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Studies of α_{s1}-Casein Molecular Structure and The Proteins Emulsifying Ability in Activated Media.

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ABSTRACT

The molecular modeling and quantum-chemical calculations of the milk protein molecule fragment (α_{s1}-casein) in drinking and electrochemically activated water (catholyte) have been performed. Positive influence of the catholyte on the protein hydration and emulsifying abilities has been determined on the molecular level. More effective usage of the powdered protein milk products hydrated by electrically activated water as emulsifiers and water-binding components has been proven by experiments.

Keywords: molecular modeling, quantum-chemical calculations, α_{s1}-casein, emulsifying ability, the electrochemically activated water.

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INTRODUCTION

At the present time the products containing milk proteins are widely used in meat, milk, confectionary and other branches of industry. For example, sodium caseinate or complex additives made on its basis designated to replace raw meat, milk powder, vegetable proteins and to consolidate finished products structure are widely used in the process of meat products production. Due to these substances application protein-fatty emulsions are stabilized; products consistency, succulence and appearance are made better; losses are reduced due to reduction of water and fat pockets formation in the process of thermal processing, and product cost is reduced.

The work objective belongs in investigation of the electrochemically activated water (catholyte at pH equal 11.2, oxidation and reduction potential equal -500 mV) influence on the milk proteins properties (by example of α_{s1}-casein) with a help of molecular modeling, quantum-chemical calculations and the experiment results review.

METHODS

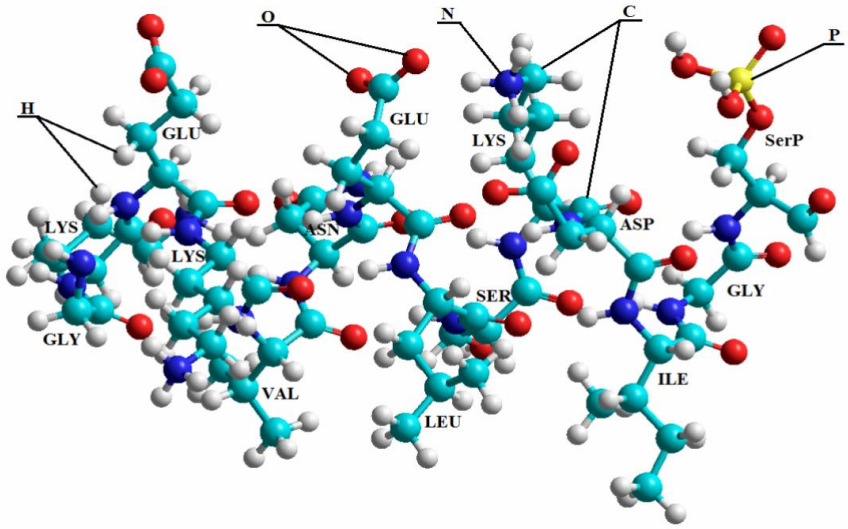
The molecular modeling and the quantum-chemical calculations have been performed with a use of HyperChem software tools. Geometry optimization for α_{s1}-casein molecule fragment (milk casein base fraction) has been performed in accordance with the recommendations [1] by AMBER molecular mechanics method developed specially for proteins and nucleic acids.

To establish electrostatic potential distribution on α_{s1}-casein molecule surface they have performed calculation of partial charges on the atoms of the protein fragment being studied using PM3 semi -empirical quantum-chemical method (modified neglect of diatomic overlap Parametric Method 3) [1].

Emulsifying ability has been determined by the method of Inklaar P. and Fourtuin J. [2, 3, 4], by means of emulsion preparation on homogenizer based on 1% of protein water dispersion at constant rate of sunflower oil adding.

RESULTS AND DISCUSSION

The sequence of 14 amino-acid residues of the genetic variant B main chain (numbers 33-46) [5, 6] covering the transition from its hydrophobic section to the hydrophilic section with strong peculiar properties has been chosen for the studies conduction on the basis of α_{s1}-casein original structure analysis having been performed (Fig. 1).



