VASSILIEV PAVEL MIKHAILOVICH

Doctor of Biological Sciences, Senior Research Fellow of the Higher Attestation Commission (Assistant Professor)

Head of Laboratory for Information Technology in Pharmacology and Computer Modeling of Drugs for Reasearch Center of Innovative Medicines,
Professor of Chair for Pharmacology and Bioinformatics,
Volgograd State Medical University

E-mail: pvassiliev@mail.ru
Researcher ID: R-9283-2016 Scopus Author ID: 7005832292
ORCID ID: 0000-0002-8188-5052 RSCI Author ID: 101402

Author of more than 440 scientific papers, including: 2 monographs; 15 chapters in books; 75 articles in WoS and Scopus journals, including 15 articles in Q1 journals; 14 copyright certificates and patents; 12 certificates of state registration of computer programs and databases.

Laureate of the Lenin Komsomol Prize in the Volgograd Region in the field of science and technology (1988), twice winner of the Volgograd Region Prize in the field of science and technology (2008, 2012).

Participated as a leader, responsible executor and key executor in 11 scientific projects on grants and government assignments from the Russian Foundation for Basic Research, the Russian Science Foundation, the Ministry of Industry and Trade of the Russian Federation, the Ministry of Education and Science of the Russian Federation, the Ministry of Health of the Russian Federation, including three major scientific projects and one international project.

Under his leadership, 5 graduate works, 6 PhD theses and 1 doctoral dissertation were successfully defended. Currently, he is the supervisor of 2 PhD theses and 1 doctoral dissertation.

Field of scientific interests.

Pharmacology – directed in silico search for pharmacological active substances, in silico study of the mechanism of action of drug compounds.

Medicinal chemistry – chemoinformatics, computer design of drugs, virtual screening.

Molecular modeling – molecular modeling of biological active compounds, docking, molecular dynamics, pharmacophore analysis.

QSAR – computer prediction of the pharmacological activity of chemical compounds.

Bioinformatics and systems biology – system pharmacology, network pharmacology, building biological networks, targeted search for multitarget and polyfunctional drugs.

Information technology – machine learning, artificial intelligence, artificial neural networks, data mining, big data, deep learning, supercomputer technologies.

Currently, the main direction of researches is related to the use of artificial intelligence technologies, systems biology, bioinformatics and supercomputer technologies to develop a methodology for building consensus ensemble neural network multitarget multidescriptor models for predicting various types of pharmacological activity of chemical compounds.

The main tools used are: artificial neural networks of various architectures, fragmental and quantum chemical approaches, molecular modeling methods, docking and molecular dynamics.

Fundamentally new methods for the in silico spectral evaluation of the affinity of compounds to biotargets are being developed.

A number of original programs for computer prediction of the pharmacological activity of chemical compounds have been created in the form of the IT Microcosm software package.

Using the developed methodology, an in silico search for new pharmacologically active compounds and repositioning of known drugs are carried out.