VMD-SS: A graphical user interface plug-in to calculate the protein secondary structure in VMD program

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Abstract:
The investigation on the types of secondary structure (SS) of a protein is important. The evolution of secondary structures during molecular dynamics simulations is a useful parameter to analyze protein structures. Therefore, it is of interest to describe VMD-SS (a software program) for the identification of secondary structure elements and its trajectories during simulation for known structures available at the Protein Data Bank (PDB). The program helps to calculate (1) percentage SS, (2) SS occurrence in each residue, (3) percentage SS during simulation, and (4) percentage residues in all SS types during simulation. The VMD-SS plug-in was designed using TCL script and stride to calculate secondary structure features.

Availability: http://science.scu.ac.ir/HomePage.aspx?TabID=13755

Background:
The secondary structures play important roles in protein structure and protein folding. Study of the protein structure helps us to understand protein function [1, 2]. There are several algorithms for secondary structure assignment. These include STRIDE [3] and DSSP [1]. STRIDE uses combined hydrogen bond energy and statistically derived backbone torsion angle data [2]. The Visual Molecular Dynamics (VMD) [4] uses the stride algorithm for the secondary structure assignment to known protein structures. VMD contains several tools for the analysis of structures and its trajectories produced by the most popular molecular dynamics simulation packages, such as NAMD [5], Amber [6] and GROMACS [7]. However, a user-friendly plug-in to calculate SS of a selected region or particular residue in a PDB and trajectory files is not available. Therefore, it is of interest to describe VMD-SS (a software program) for the identification of secondary structure elements and its trajectories during simulation for known structures available at the Protein Data Bank (PDB).

VMD-SS is a graphical user interface plug-in for protein secondary structure analyses in the VMD program to extent its application. Furthermore, calculation of the secondary structure during molecular dynamics simulation is possible using VMD-SS. Changes of secondary structure of each residue during simulation is an important parameter for documentation. Thus, we describe a user-friendly graphical user interface (GUI) plug-in under the VMD to perform analysis in a trivial manner.
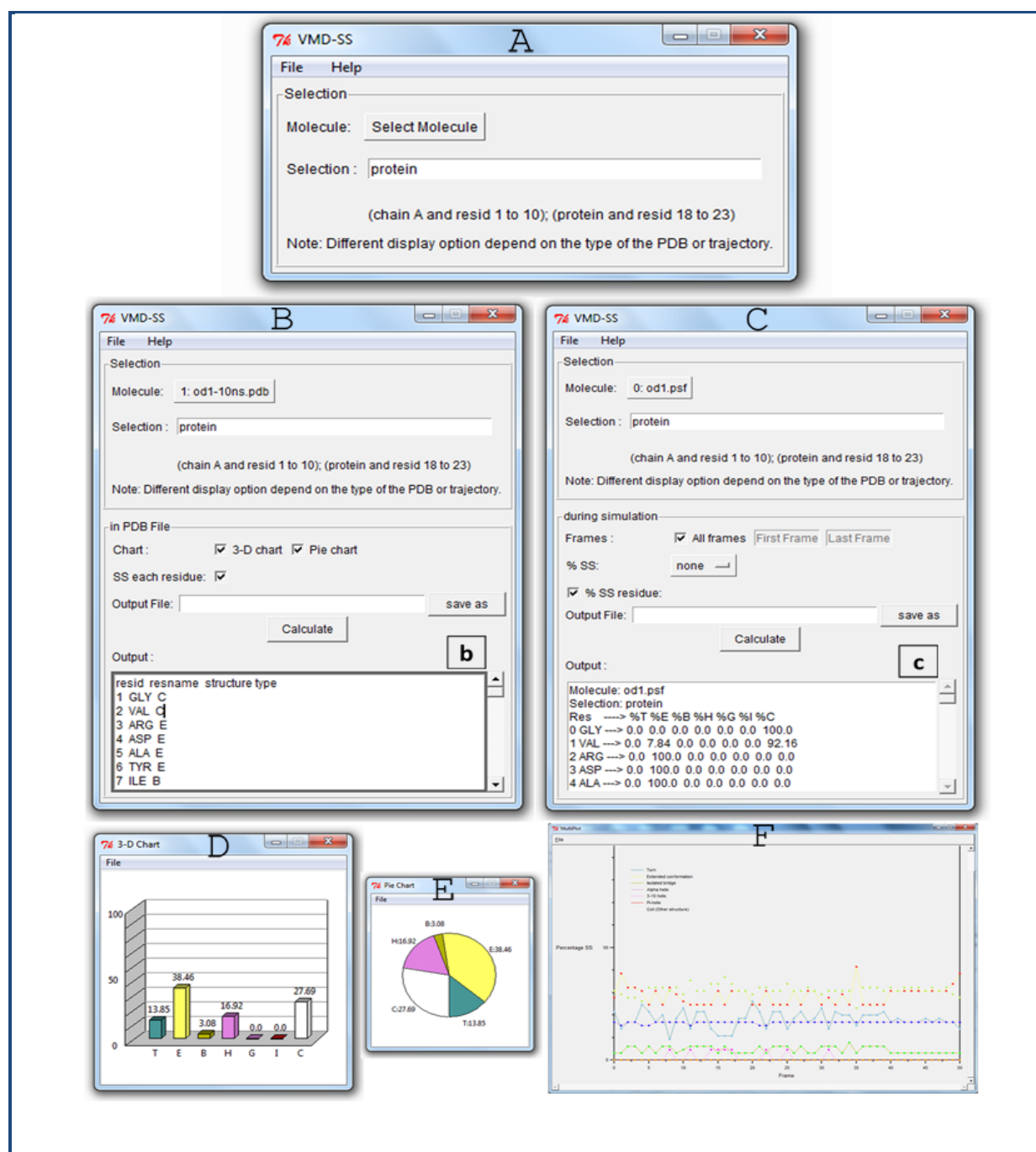
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Figure 1: (**A**) The main panel of VMD-SS; (**B**) illustration of page including options for PDB file, (**b**) this part of plug-in shows SS of each residues in a PDB file, (**C**) illustration of page including options for trajectories, (**c**) this part of plug-in shows percentage of SS of each residues during simulation, (**D**) secondary structure 3-D column chart of a PDB file, (**E**) secondary structure pie chart for a PDB file, (**F**) plot of percentage of each type of secondary structure during simulation.