-Gly-Lys-Glu-Lys-Val-Asn-Glu-Leu-Ser-Lys-Asp-Ile-Gly-SerP-

Figure 1: The fragment of α_{s1}-casein molecular structure

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For the purposes of α_{s1}-casein and drinking water interaction process modeling the protein molecule fragment has been placed to the water box center using Periodic Box tool of HyperChem software application. After the water molecules relaxation by the basic method of MM+ molecular mechanics, the protein molecule quantum-chemical calculations have been performed, its geometry has been optimized and partial charges calculation has been performed on the atoms of α_{s1}-casein molecule fragment being studied. The system minimum potential energy value -3069.997 kJ/mol at the mean-square gradient – 0.398 kJ (Å·mol) has been determined on the basis of the protein molecule fragment geometrical optimization in drinking water (Fig. 2).

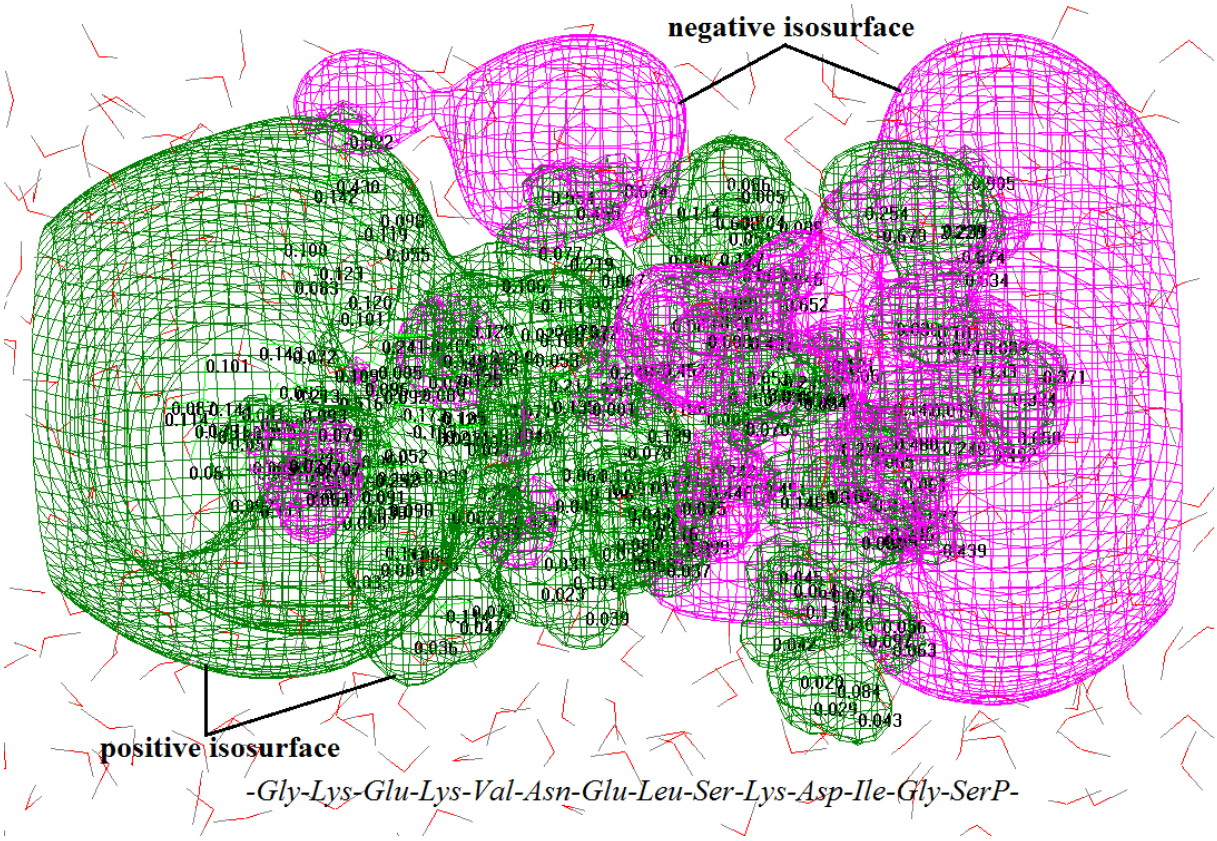

Figure 2: Three-dimensional chart of distribution of partial charges and electrostatic potential of α_{s1}-casein molecule fragment in drinking water

It was established that the high electron density areas on α_{s1}-casein molecule fragment being studied are located in the end sections of amino-acid residues with oxygen atoms and the strongest negative electrostatic potential is formed with participation of amino-acid residues of glutamic and aspartic acids as well as phosphoserine.

