AQUEOUS ENVIRONMENT INFLUENCE ON MOLECULAR DYNAMICS OF OLYGOPEPTIDES

K.V. Shaitan and S.S. Saraikin*
M.V. Lomonosov Moscow State University, Moscow, Russia 119899

The physical principles underlying dynamic behaviour of biomacromolecules are studied more than 25 years. However there was practically missed the detailed and comparative studying peptide structures molecular dynamics at various conditions. In issue comparative studied ergodic molecular dynamics trajectories of dipeptides series containing all twenty natural aminoacids residues in vacuo and in aqueous medium. In the latter case peptide put in a cube with water molecules under periodic boundary conditions. For water molecules model TIP3P is used (tab. 1). An edge of the cube is 25 A. The cube contains approximately 500 molecules of water. The quantity of water molecules varies on the investigated dipeptide size keeping of density about 1. All types atom - atom interactions are included. Technical problems of trajectories ergodicity are solved. The one-dimensional distribution functions for various tortion angles, two-dimensional distribution functions for pairs of tortion angles and Poincare sections, cumulative multivariable distribution functions for N tortion angles, free energy maps, and also dynamic correlations with the help of special kind normalized auto- and crosscorrelation functions are used and studied for dipeptides under vacuo and aqueous medium conditions. The similarity in dynamic behaviour between olygopeptides in vacuo and in aqueous medium is discussed.

Table 1. Parameters of the valent, electrostatic, Van der Waals interactions and hydrogen bonds used for water model.

Atom	Van der Waals interactions		**Hydrogen bond**		Valent bond		Valent angle		Atom charges
	ε	r_{min}, A	ε	r_{min}, A	K_{OH}, kcal/(mol *radian^2)	r_{min}, A	K_{HOH}, kcal/(mol *radian^2)	θ, degree	q, e
O	0,15	3,3	0,5	1,95	1106	0,96	94	104,5	-0,834
H	0,02	2,0							0,417

E-mail: *sara@moldyn.ru*