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THE SET OF PROGRAM MODELS FOR ECOLOGICAL MONITORING TECHNICAL SYSTEM BASED ON PRINCIPLES OF BIOPHYSICS

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Abstract—*Set of program models for ecological monitoring technical system is presented. The set includes the models based on the results of studied biophysical effects of some technical pollutants influence on the cells of living organisms.*

Index Terms—Technical system; ecological monitoring; transmembrane electrical current; program model; chemical pollutants.

I. Introduction

Area pollution by different chemical substances near airports, other industrial objects grows in contemporary world from day to day. That is why current elaboration of new technical systems supplied by kits of modern methods for ecological monitoring is topical nowadays. Also during last decades the ideas to unite together technical systems and living objects become more and more popular. Such combining them in biotechnical system may give possibilities to use in technique the advantages of technical and living systems both for the solution of different contemporary tasks.

In our previous publications were reported in details about the development of "EcoIS" technical system for ecological monitoring by Dr. Klyuchko O. M. and colleagues [1], [2]. Developed new technical system is based on computer informational technologies and directed on ecological, biochemical, biophysical data mining and processing. The system is complex one, and includes few types of subsystems. One of "EcoIS" subsystem is biotechnical device for testing of chemical substances – industrial pollutants. This subsystem with relative methods and techniques is analogous to devices developed previously for biophysical laboratory investigations of transmembrane electrical currents by intracellular dialysis, voltage-clamp, and patch-clamp methods [3] – [7]. Subsystem is supplied by original software, the set of program models that reflect a number of biophysical phenomena. Among them there are ones based on Dr. Klyuchko O. M. results of electrical properties of natural brain neurons studying [6], [7], studying of 2D neuronal complexes in culture and methods of excitable neurons marking by fluorescent drugs. Some of such program models we described previously in our publications [8] – [14]. Starting from the simplest program models like "Signal spreading along the linear fragment of DNA molecule", later were consequently developed models for "Electrical signals transmission along the neuron and its nanostrucrures", "Functioning of biologic voltage-activated nanostructures", "Auto-oscillating phenomena in neuron complexes", and some others. Below the brief review with more detailed description of some peculiar samples is given; they are interesting from the point of view of mentioned subsystem from "EcoIs".

II. Physical Model Of Planar 2D Complex Of Neurons

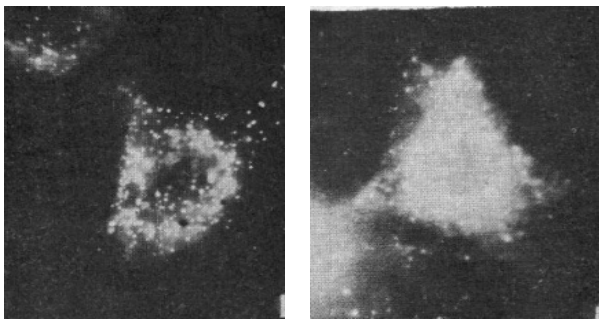
A General neuronal model description

Artificial system described below we called "quasi screen" [8], [14]. This "quasi screen" with bionic elements for biotechnical system may be imagined as 2D neuron matrix on plastic plate with cultural brain neurons in dissociated culture incorporated into electric circle with standard measuring and data stored devices. 2D neuron matrix also may be imagined as a model like chessboard (or "screen") with alternating rows and columns that separate the cells which contain optically active elements. Designing of such a "screen" in modern biophysical laboratories is absolutely real. This "screen" is specially designed plastic lining with specific "chess-like" geometric profile, armed with electrodes. The structure of such a "screen" we described previously in details [8], [11], [14]. Experimental results described in our previous articles were put in the base of our model (version of 2-dimentional network from brain neurons) [8], [14]. The sense of registered phenomena –input electric signal changes optical properties of the neuron, and luminescence of neuron become more intensive (Fig. 1) [8], [11]. Other results were taken into account during modeling – results of transmembrane electric currents studying in experi-

ments with patch-clamp, voltage-clamp, and etc. [3] – [7]. Basing on these facts the 2D neuronal model was elaborated. It looks like as screen matrix, formed by brain neurons in culture condition on plastic chess-like plate armed with electrodes. This biotechnical construction was incorporated into the electric circuit with measuring and information storage devices described in numerical manuals [3], [4], [14].

Further stages we planned were: 1 – simulation of 2D "quasi-screen" functioning (model 1), and 2 – elaboration of program for the simplest symbols coding at such screen (model 2). Obtained results are given below.

