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QUANTUM-CHEMICAL SIMULATION OF THE INTERACTION BETWEEN THE Zn^{2+} IONS WITH C-TERMINAL SITES OF KAPPA-CASEIN

Vladimir Grigorievich Kayshev[1,2], Andrey Vladimirovich Blinov[3*], Alexander Vladimirovich Serov[3], Alexey Alexeevich Gvozdenko[3], Alexander Alexandrovich Kravtsov[4,5], Anastasia Alexandrovna Blinova[3], Andrew Georgievich Khramtsov[6]

[1]RAS, Leninsky Prospect, 14, 119991 Moscow, Russia
[2]LLC "Agrofirma - Selo Voroshilova", Stavropol region, Predgorniy district, Tsentralnaya str. 91, stanitsa Suvorovskaya, Russia
[3]Institute of Engineering, North Caucasus Federal University, Kulakova str. 2, 355029 Stavropol, Russia
[4]Federal Research Center - The Southern Scientific Centre of the Russian Academy of Sciences, Chehova str. 41, 344006 Rostov-on-Don, Russia
[5]Scientific-research Laboratory of Ceramics and Techno-chemistry, Scientific-laboratory complex of Clean Rooms, Institute of Engineering, North-Caucasus Federal University, Kulakova str. 2, 355029 Stavropol, Russia
[6]Institute of Living systems, North Caucasus Federal University, Pushkina str. 1, 355009 Stavropol, Russia

[*]e-mail: blinov.a@mail.ru

Abstract

Currently, the enrichment of dairy products with micronutrients is a promising and relevant area in the food industry. Upon obtaining such food products, special attention should be paid to the study of the effect of functional additives on the stability of the colloidal system of milk.

As part of this study, we studied the interaction of zinc ions with the dispersed phase of milk. Negatively charged fragments of the C-terminal site of K-casein containing carboxyl, OH^- groups and phosphoric acid residues were simulated before and after interaction with zinc ions. The models of the C-terminal region fragments of K-casein were obtained in the QChem application using the IQmol molecular editor. The calculations were carried out on the equipment of the data processing center of the North-Caucasus Federal University (Schneider Electric). Modeling parameter was energy, method – HF (Hartree-Fock method), basis: 6-31G, convergence - 5, force field - Ghemical, modeling was performed in a vacuum.

The simulation showed that the negative charge in the considered fragments of the C-terminal site of the K-casein is concentrated on the oxygen atoms belonging to the carboxyl, hydroxyl groups and phosphoric acid residues. The interaction of positively charged zinc ions with the most negative charged regions leads to a significant redistribution of the electron density, a change in the spatial configuration and a change in the total energy of the regions.

It has been established that after the interaction of the C-terminal fragment of K-casein containing 18 amino acid residues with zinc ions, the system's energy significantly decreases from - 6517.503 to - 10066.149 kJ/mol, and changes its spatial configuration, which indicates a significant energy benefit of the Zn-casein complex existence.

***Key words**: Zinc ions, Zinc trace element, Quantum-chemical computer simulation, K-casein, C-terminal sites*