Computational structural biology and bioinformatics

Keywords: *Computational biology, structural bioinformatics, protein 3D structure, molecular dynamics, molecular docking, homology modeling, protein sequence analysis, protein-protein interactions, protein-DNA interactions, DNA replication and repair*

Vilnius
University

Research group activities

Research in our laboratory is in the field of computational biology and bioinformatics, disciplines that are playing an increasingly important role in life sciences. Recent breakthroughs in technologies have resulted in a flood of various types of biological data such as genome sequences, data on gene expression, protein-protein interactions, etc. Computational biology and bioinformatics help to make sense of all this vast biological data by providing tools for performing large-scale studies.

In addition, computational biologists and bioinformaticians utilize available experimental data to improve various analytical and predictive methods that could help answer specific biological questions.

Our laboratory carries out research projects covering a broad range of topics that can be collectively described as computational studies of protein structure, function and evolution.

There are two main research directions:

1 **Application of computational methods**

for discovering general patterns in biological data, structural/functional characterization of proteins and their complexes, design of novel proteins and mutants with desired properties. We address a variety of challenging biological problems, often in collaboration with experimentalists. The range of biological topics is unlimited, but our most extensive expertise is in studies of proteins and protein complexes that perform work in studies of nucleic acids.

2 **Development of methods**

for detecting protein homology (common evolutionary origin) from sequence data, comparative protein structure modeling, analysis and evaluation of protein 3D structure, analysis of protein-protein interactions in 3D.

Proposal

- Expertise in computational structural biology research.

- Collaborative projects in the development of computational methods.

- Partners for developing competitive research projects targeting HORIZON 2020 and other international programs.

- Collaboration with experimentalists in addressing important biological questions by combining computational and experimental techniques.

Meet our team

Our team is a mix of both young and highly experienced researchers having different scientific background including computer science, chemistry, biochemistry and molecular biology.

This enables us to use complementary approaches in solving complex research problems.

Research outcomes

Our team has developed and published a number of computational methods for the analysis and modeling of protein structure and homology detection. All these methods are implemented as open-source software packages and are available from our web site (http://bioinformatics.lt/software).

In addition to methods development, our team has also attained important achievements in applying computational methods to specific biological problems. Many of these research projects are performed in collaboration with experimentalists from both national and international research institutions from Europe, US, Japan and South Africa.

Our team has been successful in attracting both national and international competitive research funding. The head of labo-

ratory, Dr. Venclovas, in addition to managing multiple national grants, was a recipient of prestigious grant from Howard Hughes Medical Institute for two consecutive terms (2001-2005 and 2006-2011).

Computational model of CRISPR-Cas complex Kazlauskiene et al (2016) Mol Cell, 62: 295-306

Selected recent publications

- Kazlauskiene, M., et al. (2017) A cyclic oligonucleotide signaling pathway in type III CRISPR-Cas systems, Science, 357, 605-609.

- Olechnovič, K. and Venclovas, Č. (2017) VoroMQA: Assessment of protein structure quality using interatomic contact areas, Proteins, 85, 1131-1145.

- Dapkūnas, J., et al. (2017) The PPI3D web server for searching, analyzing and modeling protein-protein interactions in the context of 3D structures, Bioinformatics, 33, 935-937.

Resources

Our lab is equipped with modern personal computers and software for performing standard computational research.

In addition, we maintain Linux computer cluster for high performance parallel computing consisting of 796 Intel Cores, 40TB storage array with write/read intensive SSD drives and 1/10 Gbps interconnection.

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