SCIENTIFIC COMPUTING IN PYTHON

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Python is used in many ways. There are libraries for scientific calculations that make life easier for scientists. This language is fond of physics and mathematics for its easy to use.

Keywords: Python, MATLAB, NumPy, SciPy, Scikitlearn.

The Python programming language quite rapidly. Its scope is quite extensive, it is used in Web development, system administration, software and games, as well as in scientific research. Python is used and distributed free of charge, you can download it from official sites www.python.org. It is used in such campaigns as Google, Facebook, Dropbox, NASA, Fermilab, JPL. Using Python you can implement machine learning, an example is the prediction of the financial market. Intel, Cisco, and IBM use Python for hardware testing. The ease of this language, his love of mathematics and physics. MATLAB was originally written for scientific computing, unlike Python. But Python has many libraries that make life easier for scientists. An example of such libraries are SciPy is the library of scientific tools. It has modules to integrate and allows to solve the differential equation, signal processing, and helps in various problems that are solved in science and engineering. On top of it implemented a variety of modules for different fields of science. One of them Scikitlearn. These modules can be compared to MATLAB Toolbox. NumPy package allows you to conveniently work with vectors and matrices, the realization of all operations with them are carefully optimized. NumPy can be compared with the "core" of the MATLAB language. In the vast majority of research projects are written in Python using NumPy. Were also developed the Anaconda distribution, containing 720 packages, libraries for scientific and engineering computing.

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THE STATE OF CALCIUM METABOLISM IN RAT PLATELETS IN THE NEAREST AND LONG TERM AFTER IRRADIATION

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The investigation of the status of calcium metabolism in platelets of rats in the early and late periods after irradiation. Under the action of γ -radiation on platelets of rats revealed a change in indices of calcium metabolism in the early and late periods after irradiation (3rd, 10th and 30th day).

Keywords: calcium metabolism, platelets, irradiation.

Under ionizing radiation on the body one of the most sensory systems is the blood system. Among the cell elements, platelets play a crucial role in changing hemodynamic properties. One of the factors triggering platelet aggregation is Ca^{2+} . The calcium metabolism in rat platelets was analyzed in the experiment. Studies were carried out on mature white male rats (3 to 6 months age). Two groups of animals were studied. One group, the control group, was kept in the usual conditions of the vivarium. The animals of the second group were irradiated with

 γ -radiation in a dose of 1Gy and the state of calcium metabolism in platelets was studied on the 3rd, 10th and 30th days after irradiation.

Methods. The fluorescent pathfinder Fura-2/AMwas used for the quantitation of calcium concentration in platelets. The concentration of Ca^{2+} is calculated based on the measurement of fluorescence upon excitation of these two wavelengths according to the formula:

$$\left[Ca^{2+}\right] = K_d \frac{R_{\max 380}}{R_{\min 380}} \frac{F - F_{\min}}{F_{\max} - F},$$
(1)

where is the dissociation constant of the complex Fura-2/AM , $F = \frac{R_{340}}{R_{380}}$ – calcium – current ratio of fluorescent

signals, F_{\min} – the same ratio in the solution with low concentration of Ca²⁺, F_{\max} – the same ratio in a solution with a high concentration of Ca²⁺ (max and min when adding Triton (10 %) and EGTA (100 mmol/l), respectively). K_d = 224 nmol/l.

An increase of the basal level of calcium ions $(85,9\pm5,2 \text{ nmol/l})$ in calcium-free environment(100 mM EGTA) in platelets of rats was recorded after irradiation on 3rd day. There is a decrease in the basal level on the 10th day after exposure to calcium-free environment.

There is a greater than normal $(111,4\pm5,8 \text{ nmol/l})$ increase $(289,5\pm11,7 \text{ nmol/l})$ in the concentration of calcium ions in the platelets of irradiated rats on the 3rd and 10th day in response to the action of physiological inducers of platelet aggregation – ADP (20 mcrM) in the presence of 1 mM CaCl₂,

The content of cytoplasmic calcium by the action of thrombin (0,2 IU/ml)was increased only on day 3th $(561,9\pm12,1 \text{ nmol/l})$ and on 10th $(374,4\pm15,66 \text{ nmol/l})$ day did not differ from the norm $(383,2\pm15,2 \text{ nmol/l})$.

The concentration of calcium ions in the cytoplasm of platelets suspended in calcium-free and calcium-containing (1 mmol) in platelets of irradiated rats 30 days ($49,6\pm3,2$ nmol/l and $79,1\pm4,0$ nmol/l) after irradiation was not substantially different from the values in the control group ($44,8\pm3,6$ nmol/l and $67,6\pm7,1$ nmol/l).

Conclusion. The change in indices of calcium metabolism was revealed in the early and late periods after irradiation under the action of γ -radiation on platelets of rats: on the 3rd day after irradiation, an increase in the basal level of calcium ions in the platelets of irradiated rats in calcium-free and calcium-containing medium, and at 10-th and 30-th day its normalization. An increase in the intracellular concentration of Ca²⁺ ions under the action of ADP and thrombinis presented on 3rd and 10-th day, and did not differ from the norm on 30-th day.

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MULTIPLE CONFORMATION STATES OF HUMAN HEMOGLOBIN

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Hemoglobin (Hb) is one of the vital biomolecules in nature that plays a central role in binding, transporting and offloading oxygen from the lungs to the tissues to respiring cells, and represents the most well-defined and intensely studied allosteric protein. Hb exists in equilibrium between unliganded or deoxygenated Hb possessing low oxygen affinity, and the liganded or oxygenated Hb, which has a high oxygen affinity. Monod et al. assigned the deoxygenated Hb to the T (tense) and oxygenated Hb to the R (relaxed) states.

Our purpose is to study a number of intense and relaxed states of hemoglobin, which determine the degree of affinity of this protein to oxygen.

Keywords: hemoglobin (Hb), allosteric protein, deoxygenated Hb, oxygenated Hb, allostery, hemoglobin's affinity, conformation, ligand.