EDITORS' INTRODUCTION TO THE ISSUE

Dear Colleagues!

The thematic issue of the Biomeditsinskaya Khimiya journal contains papers presented at the XXX Symposium on Bioinformatics and Computer-Aided Drug Discovery (BCADD-2024). These annual Symposia initiated by the Full Member of the Russian Academy of Sciences Prof. Alexander Archakov have been organized by the Institute of Biomedical Chemistry (IBMC) since 1995; from 2021 they have become international and are held in an online format.

The aim of the XXX Symposium on Bioinformatics and Computer Aided Drug Discovery is to present modern achievements in the development and practical application of computer-aided methods for finding and validation of new pharmacotherapeutic targets and their ligands: in silico design of more potent and safe pharmacological agents, optimization of the structure and properties of pharmaceutical substances, rational approaches to the utilization of therapeutic agents in medical practice, as well as discussion of the scenarios for the further development of this multidisciplinary field of science.

XXX Symposium on Bioinformatics and Computer Aided Drug Discovery was held online from September 16 to 18, 2024 as part of the events dedicated to the 300th anniversary of the Russian Academy of Sciences and the 80th anniversary of the IBMC. The Symposium was organized by the Russian Academy of Sciences, Ministry of Science and Higher Education of the Russian Federation, Institute of Biomedical Chemistry, Institute of Bioorganic Chemistry of the Russian Academy of Sciences.

The topics of many lectures presented at the Symposium were directly related to the IBMC participation in the implementation of the project to create a world-class Scientific Center “Digital Biodesign and Personalized Healthcare” within the framework of the National Project “Science” aimed at the development of biomedical research according to the priorities of scientific and technological development of the Russian Federation.

The problems considered at the Symposium correspond to the two priority directions of the Strategy for Scientific and Technological Development of the Russian Federation, approved by Presidential Decree No. 145 of February 28, 2024: paragraph 21, subparagraph “c”: “Transition to personalized, predictive and preventive medicine, high-tech healthcare and health-saving technologies, including through the rational use of medicines (primarily antibacterial) and the use of genetic data and technologies”, and subparagraph “a”: “Transition to advanced technologies for designing and creating high-tech products based on the application of intelligent manufacturing solutions, robotic and high-performance computing systems, new materials and chemical compounds, results of big data processing, machine learning and artificial intelligence technologies”.

The main emphasis of the Symposium was dedicated to new “challenges” and opportunities in *in silico* drug discovery using bio- and chemoinformatics methods. Analysis of large biomedical data sets, development of machine learning and artificial intelligence approaches, as well as expansion of computational estimation capabilities serve as prerequisites for revealing mechanisms of disease onset, identification of promising biomarkers and pharmacological targets.

The application of computational methods at all stages of pharmaceutical research and development not only saves labor, time and financial resources, but also makes it possible to analyze the big data obtained by researchers, extract relevant information from them, and generate new knowledge in a multidisciplinary field. Continuous processing of large sets of biomedical data in silico, identification of target molecular targets allows to identify structure-property relationships, build and validate predictive models, and perform rational molecular design of novel lead compounds. On this grounds, the rigorous recommendations are created for diverse fields of science involved in the development and optimization, testing and application of pharmaceutical agents.

478 people from 50 countries, representing universities and colleges (62%), research institutions (22%), high-tech companies (3%), medical and regulatory organizations (3%), as well as individual researchers, graduate students, and undergraduates, registered for the XXX Symposium.

Nowadays, it is more important than ever to keep abreast of the changing landscape of the discipline world in drug discovery. The multidisciplinary atmosphere of the Symposium aims to bring together speakers and participants from different areas of drug discovery, providing an excellent opportunity to engage in an international exchange of ideas, current strategies, concepts and best practices, collaboration and cooperation, offering broad perspectives and a knowledge-enriched experience.

The program included 6 scientific sessions and the opening and closing sessions of the Symposium, as well as a poster session (http://www.way2drug.com/dr/bcadd2024/program.php). The Symposium featured 2 plenary lectures and 18 keynote lectures, 24 oral presentations selected by the International Scientific Committee from 51 submissions, as well as 18 short communications in the Young Scientist Competition (41 submissions), and 72 electronic posters (74 submissions). The speakers included both well-known scientists active in the field of computer-aided drug design and young specialists, postgraduate students and graduate students from Armenia, Australia, Belarus, Belarus, Brazil, China, Germany, Georgia, India, Indonesia, Ireland, Israel, Mexico, Nigeria, Peru, Russia, Sweden, Tunisia, Turkey, and the United States of America. Many scientific reports aroused keen interest among the Symposium participants: more than 340 questions were asked, which were answered and commented on online. Within the framework of the Symposium a competition of young scientists' reports was held: 18 reports were selected by the International Scientific Committee while considering 41 applications (abstracts and posters) for flash oral presentations. Six winners from Russia, Mexico, and India were awarded the honorary diplomas.

Most of the presentations and videos of the oral presentations are publicly available on the website of the XXX Symposium (http://www.way2drug.com/dr/bcadd2024/program.php), which were allowed by the respective speakers.

Both mature researchers working in the field for decades and young scientists making their first steps in science submitted their papers to the thematic issue of the journal.

Thus, the content of the thematic issue of the journal covers the current state of research in the wide field of bioinformatics and computer-aided drug design — from the development of various methods of *in silico* drug design to their application for the prioritization of molecular targets, search and optimization of ligands acting on them, study of molecular mechanisms of interaction between ligands and targets. Today bioinformatics is no longer just a "supplier" of mathematical methods and computer programs for data analysis. It is a multidisciplinary field of science that integrates heterogeneous chemical, biological and medical data in order to extract useful information from them and generate new knowledge on the basis of which new safer and more effective drugs can be created.

Invited Editors, Co-Chairs of the Symposium

Prof. Vladimir Poroykov

Prof. Roman Efremov