SSViewer: Sequence Structure Viewer

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Abstract- An important aspect of bioinformatics is sequence. Sequence is a discrete function which contains the combinations of amino acids in proteins and nucleotides in Dna. Important functions of Amino Acids are to serve as the building blocks of proteins, which are linear chains of amino acids. Amino acids can be linked together in varying sequences to form a vast variety of proteins. Twenty-two amino acids are naturally incorporated into polypeptides and are called protein-o-genic or standard amino acids. Of these, 20 are encoded by the universal genetic code. In the case of the DNA sequence A, T, G, C is used to represent DNA. This sequence information is analysed to determine genes that encode polypeptides (proteins), RNA, genes, regulatory sequences, structural motifs, repetitive sequences and DNA sequences can be accurately analysed using computational techniques like BLAST, FASTA which is not possible manually.

In the present study we developed a tool to visualize the 3D structure for a given sequence by using programming language Java and HTML.

Keywords: Java, HTML, Sequence, PDB, Molecular visualizaion.

I. INTRODUCTION

SSViewer is a Java-based molecular modelling application that can be used either in a stand-alone mode, or as an embedded object in webpages. Rasmol was developed in the early 1990's by Roger Sayle [1], as a standalone application and was distributed free of charge. There are many versions available for different operating systems like; Windows, UNIX and older versions of MacOS (prior to MacOS X). Chime is the another molecular viewer developed at Molecular Design Limited (MDL) and took the Rasmol code and modified it so that it could be used as a web browser plug-in to display three-dimensional, interactive molecular models from web pages. Both Rasmol and Chime use the same command library for loading and manipulating molecular models. For Rasmol, the commands are entered from a command line with a subset of the commands available from the menu bar. For Chime the commands are coded into the web page by its author. These commands are either executed when a plug-in is loaded or can be activated by a visitor to the site using buttons and other control elements. Chime also has a pop-up menu that allows a visitor to a website to execute as subset Rasmol commands. Rasmol and Chime complements each other Rasmol being used by web developers to create and test the Rasmol scripts that they plan to use with Chime.

Even though both Rasmol and Chime have wide acceptance, further development of both these applications have languished since the turn of the millennium and are now longer compatible with many of the newer operating systems and browsers. Many tools were developed for visualizing the 3D structures such as PyETV[2], PDBjViewer[3]. UCSF Chimera [4]. Our SSViewer can be a replacement for Rasmol, Chime, C3nD and Jmol. It is an open-source, Java based application that has the same look and feel as Rasmol and Chime and can interpret all of the Rasmol and Chime commands. It can be run as either a standalone application like Rasmol, Pymol or embedded in WebPages like Chime. Because it is Java based it is essentially independent of the platform that it runs on, when used from a web page it requires only a Java enabled browser. The standalone version can be obtained free of charge and runs under Windows, Linux and Mac OS X.

SSViewer is very user friendly to analyze 3D structures of proteins, DNA, RNA, and their complexes. It works within a web browser, and is designed to enable the readers of scientific journals to see the main features of 3D models. SSViewer is a user-interface to an excellent and free molecular visualization program named SSVIEWER it can display major structural features of the molecule with one click each. Initially, each chain is given a different colour, making it easy to see how many protein or nucleic acid chains are present. Residues with incomplete side chains are labelled S and non-standard residues are labelled X automatically at the outset. One-click options display secondary structure, amino(-NH2) and carboxyl (COOH) (in case of DNA 3' and 5') terminus, composition (DNA, RNA, protein, ligands and solvent), the distributions of hydrophobic, polar, and charged amino acids, salt bridges, cations, anioins and pi orbital interactions for amino acids. Non-standard residues and missing residues / side chains are flagged automatically[4]. The non-covalent interactions are automatically divided into seven categories: hydrogen-bonded water molecules, water bridges, hydrogen-bonded non-water, hydrophobic interactions, salt bridges, cation-pi-orbital interactions.

SSViewer was designed for readers of scientific journals who are already familiar with the principles of protein sequence and structure. Therefore, it lacks the extensive help, and guidance in understanding, interpreting and evaluating 3D macromolecular models that is built into www.Proteopedia.org Ease of Use. First Glance in SSViewer was designed to enable viewing a molecule in one click, in all popular web browsers and computer platforms without installing anything. Several other java-based applications that meet these criteria are offered by the RCSB Protein Data Bank. Generally, these lack the ease of use, automatically-displayed ccontext sensitive help and colour keys are provided by SSViewer, and offer a less complete set of one-click molecular overview options. SSViewer also has defined (Eg. metal, carbohydrate, non-standard residue") while other viewers typically did not over.

