ISSN: 0975-8585

Research Journal of Pharmaceutical, Biological and Chemical Sciences

Study Conformation of the Protein Molecules during Heat Treatment of the Meat Products.

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ABSTRACT

Methods of molecular analysis confirmed the feasibility of the integrated use of milk protein-carbohydrate and raw meat, because complex with a reduction in its use of energy, the system is stabilized, resulting in improved functional and technological properties of meat (FTP). Based on the thermal process modeling and analysis of physical, chemical and thermodynamic properties of molecules α-casein, lactoglobulin and myosin found that the total energy of these components in the complex is lower than offline state (Δ E = 3175,1 kcal / mol), that testifies to stabilize the system. Introduction of lactulose does not have a significant impact on the overall energy complex. Analysis of the spatial structure after the heat treatment showed the diffusion of molecules of water in the lactulose and protein complexes without breaking of covalent bonds.

Keywords: protein molecules, lactulose, α-casein, myosin

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ISSN: 0975-8585

INTRODUCTION

To date, dozens of millions of synthesized organic compounds of different chemical structure. But in practice be used only several tens of thousands. Each compound has its own characteristic physico-chemical properties. However, not all connections are experimental confirmation of their properties [1]. Therefore, an important task is to find quantitative correlations between structure and properties of chemical compounds. The study of these relationships allows you to quickly choose from the available compounds, the most desirable and determine the direction of the synthesis of new compounds. Molecular mechanics method can be used to study systems, including several thousand atoms, such as oligomers, proteins and polysaccharides. It solves problems using conformational analysis: Search stable states by minimizing the energy of a molecular system. Visualization of the spatial structure of molecules and calculation of their geometric structure will effect the forecast physico-chemical properties of organic compounds.

MATERIALS AND METHODS

In the simulation of molecular structures were determined the total energy and the dipole moment of the rms gradient. Dipole moment shows the changes of both static and dynamic parameters of the molecules.

Using Langevin dynamics module in the application HyperChem v. 7.1 simulated heat treatment process α-casein, lactoglobulin, and myosin of these proteins at 72° C, that corresponds to technological regimes curing boiled sausages [2]. The simulation processing components in water was carried out in the module Periodic boundary conditions (periodic boundary conditions). The meaning of the periodic boundary conditions in molecular dynamics is that using this method solves the problem of modeling the system consisting of a large number of water molecules. After heat treatment was take results the total energy of each molecule of the water , and the dipole moment of the gradient of the mean square.

The simulation processing components in water was performed by Langevin dynamics module Periodic boundary conditions (periodic boundary conditions). The meaning of periodic boundary conditions is that using this method solves the problem of modeling the system consisting of a large number of water molecules.

RESULTS AND DISCUSSION

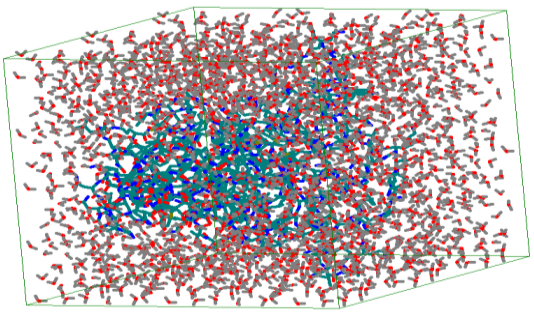

Figure 1: Cell periodicity with α-casein molecule before heat treatment

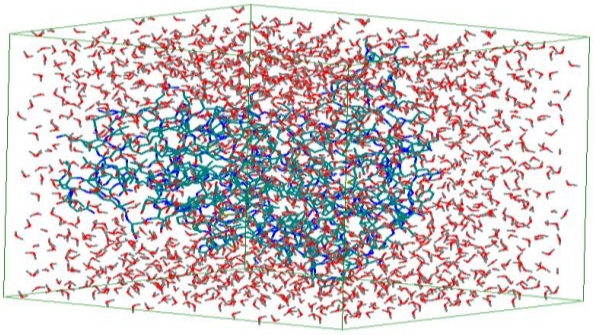

Figure 2: Cell frequency with α-casein molecule after eat treatment

ISSN: 0975-8585

The implementation of the modeling process α-casein (Fig. 1, 2), lactoglobulin, and myosin showed little change in the conformation of the molecules.

As a result of the heat treatment α-casein in water form a spatial network structure with the arrangement of water molecules in cells and beyond their borders. In addition, the modification process there is no destruction of the intramolecular bonds of the analyzed fragments.

In the simulation of the thermal treatment lactoglobulin in water (Fig. 3, 4) also observed a slight change in the conformation of the formation of the spatial structure of the entire volume of the cell hydration.