Methodology:
The user friendly plug-in called VMD-SS is designed by TCL script in TK language with the requirement of PDB or trajectory files using stride. The VMD-SS plug-in is a sub-function under the utility 'extension' of the VMD program.

Input:
VMD-SS plugin has a main page with two sections including the "Molecule" for choosing the molecule from the displayed molecule(s) under the VMD and other one is the "selection"

which gives user the ability to select particular region(s) in the protein **(Figure 1A)**. It depends on the molecule, then VMD-SS plug in contains two different options; if the molecule is a PDB or trajectories, the file page in **Figure 1B** and **1C** will be shown respectively.

Output:
Options for PDB file contains 4 sections (**Figure 1B**): section1 includes "chart" for chart drawing , which user can select pie chart and column chart for calculating secondary structure of

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protein or selected region of protein and output of this section will been shown as column or Pie chart **(Figure 1D, 1E).** Section 2 contain "SS each residue" for calculation secondary structure of each residues in a PDB file, which its output has been shown in **Figure 1b.** Section3 contain "Output file" for saving output in the DAT format in a directory and section 4 is "output" for observing results.

Options for trajectory file contains 5 sections **(Figure 1C)**: section1 is "frames" which give a selectivity to user for selecting whole frames or particular frame of dcd trajectory for calculating secondary structure of particular selection or whole protien during simulation. Section 2 is "%SS" which calculates percentage of secondary structure types in a protein during simulation. This facilitation is useful for instance in checking SS of particular region during simulation. Output of this section will be shown in a plot with different colors for each type of SS in **(Figure 1F)**.

Section 3 is "% SS residue" which calculates percentage of secondary structure types of each residue in a protein during trajectories and this facilitation may be helpful for observing changes in SS of particular residues during simulation. Output of this section will be shown in 8 columns, which first column is list of residues and other columns are percentage of SS type of each residue **(Figure 1C)**. Section 4 and 5 is as same as "Output file" and "Output" in the page of pdb file.

Discussion:

Secondary structure features are a critical characteristic for protein structure analysis. This can be displayed in timeline using sequence viewer plug-in of VMD graphically. However, there is no plug-in to calculate percentage SS of whole protein or selected region and for each residue in a pdb file or during simulation. Hence, we describe VMD-SS plug-in to support this analysis. VMD-SS plug-in can plot and give accurate data for secondary structure of a PDB file or trajectory in time-line with sequence viewer plug-ins for showing results graphically. This is trivial and robust in nature. The output data can be saved in a directory or it could be directly seen in the 'Output' section. It should be noted that the VMD program promises additional user interface plug-in as described elsewhere in VMD DisRg Plug-in **[8]**, which calculates distance and radius of gyration during simulation. Thus, these plug-ins promote the analysis section of VMD with ease of use.

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