The analysis of the model of partial charges and electrostatic potential distribution on the surface of α_{s1}-casein molecule fragment being studied (Fig. 2) allows confirming that this peptide chain has two sections with opposite properties – strong hydrophobic and hydrophilic abilities.

The protein and catholyte interaction modeling (Fig. 3) has been performed by the algorithm described above with regard to our own experimental practice and on the basis of the previously conducted investigations results [7, 8, 9]. The protein molecule geometrical optimization in catholyte allowed determining of the system minimum potential energy value -3469,697 kJ/mol at the mean-square gradient –0,391 kJ/(Å·mol). The determined potential energy value change of α_{s1}-casein molecule fragment being studied comparing to drinking water demonstrates increase of its structure-forming ability in the activated water medium.

It is known that hydration ability at the molecular level can be evaluated based on the dipole moment value being the molecule polarity measure and on the number of hydrogen bonds formed [10]. It was established that the dipole moment value of α_{s1}-casein molecule fragment being studied in catholyte has been

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reduced by 27.17 D (in drinking water – by 88.38 D, in catholyte – by 61.21 D) and the number of hydrogen bonds between the hydrophilic section of α_{s1}-casein molecule fragment being studied and the catholyte molecules has increased by a factor of 1.3 comparing to the results of the system modeling on the basis of drinking water.

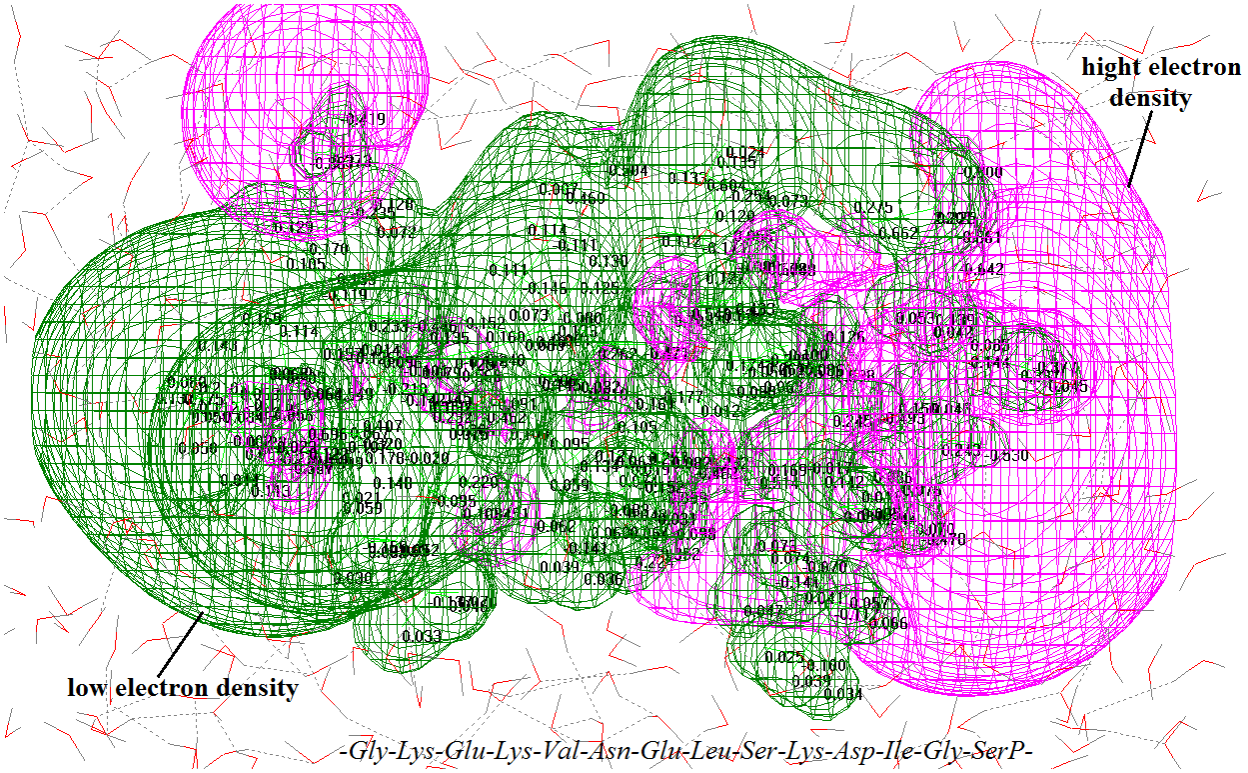

Figure 3: Three-dimensional chart of distribution of partial charges and electrostatic potential of α_{s1}-casein molecule fragment in catholyte

The conducted investigations demonstrate that catholyte while entering energetic contact with the active biopolymers sorption centers passes to the bound state in greater degree compared to drinking water which in its turn causes change of biopolymers properties at the molecular level. It is recognized that the moisture being bound in such way suffers first-order phase transition which shall be taken into consideration for the purposes of technological problems organization and solving [11].

