by computer simulation. The method named collisional molecular dynamics is applied to proteins containing Fe_4S_4 clusters: low potential protein Fd *Thermotoga Maritima* (60 a.a.) and high potential protein HiPIP *Rhodocyclus tenuis* (62 a.a.). Fe_4S_4 cluster may be in oxidized or in reduced state, having different partial charge on its atoms. After changing the redox state the system is allowed to relax. Then averaging energetical and dynamics characteristics is carried out over the trajectory of relaxation. Additional averaging is carried out using different trajectory with different starting conditions. Modified software package PUMA developed at IMPB RAN is applied for simulations. Molecules of water are included explicitly. Periodic boundary conditions are used for simulation of condensed state. System is also interacting with "collisional thermostat", which is responsible for maintaining constant temperature and reducing dynamical effects arising in small systems.

Comparing of different contributions in interaction energy of proteins containing Fe_4S_4 clusters is carried out in vacuum and in water. Simulation results demonstrate that when proteins are in water the impact of Colomb contribution is changed significantly, the value of total energy being practically constant. Being in vacuum, proteins are characterized by slightly deviations of the energy components from their averaged values. For HiPIP the energetical characteristics of protein matrix is independent on electron state of cluster and value of OVP is defined mainly by difference in interactional energy between protein matrix and the cluster and the protein with water. For Fd all energetical characteristics are depend upon electron state of cluster.

Detail analysis of structure changing and dynamics processes are carried out while electron state of proteins is changing.

This work has been supported by grants of RFBR (grant № 01-04-49302) and INTAS, (grant 99-0281).

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