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QuickPDB[5] has a elegant sequence-to-structure user interface. Java-based viewers offered at the Protein Data Bank, even without toggling on the high-quality rendering mode in FirstGlance. Nevertheless it does not provide the "publication quality" images of PyMOL or the stand-alone Protein Workshop java application. SSViewer usually obtains the molecules it displays (atomic coordinate PDB files)from the US Branch of the Worldwide Protein Data Bank (PDB), which makes freely available all published macromolecular 3D structure data. In order to display functional biological assemblies (specific oligomers), theoretical models, and other data files not available from the PDB, SSViewer can obtain molecules from any web server or you can upload your own model data.

II. IMPLEMENTATION

SSViewer is a user interface to the java applet. SSViewer is written in JavaScript, html and java. As mentioned above. SSViewer makes the visualization power built into the java applet accessible to users who do not have the time to learn the SSViewer command language, or how to embed SSViewer in web-pages. with the help of java applet SSViewer can able to read the X, Y, Z co-ordinates.
SSViewer contains a number of commands that can be used to display and highlight molecular models. For example, there are commands to produce various geometric shapes that represent atoms and bonds. Typically, atoms are rendered by spheres while bonds are rendered as sticks. Atoms and bonds can also be coloured differently to illustrate various properties. There are many Other commands like changing background colour, atom with bonds, without bonds, zoom, Rotation, surface area etc.

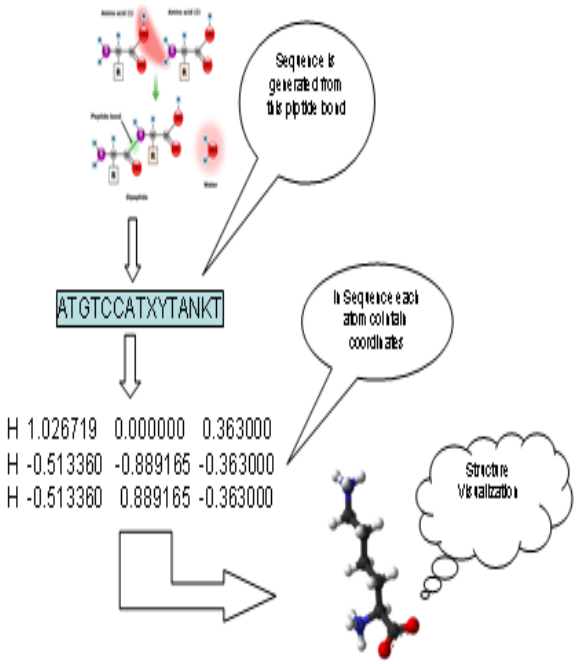

Figure.1: Flow Diagram for the SSViewer

III. RESULTS

The figure.2 shows the Home Page of the web resource. It contains various options like load the file, import, full screen, direct access of different file formats which are visible on screen used to generate the structure and it also contain search box and background colours.

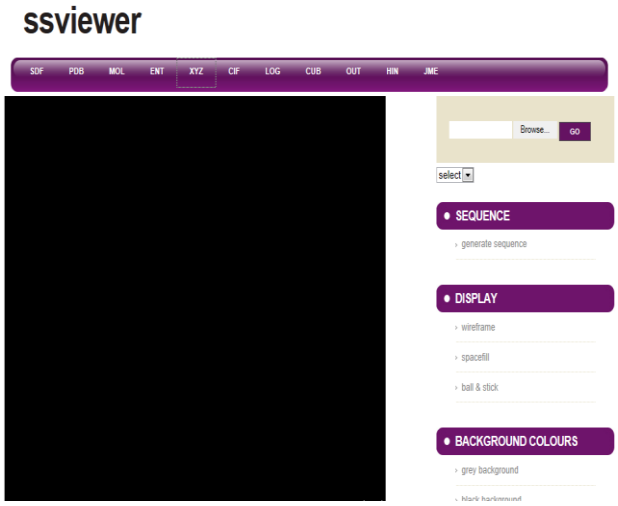

Figure.2: Home Page of SSViewer.

The figure.3 showing the structure for a given XYZ file format. If we have loaded a xyz file to the viewer it displays structure by reading its corresponding co-ordinates.

