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FORECASTING OF FUNCTIONAL PROPERTIES OF THE SOYA PROTEIN BASED ON THE MOLECULAR DYNAMICS METHOD

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Abstract

One of the global problems of the food industry is to find the new protein source that could be used for high quality and nutrients balanced foodstuffs production. Soya isolates and concentrates as well as soya flour are widely used in meat industry. From the technological point of view, the new method of functional properties regulation of plant protein should consider the water-binding capacity, emulsifying and gel-forming capabilities development. Functional and technological properties could be controlled by activated liquid systems made by electrochemical treatment and cavitational disintegration. The goal of research was to study the soya protein (11S-globulin) behavior in different medium by the method of the molecular modeling. Molecular modeling and quantum chemical calculations were provided by special computer programs complex VMD and NAMD.

It was established that significant changes in electrostatic potential distribution of 11S-globulin molecule were observed in electrochemical activated water (EAW) rather than in water. Total amount of positive charged parts of molecule was 1.2 times as much in anolyte, and total negative charged parts was 1.7 times as much in catholyte. It was established that amount of neutral parts of protein was reduced by 3.63% in anolyte and by 14.77% in catholyte in relation to the total square surface of the protein.

Results of molecular modeling could be used for methods of soya protein modification developing by activated liquids using instead of drinking water.

***Key words**: Soya globulin, Catholyte, Anolyte, Molecular modeling, Quantum and chemical calculation, Electrostatic potential.*

1. Introduction

One of the global problems of the food industry is to find the new protein source that could be used for high quality and nutrients balanced foodstuffs production. There are some kinds of plant sources of the protein that have high content of protein (20-40 %): soya, bean, chick-pea, pea, mung, lupine, lentils and etc.). Forecast of the consulting company LMC International Ltd said that the international market of soya concentrates would rapidly grow and get to 5.6 million tons in 2020 as well as soya isolate market would catch up to 1.6 million tons. It is predicted that part of the whey protein market and up to half of caseinate and casein market would be replaced by plant protein products. Soya isolates with 91.0% of the protein content, and concentrates (68% of protein) and soya flour (57% of protein) are widely used in meat industry. From the technological point of view, the new method of functional properties regulation of plant protein should consider the water-binding capacity, emulsifying and gel-forming capabilities development.

There are some problems of functional properties of meat and combined products regulations that should be solved for high quality foodstuffs production. Traditionally, water-binding and emulsifying capacities and gel-forming capability are usually controlled by the optimal physicochemical and thermodynamical parameters of processing and biotechnological methods as well as physical treatment using (Titov [1], Shazzo [2], Sarbatova [3]).

One of the ways of functional and technological properties control is activated liquid systems using for treatment of the raw material or using that water for foodstuffs production instead of the drinking water. There are some methods of activated systems making that usually use new methods of treatment like electrochemical activation (water dialysis) ultrasonic treatment, magnetic processing.

There are many different publications about benefits of electrochemical activated water using for raw material processing and foodstuffs production. From scientific point of view, there are some more interesting effects than pH level of catholyte and anolyte made by electrochemical treatment of water (which could be obtained by traditional chemical methods): energy potential which was moved out from equilibrium condition and characterized be redox potential, dielectric permeability and some other parameters (Bakhir [4], Borisenko [5]).

Research works of Borisenko A. and Bratsikhin A. [6] were dedicated to electrochemical water using for raw meat and plant material functional properties regulation in meat products manufacturing processes. It was established that catholyte could be used instead of drinking water in gelled and whole meat foodstuffs production as well as for semi-finished meat-and-plant products making. Catholyte as a base of the brine for meat salting could develop water binding and color processes that could decrease the phosphates and sodium nitrate adding into the meat product formulation.

The goal of made research was to study the different kinds of the continuous medium (drinking water, catholyte and anolyte of the electrochemical treated water) influence on the soya protein properties (11S-globulin) by the method of the molecular modeling, and quantum and chemical calculations.

2. Materials and Methods

Molecule of 11S soya globulin was downloaded from International Protein Data Bank and optimized in special computer programs listed below.

Molecular modeling and quantum chemical calculations were provided by special computer programs complex VMD (Visual Molecular Dynamics) and NAMD (Nanoscale Molecular Dynamics) [7]. Subunit of A3B4 (Adachi [8]) 11S globulin molecule was placed in the centre of virtual water box with different types of continuous medium. The geometrical optimization was made and then the modeling of system's component interaction was made by method of molecular dynamics at temperature 293 K.

3. Results and Discussion

It was established that studied subunit A3B4 had two protomers consisted of the N-terminal and C-terminal structural equivalent domains, which were connected by disulfide bond. Every protomers had two β-barrels from β-sheets, which are connected with α-helix contented three long disordered parts. These parts were created hydrophilic areas on surface of the hexamerous 11S globulin molecule.

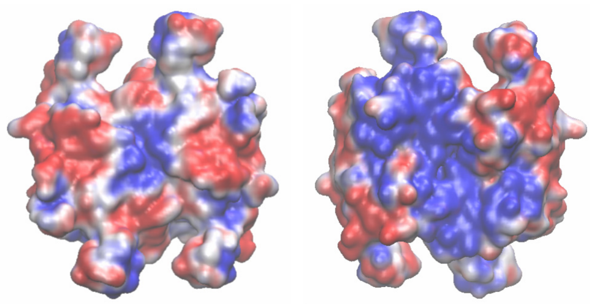
The map of molecular electrostatic potential dispersion on surface of studied molecule (11S-globulin) in water is show on Figure 1.

