DISULFIDE BRIDGES EFFECT ON DYNAMICS OF LYSOZYME. ACCORDING TO THE METHODS OF MOLECULAR DYNAMICS

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Enzymatic activity of protein is directly connected with their mobility. Therefore the considerable efforts during last decades have been devoted to studying of biopolymers dynamics with the help of computer modeling. Results of these researches have a major value for development of a technology of the molecular designing and bioengineering.

In this work the effect of disulfide bridges on conformation mobility of lysozyme has been studied by methods of molecular dynamics. Trajectories 5ns long have been obtained at temperature 300K for two variants of lysozyme: native (with S-S-bonds) and modified (without S-S-bonds). On the basis of the analysis auto- and crosscorrelation functions bending fluctuations of α-helixes in the major domain lysozyme it is possible to make a conclusion that smaller values of mean square displacements of atomic groups $\langle x^2 \rangle$ for lysozyme (in comparison with α-helix of globular protein myoglobin), are defined first of all by structural organization of lysozyme molecule (α+β-protein), instead of presence of disulfide bonds. Fluctuations amplitudes of secondary structure devices of lysozyme are practically invariable at destruction of disulfide bonds. These results are important for interpretation of available differences in values $\langle x^2 \rangle$ observed in experiments on RSMR. In the major domain of lysozyme with S-S-bonds α-helixes very fast (for times about tens picoseconds) lose the relative dynamic correlation and in further their movements occur independently. In lysozyme, in absence of disulfide bonds, the characteristic times of motions of secondary structure devices increased in 3-7 times. In absence of S-S-bonds the volume of a molecule decreases approximately on 2%, first of all because of a "gap" between the major and the small domain of lysozyme. That is, disulfide bonds in lysozyme not only "glue" the secondary structure devices of protein, but also play a role of a "rod", supporting stationary values of volume of the molecule necessary for realization of its functions.

The work is partially supported by RFFI (01-04-49302), Ministry of Industry, Science, and Technology RF (40.165.11.0102) and the Ministry of Education RF (I-0431).

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