At the next step we would like to elaborate a program model of this neuronal "quasi screen". Abstract neurons were ordered on 2D matrix and corresponded to screen pixels. All these stages of our investigations were done, and results were already published in different scientific and technical journals [5], [7], [13], [14].



a b

Fig. 1. Effect on neurons marked by primulin and activated by agonist-neuromediator GABA. Fluorescent granules contained primulin complexes with proteins: a is control. Fluorescence in the absence of agonists influence; b is enhanced fluorescence of neurons in case of gamma-aminobutyric acid (GABA) influence on the neuron (Dr. Klyuchko O. M. experiments [11])

In framework of our assumptions few program models were developed and below we suggest some of them. For our model-1 we assume that in some cells of this screen there are bionic photosensitive elements [8], [11].

B. Assumptions of the model

For model design the following assumptions were done.

1. Each screen pixel can be in 3 states, the model color coded by "red", "yellow", "achromatic".

2. Actions of a pixel can be described by a model of the 4 phases. Nature of these phases corresponds to 4 defined states of protein molecules of channel-receptor complex (CRC) that contains channel of electrical current (phase description see further).

3. The demonstrational velocity of the model has been 60 times increased: one minute of real processes in nature (as recorded in the experiment), corresponds to 1 second model.

4. Image coding occurs by the establishing of a different color points set in a given time interval.

C. Description of bionic elements

As was mentioned above, the light-sensitive elements of the screen are bionic elements with variable of optical properties. According to our experiments these bionic elements may be following:

1. complex protein molecule and molecule optically active substance (fluorochrome).

2. "luminescent" neurons described in our article [11].

Our model is designed for the second version of the screen where optically active elements are the neurons with fluorochrome molecules inside. We have developed a model based on dynamic changes in the optical characteristics of the neurons that we described previously in [8, 11].

D. Dynamics of optical neuron characteristics changes in screen matrices

According to the results of the experimental neuron reaction studying, the receipt of the excitation signal can be represented as three consecutive phases that have their physical, biochemical and physiological sense. Three states on the model are colored with white (excitation is absent), red (excitation is maximal) and yellow (excitation intensity is of middle value) colors.

III. MODEL 1

Model 1 demonstrates the activity of quasi screen with neurons for the case when activated signal is inputted to active element at the left top of neuronal matrix and then is moved to the right bottom angle. We suppose that each active element of the screen may be activated with further relaxation. Below we describe these phases of activation and deactivation of each element.

1. The first phase of bionic elements activation - the period before all system activation. Initial time moment is t_0, inputted signal before activation is absent. Moment t_0 is characterized by signal amplitude $A = 0$, fluorescence intensity is going to zero (E_0). Such pixels are achromatic at our model (Fig. 2).

2. The second phase of bionic element excitation is at time moment (t_1). Interval $t_1 - t_0 = 20$ s. During system transition from the phase 1 to phase 2 the amplitude of activated signal – electrical current grows to the maximum $A = A_{max}$. Pixel luminescence is maximal (E_{max}). At model the neurons of this phase are marked by red color (Fig. 2).

3. Additional points are characteristic (middle points) for the excitation of bionic elements at time moment (t_2, t_3) Interval $t_2 - t_0 = 30$ s and time points near it. At these time points of activated signal the amplitudes of electrical currents are going to decrease (bionic element luminescence is decreased) $A = A_{\min}$. Pixel luminescence falls to minimal values ($E_{\min}$). At model elements of this phase are marked by yellow and orange depending on current amplitudes and intensity of luminescense (Fig. 2).

4. The fourth phase of bionic element activation is at time moment t_4. Interval $t_4 - t_0 = 180$ s. The phase is characterized by signal amplitude (electric current) $A = 0$, luminescence intensity is going to zero (E_0). These elements are achromatic at model too (Fig. 2).

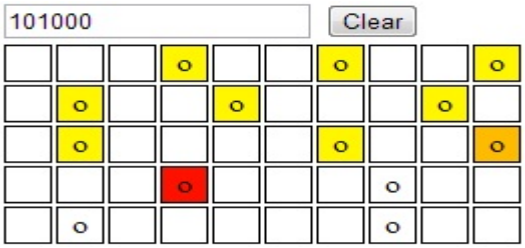


Fig. 2. Working model at 101th second from process start

At the screen on Fig. 2 the bionic elements are depicted by the circles at defined positions on screen matrix. This arrangement of bionic screen elements is determined by conditions in which the existence of bionic elements is possible under the experimental conditions. Working model at 101th second from process start is shown at Fig. 2. It is possible to see that one element is at the second phase, some other elements are at phase number three.

