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COMPUTER SIMULATION OF BIOCHEMICAL PROCESSES OF THE K-NA PUMP IN HUMAN KIDNEY NEPHRON

The development of information technologies and their application in modern medicine facilitate the work of medical workers. Visual visualization of human organs through their computer model. More detailed study of the processes occurring in them. This article deals with the model of the K-Na nephron pump of a human kidney, which shows its work and functions in regulating blood pressure and salt composition of human blood. The investigated mechanism of operation of the K-Na pump, the biochemical processes occurring in the body, leading to the action of the K-Na pump, considered algorithms in the construction of a computer model. This makes it possible to consider in more detail and study the basic processes of the human kidney.

Keywords: K-Na pump, information technologies in medicine, computer modelling, biochemical processes, bioinformatics.

Introduction. Computer modeling of biochemical processes in human organs in its everyday life on the basis of mathematical and biochemical methods for describing similar processes and a library of various patterns of changing the conditions of their flow on the basis of various scenarios for the development of the environment and the various influences of their nature constitute the subject of research and are the main goal of this article. The use of computer modeling helps to present the mechanism of operation of the studied object, its interaction and the basic biochemical reactions occurring at a certain point in time. The proposed article is a continuation of research into the processes occurring inside the kidney [1-4].

Algorithm and methods. The main objective of the study is to design a technology for visualizing the course of the physico-chemical and chemical-biological processes of the human kidney, as well as to consider the mechanism of operation of the K-Na pump inside the nephron of the kidney. To study this process, you need:

1) to study the mechanism of operation of the pump and to investigate its basic functions;
2) investigate the causes of the pump operation.

One of the many important functions of the K-Na pump is the regulation of blood pressure by monitoring the juxtaglomerular apparatus of the salt composition of human blood. Without the functioning of such a pump, most nephron cells will be destroyed, which is the cause of human diseases. Due to the increase in the Na content in the blood, the K-Na pump is automatically activated, which ensures removal of even more Na ions from the cell together with water. The main stages can be described as follows:

1. As a result of phosphorylation of the molecule, ADP is released from the active site and returns to the cytoplasm.
2. Phosphorylated protein passes into a state where sodium ions are inaccessible for metabolism, occluded.
3. The transition of the enzyme to the next stage is activated by magnesium ions. Its effect is to accelerate the transition of the phosphorylated enzyme from the sodium conformation to the potassium conformation. The transfer of sodium through the membrane is carried out synchronously with the conformational transition. As a result, sodium ions dissociate from the enzyme on the other side of the membrane, where potassium ions bind to the same center.
4. Potassium is subjected to the same occlusion as sodium, in the course of this process, the transfer of potassium ions through the membrane takes place.
5. Phosphate is available for attack by a water molecule. Water hydrolysis and the release of inorganic phosphate into the intracellular environment occur.
6. After this, potassium ions also dissociate from the binding center, releasing into the cytoplasm. Their place is occupied by sodium. The last stage of the cycle simultaneously prepares the enzyme to start a new cycle.

This is the active transport of sodium ions from the cell and potassium into the cell, and the energy of ATP is spent on paying for the transition of the enzyme from one conformation to another. [5] In total, one positive charge is removed from the cell in one cycle. Thus, the K-Na-pump is electrogenic. Transport protein performs this operation at a high rate: from 150 to 600 sodium ions per second.[6]

