



Russian-Armenian University

Institute of Biomedicine & Pharmacy RAU



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Laboratory of structural bioinformatics

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Laboratory of structural bioinformatics



Research and Development activities:

The aim of the laboratory is the investigations of the processes which take place in biomedical molecular systems by the methods of molecular modeling & computer analysis.

Tasks:

- * Computer-aided drug design (CADD) and discovery /structure & ligand based drug design/
- * Study of ADME & toxicity of newly synthesized or modified bioactive compounds.
- * *In silico* screening & target prediction.
- * Assessment of the ligand-target interactions by the methods of molecular modeling.
- * Development and modification of bioinformatics software and modules which can improve the analysis of semi-empirical results.
- * Database creation

Focus on:

- * Neurodegenerative Diseases: Study of the anti-cholinesterase activity of different nature bioactive compounds using molecular modeling.
- * *In silico* evaluation of the bioactivity of newly synthesized compounds based on structure-activity relationship (SAR).
- * Database of secondary metabolites of endemic plants.

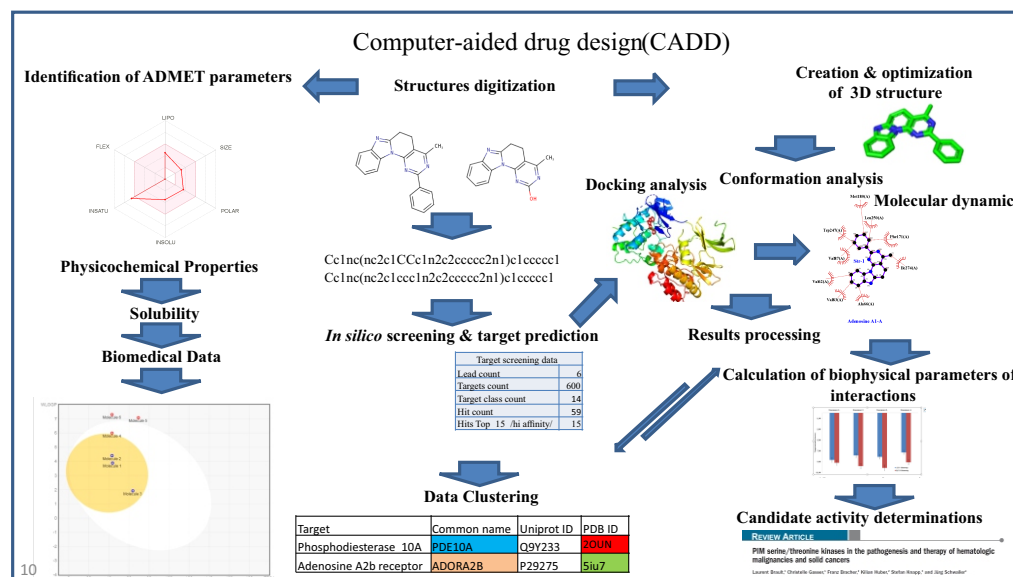
Service:

The Laboratory of Structural Bioinformatics is a platform for the implementation of the concept “Research as a Service (RaaS)”. The developed methodology of “Express Drug Research” may have a business component in the following areas:

- Pharmacy-in silico identification of lead & hit compounds, drug design, etc.
- Biotechnology - identification of the mechanisms of action for various biologically active compounds by the methods of molecular modeling.
- Biomedicine - a comparative analysis of DNA sequences and other biopolymers. Identify the mechanism of action of drug on certain targets.
- Agriculture- preliminary *in silico* assessment of the effectiveness of new insecticides, herbicides, etc. toxins used in agriculture.
- Biology- Evaluation and processing of the results of biological experiments (statistical analysis of biological big data).

Collaboration:

- * ITMO University, Russia
- * Moscow State University, Russia
- * St. Petersburg University of Peter the Great, Russia
- * Stavropol State University, Russia
- * Sumy State University, Ukraine
- * University of Tsukuba, Japan
- * Uppsala University, Sweden
- * Scientific and Technological Center of Organic & Pharmaceutical Chemistry NAS RA, Armenia
- * Bioinformatics Group of NAS RA, Armenia
- * Institute of Molecular Biology NAS RA, Armenia



Used program modules and databanks:

- * MarvinSketch
- * UCSF Chimera
- * Pass online
- * PyMol
- * AutoDock Vina
- * AutoDock Tools
- * LigPlot+
- * ClastVis
- * Gromacs
- * TargetNet
- * ExPASy
- * Protein Data Bank
- * Drug Bank
- * & Other