IV. Mathematic Model Of Activity Of 2D Neuron Assemble

Mathematic model of electric currents propagation in neuronal complexes are given below basing on [5]. Let's imagine this task as existing complex of active elements at planar 2D neuronal matrix. Signal of excitation here is going from a source as electric current that causes a number of concentric waves. Actually, such system is an artificial neuronal network where electrical currents carry excitation from one active element to another. Neuron by itself may be in 3 states: rested, excited, and refracted (analogously to the system at Fig. 2). At resting state a neuron may stay enough long if its transmembrane potential φ doesn't exceed some threshold φ_*. At moment when the potential become equal to φ_* neuron exceeds and exists in this state during time t_a, and then potential falls to "0". According to [5], if to define the "age" of neuron τ, as the time from the last excitation, the last condition may be written as

$$\varphi(\tau, t)|_{\tau=t_a} = 0, \quad (1)$$

where t is a current time. If $\tau > t_a$ neuron potential satisfies the condition

$$C\frac{d\varphi}{dt} = i - g\varphi(\tau, t), \frac{1}{2}, \quad (2)$$

where is $\tau = \tau(t)$; C is capacity, g is membrane conductance; i is summary synaptic current depended on the state of neighbors of studied neuron.

Let's suppose that the neuron threshold depends on its age $\varphi_* = \varphi_*(\tau)$, and $\varphi_*(\tau)$ is a monotonously decaying function τ, defined as $\tau > t_r$, where t_r is a refracted time. In area $\tau < t_r$, the neuron has unlimited threshold, and refracted time of this neuron is defined as the state with unlimited threshold. Variable t_r is an absolute refractivity when a neuron cannot be excited by any outer influence. Relative refractivity is described by the concrete type $\varphi_*(\tau)$. So, the neuron "lives" up to any maximal age τ_m, defined by equation

$$\varphi(\tau_m, t) = \varphi_*(\tau_m). \quad (3)$$

During the excitation a neuron "is" of age $\tau = 0$, and the cycle is repeated again. At this stage the different neuron states may be defined as:

1. $0 < \tau < t_a$ – the state of excitation;
2. $0 < \tau < t_r$ – the state of refractivity (absolute);
3. $\tau > t_r$ – the state of the rest or relative refractivity (equal notions).

Let's observe the interaction between the neurons and geometry of the links that define synaptic current. This current transmits the information signal from neuron to neuron in plane of 2D matrix in our constructed system (Fig. 2). If the velocity of nervous impulse spread is constant one, the delay in time will be r/υ, where r is a distance between the neurons; v is velocity of impulses.

Let's suppose that the current at defined synapse is $i_s(\tau_s)$ where τ_s is a time, calculated from the moment of excitable impulse income to a synapse. The distribution of neurons with the same number of parameters is $\eta = \{C, g, t_a, \varphi_*\}$, according to the age may be defined as $a_\eta(r, \tau, t)$, where r is coordinate in space. The number of synapses that reach one neuron from volume element dr' may be defined as $K(r, r')dr'$. For such a case [8], the synaptic current to neuron with coordinate (r) at moment t from neurons with parameters is:

$$di = f(\eta)d\eta\int dr\int d\tau_s a_\eta\left(r', t-\frac{|r-r'|}{v}, \tau_s\right) \times K(r,r')i_s(\tau_s), \quad (4)$$

where $f(\eta)$ is a density of neurons according to parameters. We suppose that φ_* may be defined by one or few parameters. If to find a sum in (4) according to all possible parameters, the synaptic current may be written as:

$$i(r,t) = \int d\eta\int dr'\int d\tau_s f(\eta)K(r,r')a_\eta \times\left(r', t-\frac{|r-r'|}{v}, \tau_s\right)i_s(\tau_s). \quad (5)$$

Expression of (5) is true only under the condition that duration of i_s does not exceed the maximal age. Let's suppose that $i_s(\tau_s)=0$ if $\tau_s > t_s < t_r$, so, "working time" of the synapse t_s is less than refractive time of any neuron. At the end of mathematic task formulation let's examine the distribution of changes of age. For the first, we can put a condition

$$a_\eta(r,t,\tau) = a_\eta(r,t-\tau,0),\ \tau<\tau_m, \quad (6)$$

For the second, if the total number of neurons is constant in time

$$\int_0^{\tau_m(\eta,r,t)} a_\eta(r,t,\tau)d\tau = 1. \quad (7)$$

After substitution (6) to (7) we obtain the equation for the density of neurons at initial age $a_\eta(r,t,0)$:

$$\int_{1-\tau_m(\eta,r,t)}^{t} a_\eta(r,t',0)dt' = 1. \quad (8)$$

Using (6) let's transform (5) into:

$$i(r,t) = \int d\eta\int dr'\int d\tau' f(\eta)K(r,r')a_\eta \times\left(r', t-\frac{|r-r'|}{v}-\tau', 0\right)i_s(\tau'). \quad (9)$$

