## UDK 547.854.5 DEVELOPMENT OF PH SENSITIVE MATERIALS BASED ON BARBITURIC ACID KNOEVENAGEL CONDENSATION REACTION Nebalueva A.S. (ITMO University), Timralieva A.A. (ITMO University), Shilovskikh V.V. (ITMO University), Skorb E.V. (ITMO University) Scientific Supervisor- Prof. Dr. Skorb E.V. (ITMO University)

Abstract. Nowadays there is an enhanced development of new functional materials for application in different fields. In our research we modified barbituric acid with vanillin and ethylvanillin for further using as pH controlled functional molecules with suspected bactericidal properties.

Currently the synthesis of new functional materials with properties switching under mild conditions and resistant to external influences is a raising trend in chemistry. Barbituric acid is the one of widely known model molecules for the synthesis of substances with bioactivity. It has an active methylene group located at the C-5 position in molecule. This position is a reaction center and can be easily involved in condensation reactions with aldehydes or ketones that do not contain an  $\alpha$ -hydrogen. This general type of reaction is known as the Knoevenagel condensation reaction. Knoevenagel condensation is an important and widely used method for the formation of carbon-carbon bonds in organic synthesis with numerous applications in the synthesis of carbocyclic and heterocyclic compounds of biological significance. In our research we use vanillin and ethylvanillin as aldehydes. The advantages in favor of these components are their good solubility in water and safety for human body, which allows us to obtain molecules of new substances that are safe for bio-use with suspected bactericidal properties.

The aim of our work was to study the reaction of vanillinbarbiturate and ethylvanillinbarbiturate, as well as to consider the influence of external factors on 5-(4-hydroxy-3-methoxy-benzylidene)pyrimidine-2,4,6-trione and 5 - (4-hydroxy-3-ethoxy-benzylidene)- pyrimidine-2,4,6-trione. We chose the reaction of vanillin and ethylvanillin with barbituric acid, since the reaction of colorless vanillin or ethylvaniline and barbituric acid forms a colored 5-(4-hydroxy-3-methoxy-benzylidene)-(4-hydroxy-3-ethoxy-benzylidene)-pyrimidine-2,4,6-trione, pyrimidine-2,4,6-trione or 5 respectively, which means that the reaction can be judged by the color intensity of the solution. So, the tracked sign of the passage of synthesis is the change of color from colorless to bright yellow. During the study, it was found that under the influence of alkalis, the resulting substances change color from yellow to red. Using absorption spectrophotometry, the appearance of a peak in the longwave region was observed, which correlates with visible observations. Moreover, the existence of four forms of 5-(4-hydroxy-3-methoxy-benzylidene)- pyrimidine-2,4,6-trione was revealed by spectrophotometry methods depending on the degree of protonation.

Thus, molecules of substances with pH controlled functional molecules were obtained, which, when confirming the bactericidal properties of one and/or several forms of the existence of molecules, leads to the creation of functional materials, including "smart skin" applications.

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