

Study of the mechanism of reactions catalyzed by the cytochrome C complex with cardiolipin activated by coumarin dyes

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Motivation and Aim: Modern technologies and programming tools make it possible not to simply solve the problem, but also, using simulation and complex modeling methods, to create a virtual reality for work in which researchers can consider the topic of interest in all its diversity [1]. Here we analytically solved kinetic equations, describing the oxychemiluminescent reactions in the suspension of mitochondrial membranes, and compared the obtained results with experimental data [2, 3]. The system contained cytochrome C, forming a complex with cardiolipin, activated by the coumarin dye C-525 during apoptosis. The free radical formation was constantly monitored via the oxychemiluminescence kinetics. For data analysis, we developed a special program to calculate reaction rate constants based on the known reaction scheme, and compare different calculation algorithms.

Methods and algorithms: For solving the direct problem, the law of acting masses was used; the system of differential equations for reaction rates was solved by the Euler method; the rate constants were selected manually according to the method developed elsewhere [2]. The inverse problem was solved based on the above data and the law of quantum yield constancy. Several optimization algorithms in C++ were considered and implemented. Each of them was compared step by step with the experimental data, and the most successful algorithm was selected based on the calculated oxychemiluminescence quantum yields [3].

As is known, the chemiluminescence quantum yield in the presence of coumarin dyes is several orders of magnitude higher than for spontaneous oxychemiluminescence [4, 6]. Thus, analyzing electronic states in the process of photoexcitation [5], kinetic rate constants can be determined, which subsequently allows to determine the desired reaction scheme. To visualize the process, the photon emission was calibrated in conventional units so that the calculated luminescence kinetics and rate constants could be compared with the experimental data.

Conclusion: A method has been developed for analyzing the substrate of the peroxidase reaction, which can serve as an activator of chemiluminescence when studying the effect of the cytochrome C complex with cardiolipin on cancer cells.

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