The analysis of the results of α_{s1}-casein molecule fragment quantum-chemical calculations and electrostatic potential distribution in catholyte (Fig. 3) comparing to drinking water demonstrates strong electrostatic potential concentration with high electron density center displacement to the phosphoserine amino-acid residue area (*SerP*) and allows predicting of the protein emulsifying ability increase due to hydrophilic and hydrophobic properties strengthening at the corresponding sections of the peptide chain.

The conducted quantum-chemical studies data are confirmed by the results of the full-scale experiments characterizing the influence of the dispersion medium on emulsifying ability of the powdered milk protein product “Belmiks NK” using Na-casienate as the basis. The experiments have shown that the strongest emulsions stability is observed when the catholyte of 60% fat phase percentage is used. Emulsifying ability of a protein product at the specified oil concentration in the system reaches 150 g of fat per 1 g of protein. When drinking water is used the maximum volume ratio of sunflower oil amounts 50%. When oil concentration exceeds 70% an emulsion is almost not forming in the system with drinking water (Fig. 4); at the same time it is well observed and it is quite stable with catholyte.

Therefore protein milk products hydrated with electrically activated water (catholyte) are more effective as emulsifiers and water-binding components then when drinking water is used. This allows recommending them for production of different meat products.

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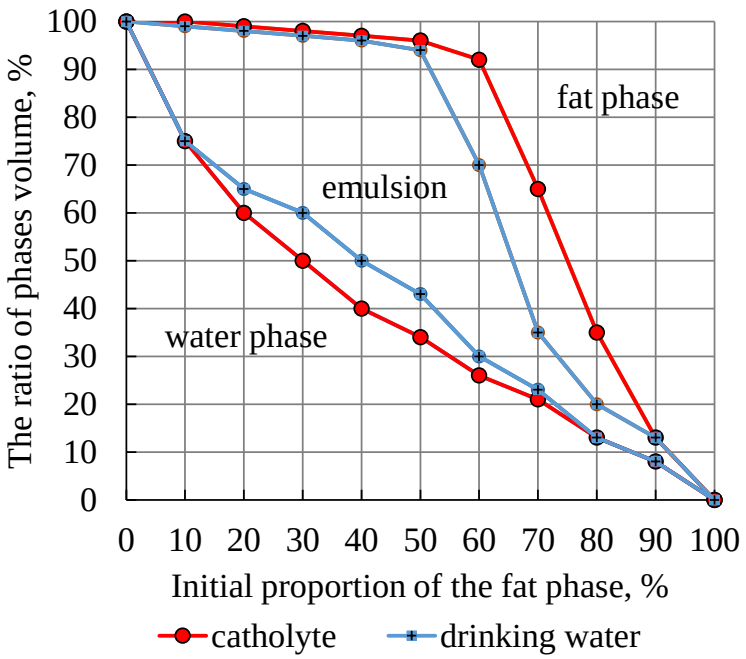

Figure 4: The diagram of the milk protein product "Belmiks NK" emulsifying ability

CONCLUSION

It is established at the molecular level that catholyte usage provides new possibilities for the protein-bearing food stuff technology as far as electrically activated water enters the bound state in greater degree (by a factor of 1.3 greater compared to drinking water) and that is why colligative properties interconnected transformations of the food raw material hydrophilic components can be predicted.

The molecular modeling and experimental studies results demonstrate that when a catholyte is used somewhat different mechanism of protein-fatty emulsions forming is observed then when drinking water is used. It is related to the specific nature of the protein molecule charges and electrostatic potential distribution in catholyte which is the reason of increase of its hydration degree and fat particles adsorption on the surface and consequently emulsifying ability increase.

The data obtained allows objective assessing of the possibilities for effective usage of powdered milk-protein products hydrated with electrically activated water in the process of emulsified food stuff production.

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