DYNAMIC PROPERTIES OF α – HELIX AND β STRUCTURES AS MOLECULAR COMPONENT OF PROTEIN AND AS ISOLATED MOLECULAR STRUCTURES IN THE VIRTUAL VISCOUS MEDIUM. ACCORDING TO THE METHODS OF MOLECULAR DYNAMICS

M.G. Mikhailyuk[a] and K.V. Shaitan[b]

[a] *Institute of Chemical Phisics, Russian Academy of Sciences, 4 ul. Kosygina, 117977 Moscow.*

[b] *Moscow State University, Vorob'evy Gory, 119899 Moscow.*

Extended elastic devices of a polypeptide frame organize fluctuation dynamics of a protein, that it is rather important for the functional activity. In a sense the molecule of protein can be presented as the reinforced drop consisting of elastic devices with various expansion and the shape, immersed in a dense medium formed from the side groups and molecules of a solvent. Devices of this construction make the restricted Brownian motion with parameters, defined by constants of a rigidity of elastic frame and microviscosity of intraprotein medium. The comprehension of physical principles of the mechanical device of protein globules and similar nanostructures is necessary for development of the molecular engineering and projection of the molecular machines.

In the given research we have studied in details the dynamics of secondary structure devices on the examples of α-helixes of myoglobin, barnase, lysozyme, polylysine and polyglycine and β-structures in barnase, GFP and lysozyme by the methods of molecular dynamics. It is shown, that devices of secondary structure are essentially nonuniform and nonlinear elastic devices. The efficient elastic modulus of α-helix and β-layer reaches a maximum at center and noticeably goes down at the terminative sections. Especially it is noticeably for N-terminus of α-helix. The dynamic structure of a α-helix reminds a spring with stretched and loosed coils on the ends. Due to it amplitude maxima of α-helix bending fluctuations are observed near first and last quarter of its length. The efficient melting of α-helix begins at N-terminus. In vacuum at temperature 700K at times about 5ns over half of aminoacid residues stays in other possible conformations at least during a half of estimated time. Elastic moduluses of the free α-helix and free β-layer, calculated in full-atomic approximation, are $E=6\div8*10^{11}$ erg/sm^3. In molecular component of protein elastic moduluses of α-helix and β-layer appear 1.5-2 times above. Because of steric restrictions at fluctuations of these devices in structure of protein there is a noticeable distinction in amplitudes in comparison with free devices of secondary structure cut out from a molecule of protein. For example amplitudes of fluctuations of free α-helix and the same α-helix in a composition of barnase differ in 1.7 times. Variations of potential field parameters at change from heavy-atomic model to full-atomic model make essentially effect on the magnitude of elastic modulus and the amplitude of bending fluctuations of secondary structure devices. These results show the sensitivity of these dynamic parameters to details of exposition of force field and, apparently, can be used for an improvement of force parameters further.

mmax@moldyn.ru