

MSProt Viewer

Friendly Environment to Visualization of Proteins

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Abstract

With the diversity of data originated from projects for sequencing genomic DNA a great number of sequences is known. In order to have a better knowledge of the molecular dynamics of organisms, proteins are extremely relevant as study targets.

For the study of protein structures, one of the most used approaches is the visualization and analysis in three-dimensional environment (1).

The knowledge, even approximate, of the three-dimensional structure of a protein is essential for understanding the details of its molecular function and gives valuable insights for the development of effective rational strategies for experiments such as studies of disease related mutations, site directed mutagenesis, or structure based drug design (2).

To make the intuitive visualization of protein structures, our research group developed a software named MSProt - Viewer. It was designed to maximize interactivity and is aimed at experimental scientists who do not have the time to deal with complex computer commands.

The database used to provide the files of the protein was the PDB (3). Several files in PDB format may be loaded simultaneously.

The workspace is divided into two windows (Fig. 1). The main window is used to display the molecules and the lower window is used to show the other features of the molecule. Using the main menu you can choose which features are to be shown in the lower window.

Each one of the loaded proteins has its data displayed in a separate table. This table contains data from positioning of axes, types of atoms, chains, type and number of each amino acid. The user can choose different ways to view the protein clicking with the mouse on the table, displaying all loaded structures or selected parts of the molecules.

The resulting code was placed in public domain using an open-source license, allowing users to freely use, access the code, modify and redistribute it.

MSProt was developed in C++ (4) using the OpenGL library (5) for 3D programming and an open-source version of the Qt library version 4.4.0 (6). Binary distributions for Windows and Linux-based systems was available since the development tools used allow porting for multiple platforms.

The display of models of proteins are based on software Swiss-PdbViewer (7) and VMD (8).

A beta version of the software is available in the address:
<http://sourceforge.net/projects/msprot/>

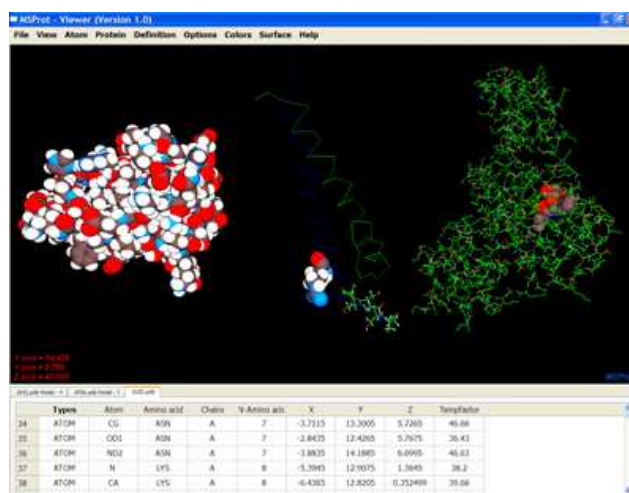


Figure 1 - Proteins viewed with MSProt. Codes PDB: 1PD6, 1IHQ and 1N2D.

References

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