status in the experiment depending on the season and the type of higher nervous activity. Experimental and clinical physiology and biochemistry. 999. N2. P.7–10.

3. Shkurupii V. A. Ultrastructure of the liver cells in stress. Novosibirsk: Nauka, 1989. 144 p.

THE STUDY OF ANTI-RADICAL ACTIVITY OF GLUTATHIONE WHEN INTERACTING WITH FREE RADICALS OF OXYGEN

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Following the analysis of the results of quantum chemical simulation of interaction between a GSH molecule and oxygen radicals •OH and $•OO^-$, it was found that it takes place through the acid-base mechanism, where GSH acts as a base towards •OH, and as an acid towards $•OO^-$.

Key words: glutathione, hydroxyl radical, superoxide-anion-radical, quantum chemical program Firefly.

ДОСЛІДЖЕННЯ АНТИРАДИКАЛЬНОЇ АКТИВНОСТІ ГЛУТАТІОНУ ПРИ ВЗАЄМОДІЇ З ВІЛЬНИМИ РАДИКАЛАМИ КИСНЮ

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На основі аналізу результатів квантовохімічного моделювання взаємодії молекули GSH з радикалами кисню •OH і $•OO^-$ встановлено, що вона відбувається за кислотно-основним механізмом, причому GSH по відношенню до •OH виступає як основа, а по відношенню до $•OO^-$– як кислота.

Ключові слова: глутатіон, гідроксил-радикал, супероксид-аніон-радикал, квантовохімічна програма Firefly

ACTUALITY. To decrease the negative effect of free oxygen radicals on a living organism practical medicine widely uses endogenous oxidants since they take part in the system of human organism protection from the aggressive action of free radicals, for example [1-2]. The lack of systematic investigations, especially at the molecular level, of antiradical activity of various antioxidants under their interaction with free radicals in biological systems not only determines availability of contradictory estimates in interpretation of the results of experimental regularities [3-5] but also creates difficulties in development of general ideas concerning the mechanisms of interaction of antioxidants with free radicals and purposeful approach to the control of these processes which are applied to medical practice [6, 7]. The above said actualizes studying the antiradical activity of various antioxidants.

Interaction of antioxidants with free radicals is determined by the influence of the great number of various interrelated kinetic processes which stabilization is rather problematic even in the experiment conditions. Thus, it seem urgent to study efficiency of the influence of endogenous antioxidants by simulating the mechanism of their interaction with free radicals by the methods of quantum chemistry in combination with experimental ones, in particular, with electrochemical method that allows not only obtaining the substantiation of the positive effect of using the antioxidants but also establishing potential significance of these substances as medical remedies.

The work objective was investigation of antiradical properties of endogenous antioxidant glutathione ($C_{10}H_{17}N_3O_6S$) by simulation of the mechanism of its interaction with free radicals (hydroxyl radical (•OH) and superoxide-anion-radical ($•OO^-$).

MATERIALS AND RESULTS OF RESEARCH. Human organism contains a nonenzymatic antioxidant system of cells protection from the influence of free radicals. The compounds with various properties appear as the system components. One of such compounds is glutathione (GSH) [8] synthesized in each organism cell, but antiradical mechanism of its interaction with active oxygen forms at the microscopic level is not completely understood, except for certain results of macroscopic medical [9] and electrochemical [10] investigations which are unfortunately of phenomenological character and do not give a purposeful approach to such processes control.

One of the key active forms of oxygen is $•OO^-$, which is formed when adding one electron to oxygen molecule in the basic state and can be a source of •OH formation in human organism; it may be the strongest oxidizer among free oxygen radicals [11], thus •OH and $•OO^-$ can exist simultaneously and be used for studying their interaction with glutathione for simulation of its antioxidant activity. The above said has determined the choice of investigation objects.

Theoretical study of the mechanism of GSH interaction with $•OO^-$ and •OH is performed with the help of the program module GAMESS (version of March 27, 2007) and program module Firefly 8 by the most modern unempirical quantum chemical method in the basis 6-31G** [12].

When GSH molecules interact with one $•OO^-$ at the point of global minimum of full interaction energy there occurs redistribution of the charge of 702e with $•OO^-$ to glutathione molecule through the atom of hydrogen H(23), indicating