

## USING OF PyMOL PROGRAM IN THE EDUCATIONAL PROCESS

**Barabash A.L., Chuk O.A.**

*National Aviation University, Kyiv*

*Scientific adviser – Baranovskyy M.M., Dr.Sc. (Agriculture), Prof.*

An indispensable condition for the training of highly qualified biotechnologist is the formation of students' ability to use modern information technologies. Recently, molecular modelling in specialized software packages is widely used in the field of biotechnology. PyMOL program is one of those system, where it is possible to create high-quality three-dimensional images of both small molecules and biological macromolecules, primarily proteins. Moreover, about a quarter of all images of protein structures published in the scientific literature were made by the use of PyMOL [1].

In the second semester of the 2020-2021 academic year, students of the Biotechnology Department of NAU had the opportunity to study the facultative course “Antibiotics: Molecular Mechanisms of action and Biotechnology” in English from Dr. Matthias Höhne as the part of international cooperation with University of Greifswald, Germany. Each lecture was accompanied by a demonstration of the practical use of the PyMOL software environment for molecular modelling of the mechanisms of action of antibiotics. Features of PyMOL software allow you to build a molecular model of antibiotics and predict their physical and chemical properties. These functions are integral components of the development of new drugs and the development of science in general.

It is important to have basic theoretical knowledge before using of PyMOL program in such disciplines as: organic chemistry, biochemistry, physics, pharmacognosy etc. Therefore, to introduce the use of molecular modeling in the educational process is possible in 3-4 courses.

The use of PyMOL software significantly helps to learn biotechnology interactively and retain information more effectively. It should be mentioned that PyMOL software is distributed under a license.

Summarizing the information about the tools of the PyMOL software environment, we can define such ways of its application in educational process:

1. Creating three-dimensional models of drugs;
2. Forecasting mechanisms of molecule action;
3. Gain skills in developing illustrative material for scientific publications.

### **Reference:**

1. Rachel E. R., Alison B. P. Using the PyMOL application to reinforce visual understanding of protein structure. *Biochemistry and molecular biology education*. 2016. Vol. 44, Is. 5. P.433-437. URL: <https://doi.org/10.1002/bmb.20966>