

## 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 cavitation 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.