BIOINFORMATION
Discovery at the interface of physical and biological sciences

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Volume 8(7)

VMD DisRg: New User-Friendly Implement for calculation distance and radius of gyration in VMD program

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Received March 10, 2012; Accepted March 21, 2012; Published April 13, 2012

Abstract:
Molecular dynamic simulation is a practical and powerful technique for analysis of protein structure. Several programs have been developed to facilitate the mentioned investigation, under them the visual molecular dynamic or VMD is the most frequently used programs. One of the beneficial properties of the VMD is its ability to be extendable by designing new plug-in. We introduce here a new facility of the VMD for distance analysis and radius of gyration of biopolymers such as protein and DNA.

Availability: http://trc.ajums.ac.ir/HomePage.aspx?TabID=12618&Site=trc.ajums.ac&Lang=fa-IR

Keywords: VMD, plug-in, radius of gyration, distance, center of mass.

Background:
Molecular dynamic simulations of biological macromolecules are practical tools for exploring physical basics of structures and functions **[1].** There are several programs for visualization and analysis multiple bimolecular structures such as visual molecular dynamic (VMD) **[2].** The VMD contains a lot of setting to visualize and is a powerful tool for analysis the structure and trajectories that have been produced by most popular simulation packages, such as NAMD **[3],** CHARMM **[4],** Amber **[5]** and GROMACS **[6]** that have built-in scripting systems.

Furthermore, distance analysis of two selected regions of biopolymers is important in molecular dynamic simulation. For instance, the exact calculation of distances between atom pairs, between N-ter and C-ter, between Cα of two residues, between center mass of two chains in dimers, and between ligand and receptor are critical in molecular investigation **[7, 8].**

Generally, the center mass indicator might be evaluated by the formula **(Please see supplementary material for equation (I)).**

Other significant point for analysis of molecular structures is the Radius of gyration. With other words, Structural changes in a time dependent manner that determines the protein structure compactness **[9].** The Rgyr of a protein is indicated as the root mean square distance from each atom of the protein to its centroid, which is calculated by the formula **(Please see supplementary material for equation (II)).**

Distance calculation and Radius of gyration are two significant indicators being frequently used in structural analysis. But, there is no graphical user interface implement within VMD software to calculate the above mentioned parameters. Therefore, we aimed to design a new plug –in for VMD software to extent its application. The new user friendly plug-in is designed under the VMD program by the TCL script in the TK language with the requirement of PDB or trajectory

files. We termed the new plug-in to VMD DisRg, which makes the use of different programs unnecessary. The VMD DisRg plug-in is a sub-function under the utility 'extension'.

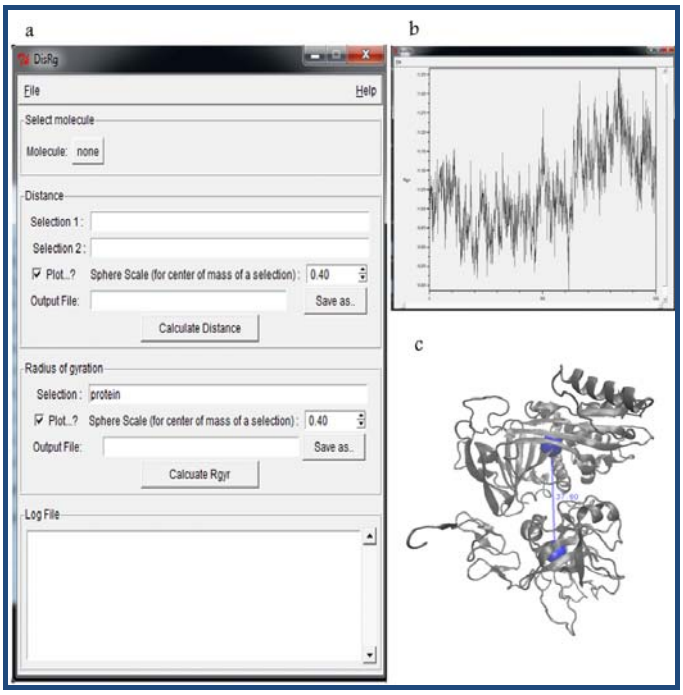

Figure 1: (a) The main panel of VMD DisRg; **(b)** Illustration of radius of gyration during simulation; **(c)** The distance of the center mass is shown graphically (the distance between two chains of a complex are calculated).

Software Input:
The Plug-in DisRg consists of 5 sections **(Figure 1a):** Section1 contains the "select molecule" for choosing molecule from displayed DCD trajectory or PDB under the VMD. Section2 has the facility for the distance analysis with the ability of selectable regions of interest. Section3 is for investigating the radius of gyration. For both section 2 and 3, there are two optional plot and sphere scale. By the use of plot (active form), a graphic output is provided during entire simulation.

Software Output:
Section 2 or the distance section calculates the distance based on selections including: 1) Distance between two single atoms; 2) Distance between center of mass of residues; 3) Distance between center of mass of two chains, and 4) Distance between center of mass of ligand and chain or regions. In addition, radius of gyration can be calculated for displayed structure and trajectories in section3 **(Figure 1b).**

Section 4 is designated as "log file" for observing the results. Autonomously, the output file can be saved in the directory being accessible by a DAT file that is compatible with other script formats. Technical implementation of the plug-in is the visualization of the selection region in two forms for atoms and center mass of given sphere **(Figure 1c)**. The User has the ability to change the radius of sphere by handling the sphere scale.

Caveat & Future development:
VMD is a practical tool for biopolymers study that has been applied by many researchers with the aim to calculate some structural features with reasonable graphical visualization as output results. One of the interesting facilities in the VMD is the modus 'extension' by its assistance the software can be extended by new plug-ins **[2].**

Moreover, distance and Rgyr are two critical characteristics for protein structure analysis, which can be calculated by VMD but with no graphically plug-in. Therefore, we aimed to add a new plug-in under the VMD to calculate these mentioned analysis, easily. We developed a friendly graphical user interface (GUI), which has some advantages: Calculation of distance and Rgyr during trajectories by drawing plot, User's selection is showed in OpenGL Display of the VMD; as a result, the User can monitor distance of COM selections (displaying COM is a novel graphical facility for User). Further advantage is that the output data can be saved in a directory or would be directly seen in the window 'log file'. With this plug-in the User can calculate some properties with easy clicks, so that an inexperienced User might have success with these new conveniences. It is to remark that the VMD program promises additional user interface plug-in.

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Edited by P Kangueane
Citation: **Falsafi-Zadeh *et al.*** 8(7): 341-343 (2012)

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Supplementary material:

The center mass indicator might be evaluated by the following formula:

$$x_{CUM} = \sum m_i x_i / \sum m_i \quad \text{(I)}$$

where X_i is the x cartesian coordinate of the atom i and mi is its atomic mass (at the same way, the y and z coordinates of the center of mass can be calculated).

The Rgyr of a protein is indicated as the root mean square distance from each atom of the protein to its centroid, which is calculated by the formula:

$$r_{gyr}^2 = (\sum_{i=1}^{n} w(i)(r(i) - \bar{r})^2)/(\sum_{i=1}^{n} w(i)) \quad \text{(II)}$$

where $r(i)$ is the position of the i atom and $\bar{r}$ is the weighted center as computer by measure center.