## Науково-практична міжнародна дистанційна конференція, Мікробіологічні та імунологічні дослідження в сучасній медицині, 22 березня 2024 року, Харків

needed to elucidate the specific mechanisms underlying the antibacterial activity of linden honey.

Our study demonstrates the significant antibacterial efficacy of natural linden honey against several *E. coli* strains *in vitro*. This finding highlights the potential of linden honey as a natural antimicrobial agent against bacterial pathogens. We observed variations in the antibacterial activity of different samples of linden honey against the tested *E. coli* strains. These differences can be attributed to variations in the botanical and geographical origin of the honey samples, as well as differences in their chemical composition. These findings contribute to our understanding of the therapeutic potential of linden honey as a natural antimicrobial agent and pave the way for its further exploration in clinical settings.

## VIRTUAL STUDY OF THE POTENTIAL OF ACTIVITY AGAINST P.AERUGINOSA IN THE SERIES OF [3-(2-METHOXYETHYL)-4-OXO-3,4-DIHYDROQUINAZOLIN-2-YL]THIOACETIC ACID DERIVATIVES Idoumghar W.

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**Introduction.** Pseudomonas aeruginosa can infect patients with impaired barriers against bacterial invasion or immunodeficiency and is prone to the rapid formation of antibiotic resistance. Undoubtedly, interesting ways to overcome antibiotic resistance are exposure to new protein targets, effective inhibitors of which, if created, may even form a new class of antibiotics. Bacterial TrmD, which has critical differences from its ortholog in eukaryotes and archaea, is attractive in this regard and may serve as a target for the development of inhibitors with antimicrobial properties. The work was carried out under the supervision of prof. Vlasov S.V. at the department of pharmaceutical chemistry (NUPh). The aim of our work was to analyze the potential of antimicrobial activity as the new possible antibiotics for quinazolones modified at position 3 with methoxyethyl fragment through the mechanism of inhibition of TrmD.

**Materials and methods**. The structures of the compounds were drawn using ACD/ChemSketch (freeware) and saved in .pdb format using Discovery Studio Visualizer 2021. AutoDockTools-1.5.7 was used to convert .pdb files to .pdbqt, the number of active rotatory bonds was set by default. AutoDock Vina was used to calculate molecular docking. Discovery Studio 2021 was used for visualization. Biotarget macromolecule was selected from Protein Data Bank (Protein Data Bank): PDB ID – 5ZHN.



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**Results and their discussion**. As a result of docking studies in the active site of TrmD isolated from *P. aeruginosa* for [3-(2-methoxyethyl)-4-oxo-3,4-dihydroquinazolin-2-yl]thioacetic acid derivatives, it was found that the best binding parameters were typical for benzyl amide of this acid. However, the pose in the active site of the benzyl derivative was the most similar of that to the native ligand.

**Conclusions**. According to docking simulation to TrmD isolated from *P*. *aeruginosa*, it was revealed that *N*-benzyl-2- $\{[3-(2-methoxyethyl)-4-oxo-3,4-dihydroquinazolin-2-yl]thio}$  acetamide can be the antibacterial agent (active agains *P*. *aeruginosa*) with an innovative mechanism of action.

## IMMUNOLOGICAL AND GENETIC TESTS FOR THE DIAGNOSIS OF BLOOD-BORNE INFECTIOUS AGENTS IN DONORS OF BLOOD AND BLOOD COMPONENTS

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Research into blood-borne infectious agents is the basis for the safety of blood and blood component transfusions. The first research in this area was carried out in the 1970s and concerned the determination of the Hbs antigen by immunological methods. In 1981, a-HIV tests were introduced, followed by a-HCV tests in 1992. In 2002, molecular biological methods were introduced into blood donation, allowing the detection of the genetic material of the HCV virus, and in 2005, the HBV and HIV viruses were introduced [Grabarczyk and Tkaczuk, 2016]. Blood samples for testing for infectious agents are taken from the same injection site from which the donation was made, during or after the donation, in disposable vacuum tubes, and negative test results are the basis for qualifying blood and its components for clinical use [Grabarczyk and Sulkowska, 2023].

In most countries of the world, blood and blood component donors are tested for markers of HBV, HCV, HIV and spirochete infection. Markers for other infectious agents are only tested in a few countries, e.g. in Japan, the USA, France and the Netherlands, donors are tested for HTLV virus, in the USA and Canada for West Nile virus infection and for the protozoan *Trypanosoma cruzi*. In Colombia, donors are tested for brucellosis, and many countries test for the presence of a-CMV antibodies [Korsak and Łętowska, 2009].

Blood donors are screened using immunological techniques, which detect antibodies to the infectious agent (a-HCV, a-HIV) or antigens (a-HBsAg, a-p24), and

