Komarovska-Porokhnyavets O.Z., Vasylyuk S.V., Petrina R.O., Gubrii Z.V., Fedorova O.V., Havryliak V.V., Shved O.V., Novikov V.P.
Lviv Polytechnic National University, Department of Technology of Biologically Active Substances, Pharmacy and Biotechnology, Lviv, Ukraine
volodymyr.p.novikov@lpnu.ua

DISSEMINATION OF KNOWLEDGE OF SOCIETY ABOUT THE WAYS OF ENVIRONMENT PROTECTION

Проведен сравнительный анализ использования альтернативных биотехнологических методов при экспериментальных исследованиях биологической активности синтезированных субстратов, при проведении процессов биоочищения и утилизации лабораторних отходов. Для прогнозирования биологической активности была использована компьютерная программа PASS. Для прогнозирования острой токсичности использовалось компьютерное обеспечение GUSAR. Оптимизированы исходные вещества для синтеза антибактериальных соединений для защиты от загрязнений и патогенных инфекций.

The necessity of dissemination of knowledge about biosafety during research in the field of biotechnology and bioengineering was substantiated.

Ключевые слова: биобезопасность; прогнозирование биологической активности; биологически активные субстанции.

Keywords: biosecurity; prognostication of biological activity; biologically active substances.

Introduction. The current state of research projects and commercial biotechnology in Ukraine on the development of gene therapy, stem cell therapy, and the level of development of biotech production, especially in the industrial and agro-biotechnology sector, requires new innovative ways to enter into safe study, investigation, production, consumption and the use of biotech products and the application of cell manipulation and biosecurity advanced technologies. The achievements of cellular and genetic bioengineering are sometimes the source of social fears, the subject of polar discussions and protests, which in the history of industrial society will not be found in another industry because of possible bio-threats in the unprofessional or criminal use of its achievements.

The purpose of the work. To disseminate a knowledge about biosecurity in various experiments on determination of the biological activity of synthesized substances and plant extracts, carrying out the bio-clearing process through complex microbial and phytoremediation, growing of callus masses for obtaining biologically active regulators and biostimulants, as well as possible microclonal reproduction of rare plant species, as well as utilization of laboratory drains taking into account the principles of stage development.

The results of work. Conducting educational activities and investigation in biotechnology and bioengineering, as well as pharmaceutical technology, provides students with an understanding of the specifics of safety standards observance during experiments, which we have taken into account when developing profiles of educational programs for training specialists and professionals in pharmacy, biotechnology, and bioengineering at Bachelor's, Master's and doctoral levels in higher education. In the educational process, our main task is to inform students about the need to adhere the bioethical and bio-safe principles in the scientific and industrial field, the introduction of basic principles of bio-protection regulation in the field of biotechnology, and the use of materials and methods that can cause unforeseen dangers of dual-use and negative affect human and environmental safety [1].
The main areas of the Department's work is to find biologically active substances as the basis for medicinal preparations and plant protection products, for the production of biologically active additives, the development of a technology for the restoration of water and soil ecosystems, the study of callus genesis for micropropagation of rare plant species [2]. In recent years, approaches to

the selection of structures for purposeful synthesis have been considerably expanded, based on mathematical models that allow establishing a relation between the structure of molecules and their biological action (Methods for Structure-Activity Relationships (SAR), Quantitative Structure-Activity Relationships (QSAR)). Most computer methods of molecular modeling and relationships analysis are used to study the interaction of the "ligand-receptor" and to optimize the properties of the basic structures formed on the analysis of the quantitative ratios "structure-activity" within a single chemical class.

In order to predict the biological activity of synthesized compounds that can be used to protect materials from biodeterioration, as growth stimulators for technical agriculture, the PASS program (Prediction of Activity Spectra for Substances: http://www.pharmaexpert.ru/ PASSOnline/) was applied [3].

This program makes it possible to determine the relationship between "structure-activity" for substances from a training sample containing substances of known drugs and biologically active compounds and on the basis of structural formula of chemical compound predict their probable type of biological activity, taking into account the main and secondary pharmacological effects, mechanisms of action, mutagenicity, carcinogenicity, teratogenicity and embryotoxicity [3].

According to statistical calculations, the average accuracy of the forecast for the PASS program is about 85 %, which is enough to apply it in practice to predict the spectrum of biological activity of new substances [3]. An important characteristic of the new medical, veterinary and agro products is an assessing their acute toxicity in laboratory animals. However, such experiments are quite expensive; in addition, they are constantly criticized for ethical reasons.

The European Community Guidelines for Chemicals and Safe Use (REACH), starting in 2007, provide for the development of computerized methods for analyzing the relationship between "structure-activity" and the study of toxic effects. Therefore, scientists of the Institute of Biomedical Chemistry of the Russian Academy of Medical Sciences developed a new method for the simulation of acute toxicity in rodents QSAR, implemented in the software GUSAR [4].

Using the free available web service (http://www.pharmaexpert.ru/GUSAR/AcuToxPredict/), we can predict the acute toxicity of synthesized compounds for rats. The most promising candidate-substances selected with PASS and GUSAR services are investigated for their predicted biological activity, which promotes the rapid application of new, effective, environmentally safe substances.

Conclusions. The combination of methods for predicting biological activity of *in silico* and microbiological testing *in vitro* in the framework of the scientific work of our Department made it possible to optimize the base compounds, improve their activity, and determine the specificity of their action, as a result, to offer effective antibacterial substances for protection against contamination and pathogenic infections.

References

1. Інформаційно-інтеграційні підходи до якості освіти згідно з принципами екобіотехнологій/ І. І. Губицька [та інш.] // Актуальні проблеми синтезу і створення нових біологічно активних сполук та фармацевтичних препаратів : матеріали доп. та зб. наук. ст. нац. наук.-техн. інтернет-конф. з міжнар. участю, 23–25 квіт. 2013 р. Львів, 2013. С. 98–102.
2. *Стадницька Н. Є., Швед О.В., Червецова В.Г., Монька Н.Я., Лубенець В.І., Новіков В.П.* // Збірник наукових праць IX з'їзду УТГіС «Досягнення і проблеми генетики, селекції та біотехнології». - Т 4. Київ: Логос, 2012. С. 609–612.
3. *Filimonov D.A., Poroikov V.V.* // Rus. Chem. J. 2006. V. 50. P. 66-75.
4. *Lagunin A., Zakharov A., Filimonov D., Poroikov V.* // Molecular Informatics. 2011. V. 30. № 2-3. P. 241–250.