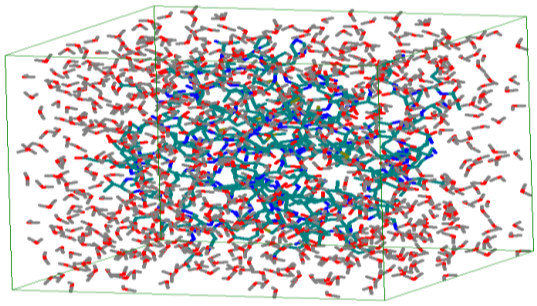

Figure 3: Cell periodicity lactoglobulin molecule before heat treatment

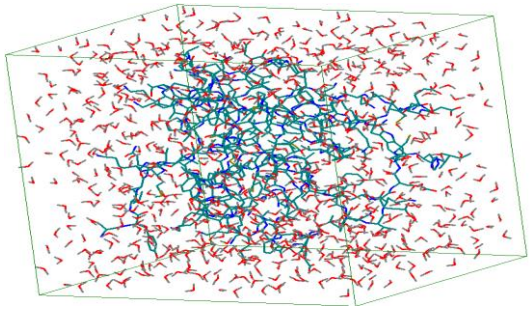

Figure 4: Cell periodicity molecule lactoglobulin upon heat treatment

After the process computer simulation heat treatment in water myosin (Fig. 5, 6) observed a more major modification in the conformation of the system.

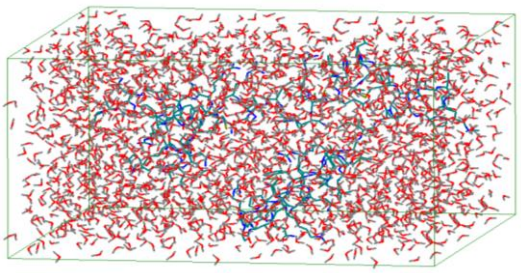

Figure 5: Cell periodicity myosin molecule to a thermal treatment

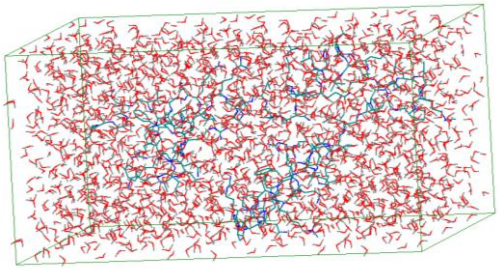

Figure 6: Cell periodicity myosin molecule after heat treatment

Analysis of the heat treatment process, the protein molecules α-casein, lactoglobulin and myosin in water showed that a reduction in the total energy without breaking the covalent bonds (Table 1).

Table 1: Some of the physicochemical properties of systems: α-casein -water, lactoglobulin – water and myosin - water

Type of system	Total energy, kcal / mol	Dipole moment, Debye	Rms gradient kcal / Å×mol)
α-casein -water	13945,1	74,3	18,9
lactoglobulin – water	6865,7	46,6	19,7
myosin - water	9027,4	69,1	16,4

Based on the magnitude of the dipole moment may be assumed hydrogen bonding. RMS gradient testified to the effective implementation of the procedure of computer simulation.

Based on the analysis decided to examine the molecular properties of these compounds in the complex. Protein molecules of α-casein, lactoglobulin and myosin were placed in a module with periodic boundary conditions and conducted its geometric optimization (Fig. 7, 8).

ISSN: 0975-8585

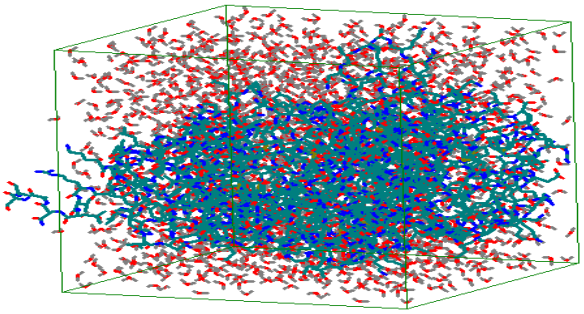

Figure 7: Periodicity cell with the protein system to geometric optimization

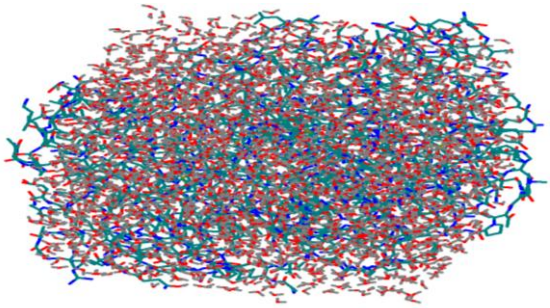

Figure 8: Periodicity cell with the protein system after geometric optimization

After geometry optimization of the system changes its conformation. Using the module Langevin dynamics defined thermodynamic and physicochemical properties of the system - the energy was 26663.1 kcal / mol, which is lower than the total energy systems in off-state (ΣE = 29838.2 kcal / mol).

