



LABORATORY of INFORMATION TECHNOLOGIES

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Room. 407

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A Software Complex for the Map-Making and Research of Proteins and Nucleic Acids

A software complex with a suitable graphic interface has been designed for cartography and studies of the surface of globular proteins, helix chains of proteins, DNA, and RNA on the basis of PDB files within the Windows environment. It is possible for the proteins to obtain maps with a functional atom and relief coloration in Antov-Hammer projection (SURFACE-2008 program) or else in an original cylinder projection (PROT-Z program). The helix-DNA program provides obtaining the maps of the surface of the DNA/RNA spiral molecules as an orthogonal projection of a 3D structure on the plane perpendicular to the long axis of the DNA helix. This software complex includes a modified program SURFACE developed earlier in the OS DOS environment for mapping the surfaces of globular proteins in the Antov-Hammer projection. The complex comprises the compact versions of the mentioned computer programs, namely SURFACE-compact, PROT-Zcompact and helix-DNA-Zcompact programs. A graphic interface has been excluded from the package as the mentioned programs are used only to organize a mass calculation of the maps in a distributed computing environment. Thus, one can reach a significant saving of both computing resources and computing time, when studying single-type data structures. In order to obtain graphic images of the maps, one should use the full versions of corresponding programs. To manage jobs within the distributed computing environment, a specialized monitoring program NetdBBio working in OS Windows has been created.