MODELING OF THERMODYNAMIC PARAMETERS OF CHEMILUMINESCENCE ACTIVATED BY COUMARIN C-525 UNDER THE ACTION OF CYTOCHROME C COMPLEX WITH CARDIOLIPIN

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This work is devoted to the mathematical modeling of the free energy, entropy and enthalpy of the chemiluminescence activated by coumarin C-525 under the action of the cytochrome C complex with cardiolipin. The presentation of the optimal process model allows the use of CL methods for the analysis of thermodynamic characteristics, which can be used as the main one that determines the state of the system.

Physical activators enhance the glow by 2-3 orders of magnitude without affecting the chemical processes taking place in the system. Mathematical modeling of the entropy of the natural dye C−525, which intercepts the excitation of triplet-excited ketones, while having values of CL 3-4 orders of magnitude higher than the excited ketones themselves, we obtain CL activated by coumarin C−525, which shows an intensity value ~1500 times higher than spontaneous CL of lipids, when it does not differ from it in terms of kinetic curve parameters and has velocity constants of the same order. The accuracy of the calculation of entropy, entropy and free energy is determined by the presence of cardiolipin for pH stabilization, the quenching of Fe^{2+} and the presence of a physical activator C−525. Among the factors that distort the value of entropy, enthalpy and free energy, there is insufficient addition of hydrogen peroxide, excessive amount of nitrogen (II) , methanol, protein denaturation, and a change in the formation of CytC in the Cyt−CL complex.

In search of optimal excitation conditions, the systems of lipoperoxidase and quasi-lipoxygenase reactions activated by natural coumarin C−525 were analyzed.

In our work, based on the analysis of the parameters of cytochrome C with cardiolipin, the physical activator C−525, horseradish peroxidase and luminol, studies were conducted comparing mathematical modeling of the thermodynamic parameters of the system: entropy, enthalpy and free energy obtained from experimental data with the parameters obtained based on theoretical calculations.