South Ural State University | National Research University

Laboratory of Computational Modelling of Drugs

The laboratory develops methods and software for analyzing and predicting the biological activity of compounds. Carries out complex theoretical and computer research of drugs, using a wide range of methods and approaches, starting with traditional statistical, regression, polynomial, PLS modeling, and finishing with the most modern 3D / 4D QSAR modeling, molecular docking, data mining. In addition to continual methods, various classification algorithms, discriminant analysis, and pattern recognition are used. The studies are carried out in a multiconformational-multitautomeric mode (proposed by the laboratory staff M. A. Grishina and V. A. Potyomkin), taking into account the multi-stage action of the drugs, i.e. taking into account their metabolism, transmembrane penetration, etc. The laboratory develops 3D/4D QSAR methods and software for modeling, molecular docking and virtual drug design. A number of antitumor and tuberculostatic drugs proposed by the laboratory have now been successfully tested in vitro. In addition, research results can be used to analyze food products and build diet schemes that help prevent a number of diseases and / or provide additional therapeutic effects on the body of sick people.

Some results:

• Models for predicting biological activity in a multiconformational-multitautomeric mode were created using the BiS and CiS algorithms developed at the Laboratory.

• Highly predictive models have been developed for assessing the ADMET properties of molecules and the possibility of their synthesis, which are important for drug research projects.

• Polypharmacological models have been developed for predicting the biological activity of compounds.

• Developed new 3D/4D QSAR approaches based on the molecular interior and exterior.

• Molecular docking to determine the characteristics of the active compounds.

• Quantum calculations for the “drug-enzyme” complexes for elucidating the fine features of the electronic structure of active substances.

• Molecular design of new drug candidates.

• The web-portal www.chemosophia.com for on-line calculations of biological activity, ADMET and physico-chemical properties is created.

The laboratory is located in 4 rooms, 3 of which are equipped with 11 high-performance personal computers based on i7 processors. The fourth room - a conference room for presentations, lectures, seminars. It is possible to perform calculations on supercomputers and clusters of the SUSU “Tornado SUSU”, “SKIF-Aurora SUSU”, “SKIF Ural”.

The salary for postdoc positions is 100 000 rubles (~ 1350 EU) monthly in hands.

Laboratory Staff:

Head of Laboratory Dr. Vladimir Potemkin (Russia) 

Principal Scientist Dr. Maria Grishina (Russia) 

Senior Scientist Dr. Brijesh Rathi (India) 

Senior Scientist Dr. Poonam (India) 

Senior Scientist Dr. Edelmiro Moman Noval (Spain) 

Senior Scientist Dr. Prateek Pathak (India) 

Senior Scientist Dr. Jurica Novak (Croatia) 

Senior Scientist Dr. Mohd Shahbaaz (India) 

Researher Nadezhda Palko 

Researher Vladislav Naumovich