Equations (2), (3), (8), (9) together with additional condition (1) describe the dynamics of neuron network completely, if respective initial conditions are put. Such conditions are defined by function $a_\eta(r,t,0)$, at enough large interval at the space $\{\eta, r\}$ [5].

V. Model 2

This model we have presented previously in [8], [11], and above, it is a prototype for our novel program model. Next step of model development is to state that activated neurons in some positions mean some symbols. The same phenomena may be basic for images recognition by natural brain, and in technical systems it may be used also. Figures 3 – 5 demonstrate how symbols CIRCLE and TRIANGLE may be coded in framework of our assumptions.

At initial phase of model function all neurons in all positions are not active: electrical currents are absent and luminescence is absent also. The second phase of model functioning is demonstrated on Fig. 3. Neurons only on first 13 positions are active (the first and partially the second line). It means that electric currents in them are present and luminescence is present also. Values of electric currents amplitudes and intensity of neuron luminescence are described in [8], [11], [14]. Only one neuron at 13 positions demonstrates maximal values of electric current amplitudes and intensity of neuron luminescence. This order of maximally luminescent neurons is coded by the CIRCLE.

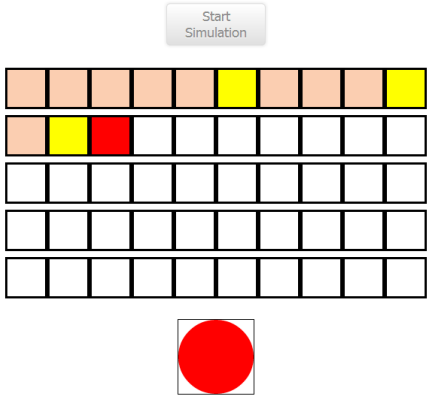


Fig. 3. Phase of the circle coding (explanation see in text)

On Figure 5 the third phase of model functioning is demonstrated (phase of triangle coding 1). Again, similarly to the previous case, the neurons at first 14 positions are active (the first and partially the second line). It means that electrical currents in them are present and luminescence is present also. The values of electric currents amplitudes and intensity of neuron luminescence are described in [8], [11]. Two neurons in positions 10 and 14 demonstrate maximal values of electric current amplitudes and intensity of neuron luminescence. But in this case this phase is coded by the TRIANGLE. On Fig. 5 the fourth phase of model functioning demonstrated (phase of triangle coding 2). Neurons at all 50 positions are active (all lines and columns). It means that electrical currents in them all are present and luminescence is present also. As in cases of Figs 3 and 4, the values of electric currents amplitudes and intensity of neuron luminescence are described in [8], [11]. Two neurons in positions 13 and 17 demonstrate maximal values of electric current amplitudes and intensity of neuron luminescence. This phase is also coded by the TRIANGLE.

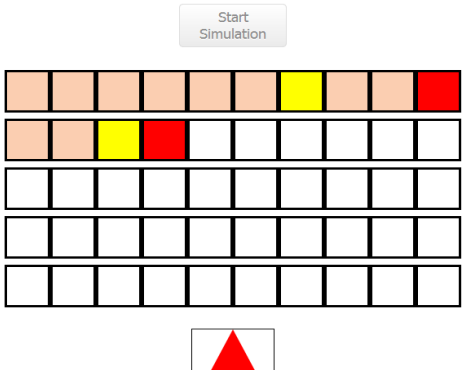


Fig. 4. Phase of triangle coding 1 (explanation see in text)

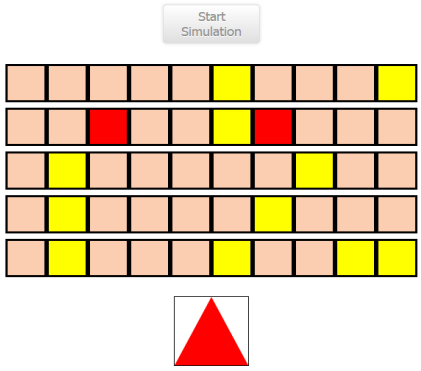


Fig. 5. Phase of triangle coding 2 (explanation see in text)

Difference between TRIANGLE 1 and TRIANGLE 2 is in fact that two active neurons are coding triangles, independently on activity of all other neurons in all other 48 positions.