Blue color on Figure 1 shows the part of molecule, which have positive potential in range [1, +∞), white color – fields of potential in the (–1; +1), and red color – for negative potential in range (–∞; –1]. The analysis of the Figure 1 shows that hydrophobic interactions and numerous hydrogen bonds have the most important role on molecule structure forming. Positive and negative charged parts of the protein molecule are its active centers in water solutions and determine good hydrational capacity of 11S-globulin.

It is known that systems, which have the molecules contented asymmetrical polarized group in addition to the non-polar ones, provide emulsifying properties. They could easily adsorb on the phases boundary and create gel-structured layer that prevents fat globes agglomeration.

Presents of the visual hydrophilic and hydrophobic parts allows the 11S globulin molecules adsorbing on the protein-fat phase boundary with gel structured layers creating, which produces the emulsifying ability and other functional properties of the protein.

It is known that continuous medium pH-level changing provides recharging of the colloidal systems as hydrogen and hydroxide ions have high capability to adsorption. Hydrogen ions have the small radius as well as hydroxide ions have dipolar moment so that allows them moving closely to the molecule surface. Based on the listed knowledge and obtained results on the modeling, it could be supposed that there would be increasing of the centers with excess or deficiency of electron density when the pH-level would be changed because of the nucleophilic (electrophilic) attack oriented on the positive (negative) charged terminal groups of the amino acids residues of 11S-globulin molecule. Therefore, controlled shifting of the pH-level and additional energy transferred into continuous medium after activation process makes it possible to regulate the protein functional properties directionally.



a) b)

Figure 1. Map of molecular electrostatic potential dispersion on surface of 11S-globulin molecule in water: *a* - face view; *b* - rear view

Practical realization of the mentioned method could be solved by the searching and finding of the universal internal interaction methods, which might be used for real changing of the continuous medium parameters that should be connected with the technological characteristics of the produced foodstuffs.

Comparative analysis of electrostatic potential distribution on the 11S globulin molecule in different kinds of water medium was made based on results of spot square calculation, which were created by the zones with the different potential (Figure 2). It is known that for far interaction like Coulombic ones, concave and convex surfaces are approximated by their projections on the plane that is perpendicular to the vector of their direction (Saburova [9]). That is why, the surfaces square were determined as square of their projections on the respective plane in specific coordinate system, which was chosen according to the square of spot projection that must be the highest.

It was established that significant changes in electrostatic potential distribution of 11S-globulin molecule were observed in electrochemical activated water (EAW) rather than in water. It was noted from the shape and sizes of the areas with a different potential analysis (Figure 1 and 2). It was fixed that there were changed condition in ratio between areas with a different potential in EAW: the total amount of positive charged parts was 1.2 times as much in anolyte, and total negative charged parts was 1.7 times as much in catholyte. It addition, it was established that amount of neutral parts of protein was reduced by 3.63% in anolyte and by 14.77% in catholyte in relation to the total square surface of the protein (Figure 2).

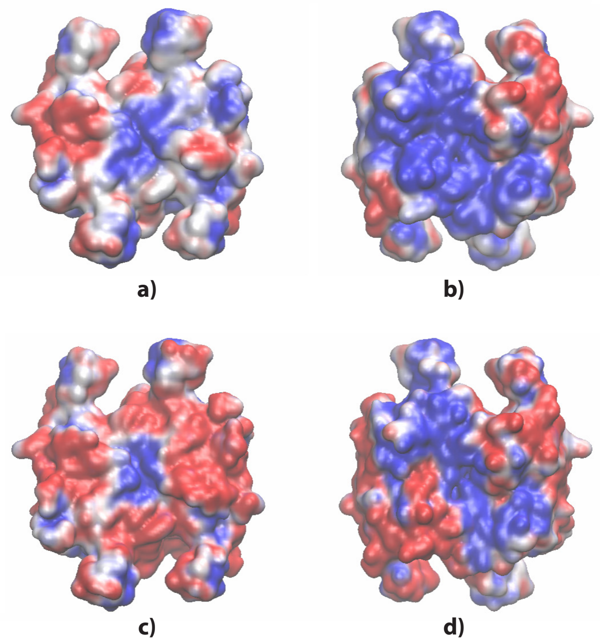


Figure 2. Map of molecular electrostatic potential dispersion on surface of 11S-globulin molecule (principle and rear views) in different medium: *a,b* - in anolyte (pH = 2.0); *c,d* - in catholyte (pH = 11.0)

Represented results could predict developing of the hydration capacity of 11S-globulin molecule in EAW because of the total square of the active centers increasing on the molecule surface, which could be attacked by electrophilic and nucleophilic agents. In addition, established developing of the surface hydrophilic properties in EAW (increasingly in the catholyte) should provide their position in oil-and-protein emulsion around the drops of continuous phase to the largest part of the surface from the external side, and it could prevent coalescence phenomena and might be one of the factor of the emulsion stabilizing.

4. Conclusions

- Methods of molecular modeling and quantum-chemical calculation could be effective using for forecasting of proteins behavior and their functional properties forming at different conditions.

- Stable protein-and-fat emulsion could be formed when the catholyte with pH = 11.0 would use instead of drinking water. Recharging of 11S-globulin molecule provides its electrostatic potential changing that is the reason of the protein's hydration development as well as its emulsifying capability.

- Results of molecular modeling could be used for methods of soya protein modification developing by activated liquids using instead of drinking water, before it would be added to the formulation of the meat-and-plant products for their balancing on amino acids content.

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