This result indicates that the integrated use of these components helps to reduce energy and stabilize the system.

Due to the fact that, in formulations developed products assumed the use of lactulose having prebiotic properties investigated its influence on the physico-chemical properties of the protein. The amount of added lactulose was 3% of the molecular weight of the protein complex. As in the previous case, the first geometrical optimization was performed, and then simulation heat treatment Langevin dynamics module (Fig. 9, 10).

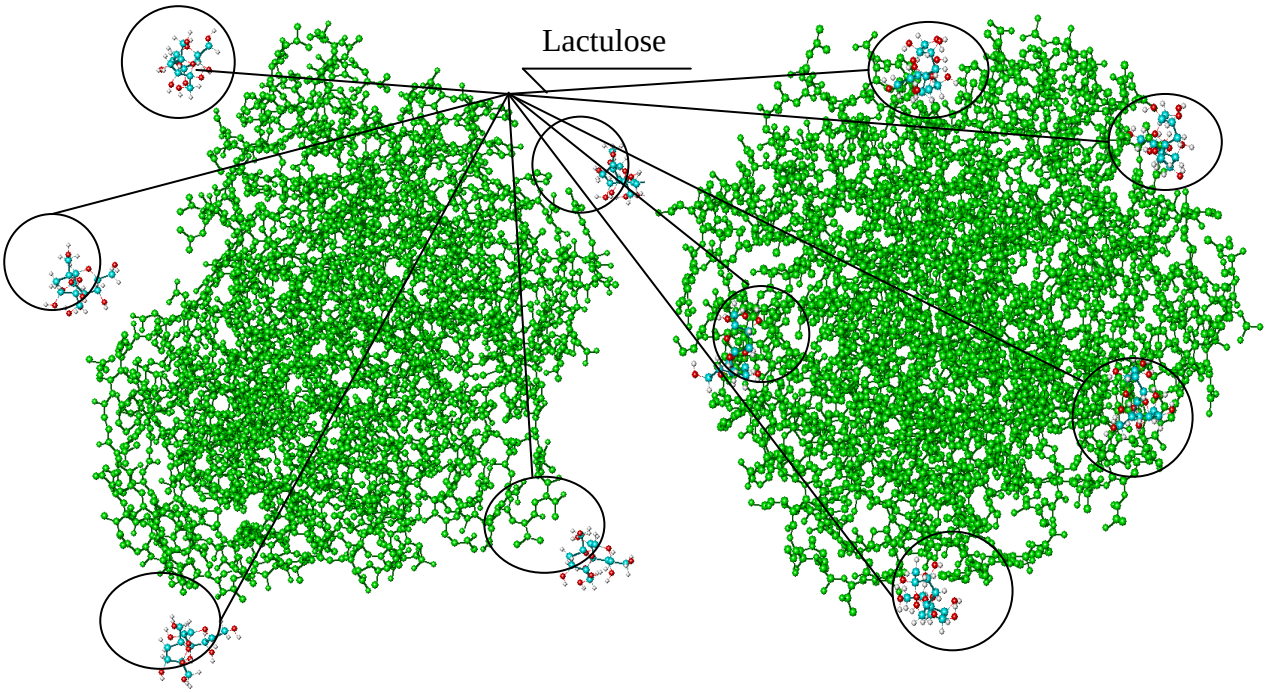

Figure 9: Periodicity cell with the protein system to geometric optimization

Figure 10: Periodicity cell with the protein system after geometric optimization

Analysis system configuration (Fig. 9, 10) showed that there is a diffusion heat treatment in the lactulose molecule protein, but does not result in a chemical reaction. Lactulose retains its structure and activity.

The total energy of the complex was 28361,2 kcal / mol, at 1698,1 kcal / mol higher than that of lactulose without complex proteins, but 1477,0 kcal / mole lower than the total energy in the system offline.

ISSN: 0975-8585

CONCLUSION

Thus, based on the heat treatment process simulation and analysis of the physicochemical and thermodynamic properties of the molecules of α-casein, lactoglobulin and myosin found that the total energy of these components in the complex is lower than offline state (ΣE = 3175,1 kcal / mol), indicating that the stabilization of the system. Introduction of lactulose does not have a significant impact on the overall energy complex. Analysis of the spatial structure after the heat treatment showed the diffusion of molecules of water and the lactulose in protein complexes without breaking of covalent bonds.

The results of computer simulations can provide the basis for the development of prescription formulations meat with dairy protein and carbohydrate drugs.

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