Conclusions for II-V

1. Program model of 2-dimential neuron matrix functioning is developed (model 1).
2. Some assumptions of presented program models may be followed by previously developed mathematic models [5].
3. Program model symbols coding by 2-dimential neuron matrix is developed (model 2). In developed original model of biotechnical system two figures: triangle and circle may be coded (model 2).
4. Systems which may be described in such a way potentially are systems with "memory" if system can stay in some of the states longer than in other states. Thus, the proposed model can be extended for modeling the screen with elements that have properties of memory.
5. The same phenomena may be basic for images recognition by natural brain, and in technical systems it may be used also.

VI. Model Of Chemosensitive Channel-Receptor Complex

The next model is important for the studying of the influence of some industrial chemical pollutant on cell molecular structures; that is why such model is useful in the set of software for ecomonitoring system we wrote at the beginning. It is known that after the activation of membrane chemosensitive channel-receptor complex (Ch-CRC) by agonist the transmembrane electrical currents are initialized. That is why such molecular structures are called sometimes "current nano-generator of Ch-CRC type". Membrane in brain cells is dotted by approximately 18- to 40 thousands of channel-receptor complexes (CRCs), inquired into the membrane. Principles of their performance are following.

1. While the CRC maintained in state of rest it doesn't let ions come across through the ionic channel. In order to make the ionic channel let the flow of ions come across it the agonist is needed to be attached to the CRC`s receptor.
2. The generation of ionic currents is useful for the propagation of action potentials, and requires the movement of significant numbers of ions across the membrane in a relatively short period of time. The rapid rate of ionic flow occurring during the generation of an action potential is far too high to be achieved via an active transport mechanism. Rather it results from the opening of ion channels.
3. An agonist is a chemical that binds to a receptor of a cell and triggers a response by that cell.
4. Antagonist is a type of receptor drug that does not provoke a biological response itself upon binding to a receptor, but blocks or dampens agonist-mediated responses. For the activation of Ch-CRC its interaction with agonist is necessary that is followed by electric current appearance. On Fig. 6 the realization of functions of Ch-CRC (nano-generator) is shown in dynamics. Let's make some explanations to this program model. On the base of this model information from other publications presented above is put as well as results of original experiments. Curves with results of original experiments one can see at the centre of Fig. 6. There are demonstrated the results of Ch-CRC activation by agonist kainate (KK) that caused the influx of non-inactivated inward current (on example of receptor of glutamate). At the second stage KK-activated current is blocked by JSTX-3 – specific substance (phenol derivative with polyamine radical) with well-known toxic activity [7]. JSTX-3 decreases maximal amplitudes of inward electric currents to minimal values (but not to zero). At the third stage JSTX-3 is removed from Ch-CRC and KK-activated electric current amplitude increased (but not to the primary values!). Main stages of these processes one can see as 4 pictures around recorded experimental results. Indeed, expressions of these functions are similar to ones of "generator" – but biological "nano-generator". Performances of these processes permit us to see in dynamics all

stages of Ch-CRC; block of KK-activated currents permit us to control of "nano-generator" at molecular level. Mathematic model of this phenomena is given in [8], [11].

Conclusions for VI

Original program model of molecular nano-generator functioning for electro-activated channel-receptor molecular complex (Ch-CRC) is described. Performances of its functioning permit us to see all stages of Ch-CRC in dynamics. Block of KK-activated currents by toxin JSTX-3 permit us to control the functioning of this "nano-generator" at molecular level.

Program model permits us to see functioning of Ch-CRC (nano-generator) in dynamics. Main four stages of these processes one can see as four pictures around recorded experimental results on Fig. 6.