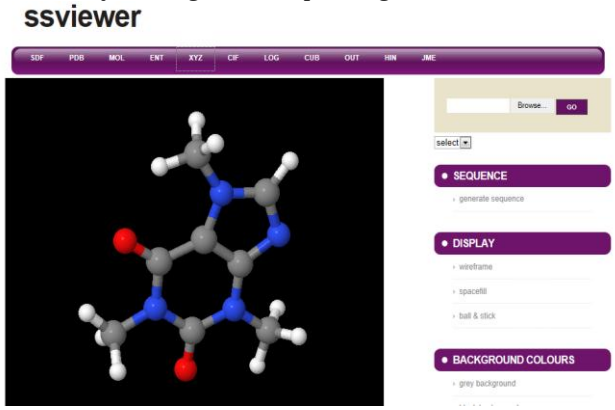

Figure.3: Visulization of the Small Molecule.

The tool is used to visualize the Sequence, while displaying it we can adjust the background colours to highlight the necessary part of the molecule. Tool has the applications to choose the appropriate colour as background with the help of a button on the right click of the mouse, it will show the various options to represent the molecule, molecular geometry, geometry optimization, H-bonds, Hydrophobicity.

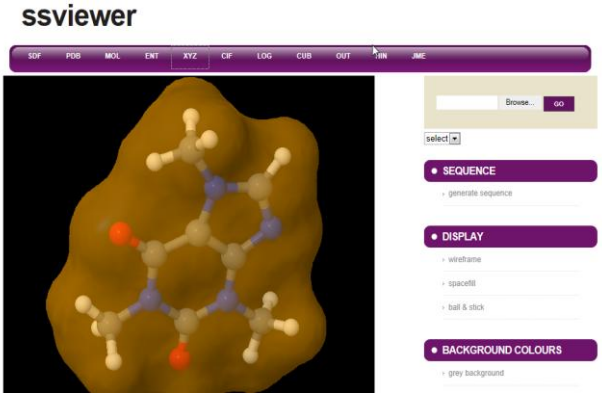

Figure.4: Solvent accessiable surface.

Solvent surface around molecule is a surface where molecule can interact with other molecules when it enter in this surface.

when right click of a mouse is selected, tool box is generated which contains the surface representation and identify molecular solvent accessibility. when you click on surfaces we get different surface options like dot surface, van -derwaals surface, electron cloud etc., there we can select the Solvent accessible surface as shown in the figure.4.

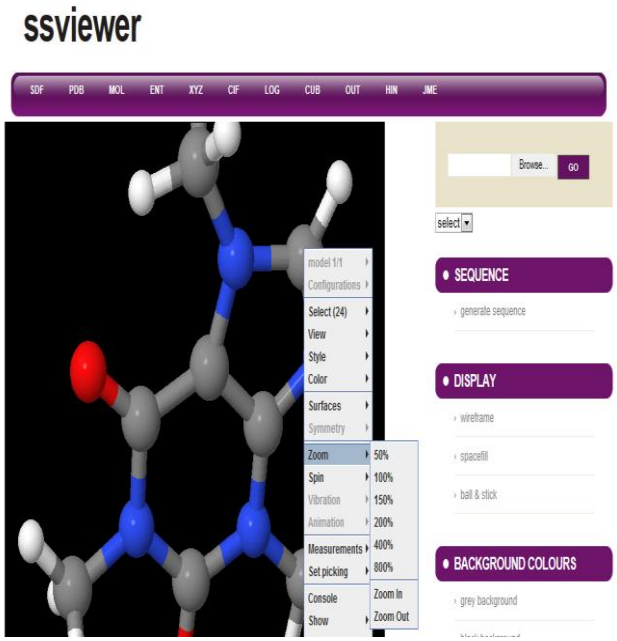

Figure.5: Zoom in and Zoom out.

Upon right click, a tool box is generated containing the zoom option. which can be used to increase and decrease the structure.

IV. CONCLUSION

SSViewer is the integration of different file formats to view their 3D Structure. especially our developed tool supports more than ten file formats like PDB, MOL, ENT, XYZ, CUBE, HIN, JME, CIF, SDF, LOG, MOL2, CHK. SSViewer having significant feature which generates output for a given random sequence by the user and it also displays the length of sequence.

FUTURE DIRECTION

New version of SSViewer can also integrate many more file formats so that we can view the structure for every file format in this tool itself. We can generate a structure for long length sequences also.

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