МЕДИЦИНСКИ УНИВЕРСИТЕТ - ВАРНА
„Проф. д-р Параскев Стоянов“
Ул.“Марин Дринов“ 55, Варна 9002, България
Тел. : 052/ 65 00 57, Факс: 052/ 65 00 19
e-mail: uni@mu-varna.bg, www.mu-varna.bg

MEDICAL UNIVERSITY - VARNA
“Prof. Dr. Paraskev Stoyanov”
55, Marin Drinov Str., 9002 Varna, Bulgaria
Tel.: +359 52/ 65 00 57, Fax: + 359 52/ 65 00 19
e-mail: uni@mu-varna.bg, www.mu-varna.bg

Fund “Nauka” Project № 25001 Resume – Competition-based Session 2025:
“Predictive *in silico* modeling of natural molecules to support public health”
Project leader: Assoc. prof. Silviya Georgieva Mihaylova, PhD

Modern *in silico* methods represent an effective tool for predicting the pharmacological activity of novel molecules while simultaneously significantly reducing the time and costs associated with drug development. These approaches are particularly important in the study of natural products, which constitute a valuable source of bioactive compounds with demonstrated antimicrobial, anti-inflammatory, neuroprotective, and other biological properties. Despite their high potential, the chemical diversity and complex composition of natural products necessitate the development of new analytical strategies for their systematic evaluation, prioritization, and integration into the drug design process.

The present project aims at the development and validation of an integrated *in silico* approach based on state-of-the-art machine learning (ML) and deep learning (DL) methods for the prediction of the biological activity of molecules of natural origin.

The main objectives include a systematic review and the construction of a database of structural and pharmacological characteristics of natural compounds; the development and validation of machine learning and deep learning (ML/DL) models for activity prediction; and the evaluation of the applicability of these models to socially significant diseases associated with chronic inflammatory and neurodegenerative processes, as well as to major public health challenges.

The expected outcomes include the development of a database containing key structural and pharmacological characteristics of molecules of natural origin; the creation of a software tool to predict their biological activity; the identification of potential molecules for the prevention of socially significant diseases, including multidrug-resistant bacterial infections, chronic inflammatory conditions, and neurodegenerative processes; and the development of a methodology for integrating natural sources and artificial intelligence into the drug design process.

The project will make a scientific contribution through the development and validation of novel predictive models, as well as a practical impact by accelerating the discovery of new bioactive compounds. Long-term, the results are expected to support the development of safer and more effective therapies, thus exerting a direct positive impact on public health.

Expected results:

1. Scientific Outcomes

- A developed and systematically structured database of natural molecules exhibiting antimicrobial, anti-inflammatory, and neuroprotective activity;
- Developed and validated machine learning (ML) and deep learning (DL) models for the prediction of the pharmacological activity and pharmacokinetic profiles of natural compounds;
- Identification of novel potential molecular candidates for inclusion in the treatment of multidrug-resistant infections, chronic inflammatory diseases, and neurodegenerative disorders.

2. Applicable Outcomes

- Development of recommendations for priority molecules suitable for subsequent experimental and clinical studies;
- Creation of a methodological framework for the application of AI-based *in silico* technologies in drug design from natural sources;
- Preparation of scientific publications based on the results obtained.

3. Educational Outcomes

Training and professional development of undergraduate students, doctoral candidates, and early-career researchers in the interdisciplinary field of bioinformatics. The project activities will provide opportunities for researchers to expand their knowledge and acquire practical experience, which will support the development of educational modules and seminars on the application of artificial intelligence in drug design for students enroled in the “Assistant Pharmacist” programme.