DETERMINATION THE QUANTITATIVE "STRUCTURE – ANTIBACTERIAL ACTIVITY" RELATIONSHIPS IN A SERIES OF NSUBSTITUTED AMINO ACIDS

Dudka K. I.

Scientific Supervisor: assoc. prof. Golik M. Yu., assoc. prof. Kolisnyk O. V. National University of Pharmacy, Kharkiv, Ukraine kolisnikov1@gmail.com

Introduction. The presence of the antibacterial and antifungal activity in derivatives of amino acids is determined by different mechanisms; therefore, a promising field of research is to obtain new N-substituted amino acids and study their antibacterial action.

Aim. To determine the quantitative "structure – antibacterial action" relationships in a series of N-substituted amino acids.

Material and Methods. The quantitative dependencies of the antibacterial action of the compounds studied on AlogPs values were calculated using the STATISTIKA 8 program.

Results. The satisfactory values of the levels of correlation of AlogPs parameters calculated with the experimental data of the antibacterial activity of N-substituted amino acids against *S. aureus*, *E. coli*, *P. vulgaris*, *P. aeruginosa*, *B. subtilis*, and *Cl. perfringens* are statistically significant. The absence of the relationship between the antibacterial effect against *C. albicans* and the structure of threonine derivatives may indicate a possible role of the latter in the metabolism of these fungi.

Conclusions.

- 1. To determine the quantitative "structure antibacterial action" relationships the correlation and regression analysis of the AlogPs values calculated for N-substituted amino acids taking into account the results of the experimental study of the antibacterial action of the compounds under research has been conducted.
- 2. The statistically significant correlation values of AlogPs with the values of the antibacterial action of N-substituted amino acids against *S. aureus*, *E. Coli*, *Pr. Vulgaris*, *P. Aeruginosa*, *B. Subtilis*, *C. Albicans* and *Cl. perfringens* have been determined, and it quantitatively confirms the earlier assumptions of the existence of the "structure–action" relationship in this series of compounds and the degree of its manifestation.