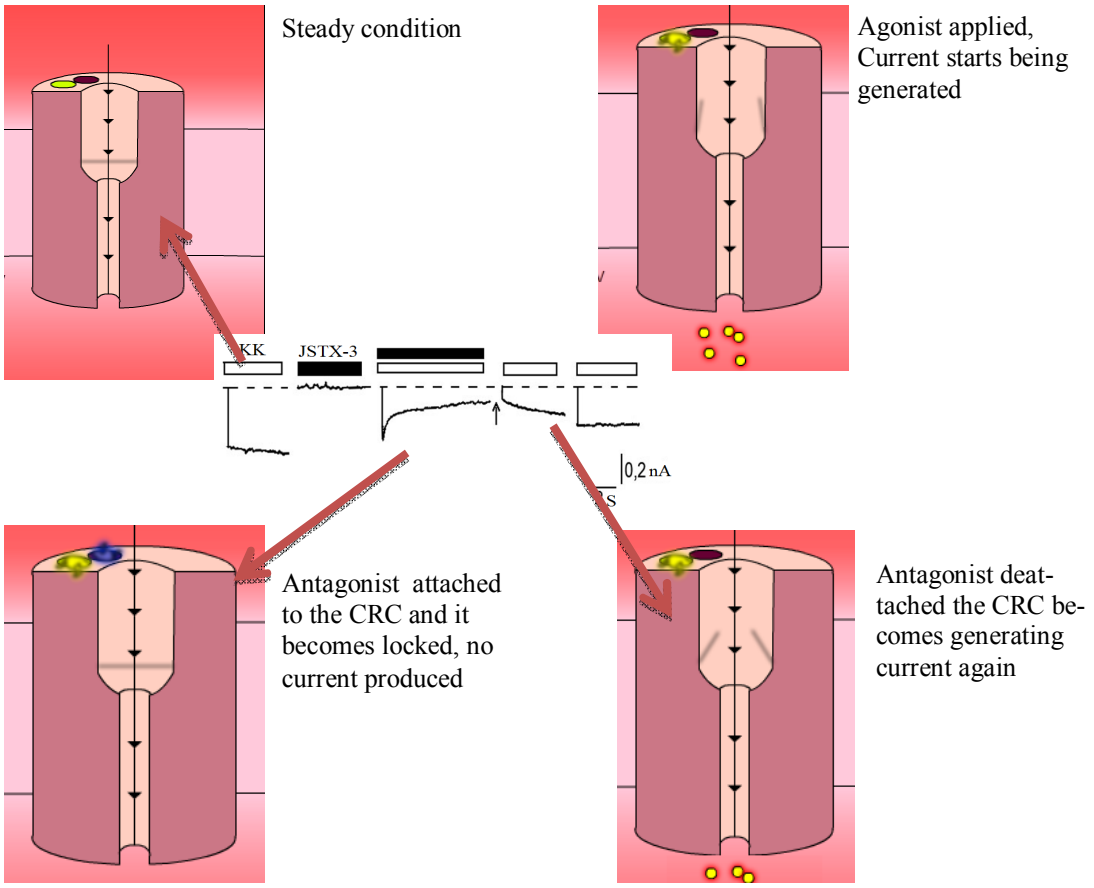


Fig. 6. Program model of Ch-CRC (nano-generator) performance in dynamics. Four phases of its action are shown (explanation see in text)

CONCLUSIONS

Some program models are described in present article. They were elaborated for the software kit of technical system for ecological monitoring "EcoIS". One of "EcoIS" subsystem is a device for testing of chemical substances as well as possible industrial pollutants. This subsystem is analogous to devices developed previously for biophysical laboratory investigations of transmembrane electrical currents. The influence of different chemicals on such currents may be studied; such data may be monitored reflecting the state of ecology in polluted area. Subsystem is supplied by original software, some of program models reflect biophysical phenomena.

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О. М. Ключко, В. М. Шутко, Д. О. Навроцький, А. М. Миколушко. Набір програмних моделей для технічної системи екологічного моніторингу, що базуються на принципах біофізики
Описано набір програмних моделей для технічної системи екологічного моніторингу. У цьому наборі представлено моделі, розроблені на базі результатів досліджень біофізичних ефектів впливу деяких технічних забруднювачів на клітини живих організмів.
Ключові слова: технічна система; екологічний моніторинг; трансмембранний електричний струм; програмна модель; хімічний забруднювач.

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Напрям наукової діяльності: біофізика, науки про мозок, біоінформатика, екологія.
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Е. М. Ключко, В. Н. Шутко, Д. А. Навроцкий, А. Н. Миколушко. Набор программных моделей для технической системы экологического мониторинга, базирующиеся на принципах биофизики

Описан набор программных моделей для технической системы экологического мониторинга. В этом наборе представлены модели, разработанные на базе результатов исследований биофизических эффектов воздействия некоторых технических загрязнителей на клетки живых организмов.

Ключевые слова: техническая система; экологический мониторинг; трансмембранный электрический ток; программная модель; химический загрязнитель.

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