

**Coordinator of infrastructural program****Prof.Dr. Dušan Turk**E-mail [dusan.turk@ijs.si](mailto:dusan.turk@ijs.si)

Tel. +386 1 477 3957

**Research institution**

Centre of Excellence for Integrated Approaches in Chemistry and Biology of Proteins

**CIPKeBiP**

Jamova cesta 39, Ljubljana (seat at Jožef Stefan Institute)

**Title**

Code IO-0048

**Analysis and protein production and biologically active molecules of medical importance****Duration of the program**

Part one: 1. January 2013 - 31. December 2014

Part two: 1. January 2015 - 31. December 2020. The program was extended until 31 December 2021 due to a declared pandemic due to COVID-19 disease.

**Abstract of the infrastructure programme**

In the second decade of postgenomic era sequencing of genomes and development of new technologies completely changed the concept of research in biological sciences. Nowadays we witness integration of approaches, which at one side gather data and analyze processes in cells and organisms as whole, and on the other side monitor and analyze increasingly complex molecular processes „in tube“, which are approaching the situations in cells. In this process of integration of knowledge and information the computational tools are turning into the crucial component of science and development. In order to follow the contemporary trends in science and enable researchers from academic and industrial environments to access the contemporary, high-end research technologies, in the Centre of excellence for Integrated Approaches in Chemistry and Biology of Proteins (CIPKeBiP) we have established a technological and scientific platform. The platform is an essential infrastructure. It enables identification of carriers of individual physiological and pathological processes, characterization of their biochemical and biophysical properties and structure, and exploitation of the gained knowledge for commercial purposes.

The infrastructure established within the frame of Centre of excellence CIPKeBiP encompasses the world-class cutting edge research and development equipment. Additional means for support of the proposed Infrastructural program will provide a possibility to open access to this top research infrastructure and expertise also to other Slovenian academic and industrial research groups. A number of academic and industrial projects can be supported by simultaneous raise of their competitiveness. In particular we want to stress that local availability of such infrastructural support to Slovenian industry (pharmaceutical and biotechnological companies) will allow them to carry out the necessary research and analysis within Slovenia instead of having to outsource such research abroad.

In order to use this most advanced research infrastructure of the Centre of excellence we propose the infrastructural program for „Analysis and protein production and biologically active molecules of medical importance“. It is a biomedically oriented. The proposed infrastructural program has the potential to support of the most advanced and demanding research and development projects. It will provide support to the leading academic and industrial institutions

in Slovenia targeting development of new biological drugs as well as biologically active organic compounds. The infrastructure is organized in five segments:

1. Visualization of molecules and their interactions in cells alone or in tissues and organisms with high resolution light microscopy;
2. Analysis and identification of protein composition in complex samples and analysis and identification of individual biological molecules and their modifications by mass spectroscopy;
3. Analysis of interactions, structure and properties of biologically active molecules (proteins and small organic molecules);
4. Development of novel potential biological drugs and drugs on the basis of biologically active organic molecules (studies at the levels of function of organelles in cells, identification and characterization of molecules with clinical potential, and expression, purification and optimization of production processes of biologically active molecules);
5. Demanding computational analysis of complex biological and other experimental data in the sense of integration of knowledge as well as optimization of experimental approaches and technological processes.

Research of the mechanisms of viral infections to prevent the spread of COVID-19 disease

We will investigate interactions between potential protein inhibitors and proteolytic enzymes of the SARS-CoV-2 virus. We will prepare a recombinant protease from the virus and, using proteomic methods, determine its specificity for natural substrates from the lung epithelium and try to identify some potentially critical human substrates.

Theoretically, on the basis of developed SVM models, the possibilities of cleavage of the S protein of the SARS-CoV-2 virus (with which the virus enters the cell) with endosomal proteases are examined.

When studying the action of SARS-CoV-2 viral proteins in cells, we will also focus on the possibility of inhibiting the replication of the virus. In this context, the role of autophagy and lipid droplets and the influence of potential drugs on the action of viral proteins would be studied, among others.

**Key words**

proteins; small organic molecules; visualisation of molecules; structural biology; protein production, mass spectroscopy; demanding computational analysis;