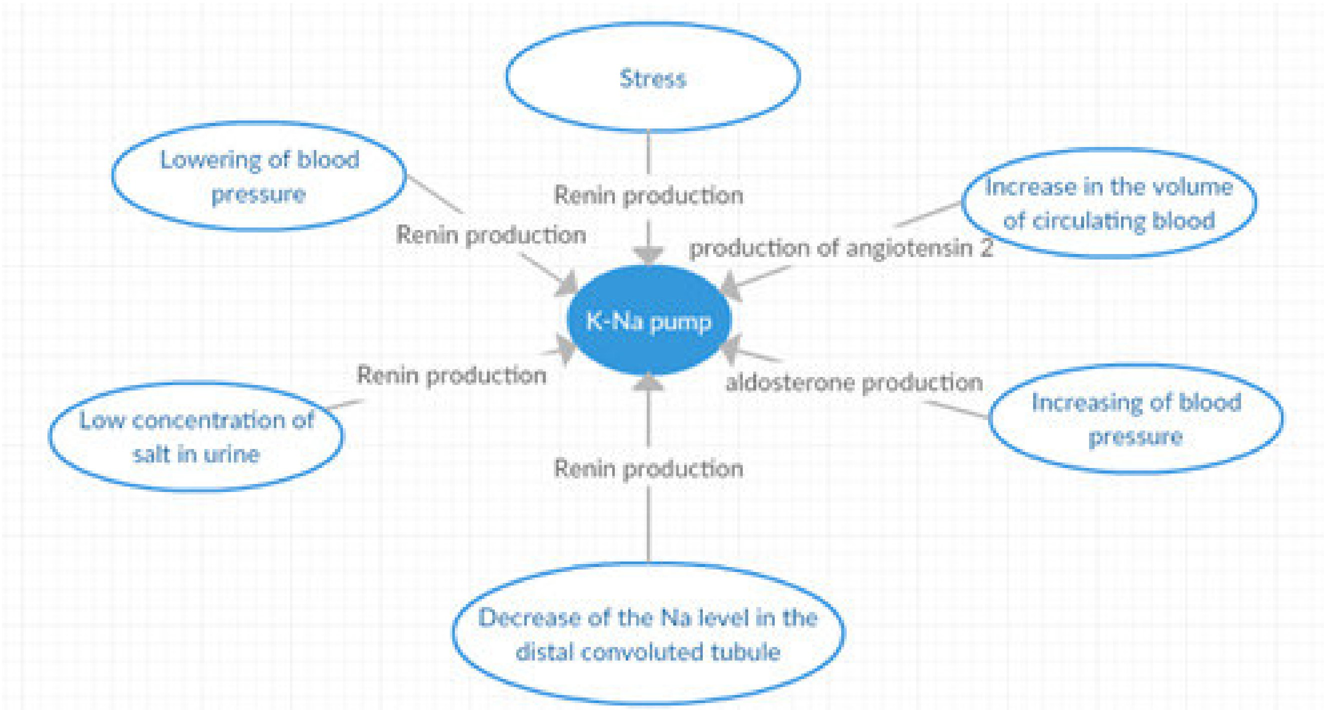

Figure 1. Influence of external factors on the operation of the K-Na pump

To study the reasons for the onset of the operation of the K-Na pump, it is necessary to consider the processes of action of the renin-angiotensin-aldosterone system, which is triggered by the production of renin in juxtaglomerular kidney cells. There are several mechanisms of stimulation of renin production:

1) It works if the intake of sodium ions in the distal convoluted tubule decreases;

2) Yuxtaglomerular cells are baroreceptors, they perceive the stretching of the walls of arterioles, and accordingly react to pressure reduction by renin production;

3) Yuxtaglomerular cells are innervated by the sympathetic nervous system, and as soon as they receive a signal, they immediately begin to synthesize an enzyme that promotes increased pressure. That is why under stress, psychoemotional stress arises hypertension.

Then the renin enters the bloodstream. There, it acts on the glycoprotein angiotensinogen, produced by the liver. Thus, angiotensinogen is converted into angiotensin I. Under the influence of angiotensin converting enzyme (ACE), the dipeptide is split off in angiotensin I, and it becomes the most potent vasoconstrictor - angiotensin II. In addition to causing spasm of smooth muscles, it stimulates the synthesis of aldosterone. This hormone, produced by the adrenal glands, retains sodium ions and water, removes potassium and enhances the synthesis of ATPase by acting on DNA, while stimulating and starting the process of K-Na pump operation. [7]

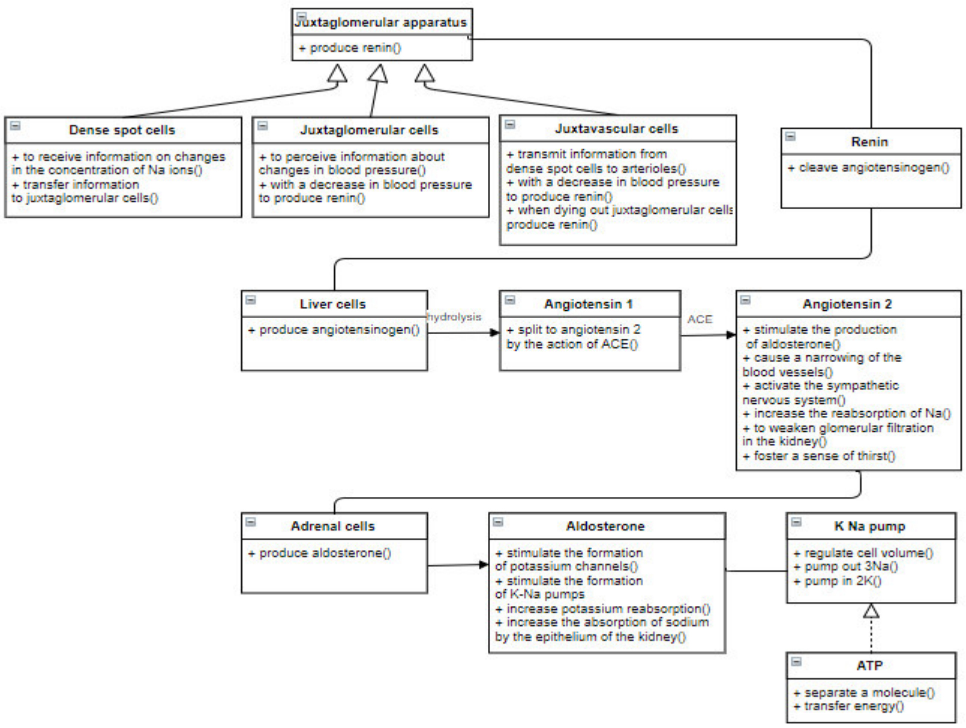

Figure 2. Renin-angiotensin-aldosterone system

Conclusion. The proposed article describes methods for describing various processes using the example of the functioning of the K-Na nephron pump of a human kidney. This article contains the results of a study on computer modeling of the chemical-biological processes occurring in a nephron as a result of the operation of a K-Na pump. The reasons for the K-Na work of the kidney nephron pump, the mechanism of its work are considered.

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