BHARATHIDASAN UNIVERSITY

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Unit-IV

TOPIC: Protein Structure Visualisation tools -RasMol Viewer

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PROTEIN STRUCTURE VISUALISATION TOOLS -RASMOL VIEWER

INTRODUCTION

The software used to examine and display structure information of biomolecules like amino acids and protein are called ***structure*** *visualization tools.*

The computer graphics help to analyze and compare protein structure to gain the functions of protein.

Molecular visualization helps the scientists to bioengineer the protein molecules.

TOOLS FOR MOLECULAR VISUALIZATION

There are a number of software's both free and commercial are available to visualize the biomolecules.

The most commonly used free software are;

- ***RasMol***
- ***Chime***
- ***MolMol***
- ***Protein explorer***
- ***Kinemage***
- ***Ribbons***
- ***Swiss-PDB viewer***

RASMOL

♡Rasmol is a Protein structure visualization tool.

♡This site was established in mid-September 2000 to provide a home for developers of Open Source versions of RasMol.

♡RasMol is an important scientific tool for visualisation of molecules created by Roger Sayle in 1992.

♡RasMol is used by hundreds of thousands of users world-wide to view macromolecules and to prepare publication-quality images.

RASMOL

♡RasMol is a molecular graphics program proposed for the visualization of proteins, nucleic acids and small molecules.

♡The program is aimed at display, teaching and generation of publication quality images.

♡The program reads in molecular coordinate files and interactively displays the molecule on the screen in a variety of representations and colour schemes.

♡RasMol runs on wide range of architectures and operating systems including Microsoft Windows, Apple

SUPPORTED INPUT FILE FORMATS

♡Protein Data Bank (PDB)

♡Mol2 formats

♡Molecular Design Limited's(MDL) Mol file format

♡Minnesota Supercomputer Center's (MSC) XYZ (XMol) format

♡CHARMm format CIF format

♡mmCIF format files

INPUT FILE FORMAT:

☺ **The input file can be in PDB format and can be downloaded from the PDB structure database.**

PDB File Format

Residue Name

Atom # | Atom Name | Residue # | X coord (Å) | Y coord (Å) | Z coord (Å) | Occupancy | B-factor

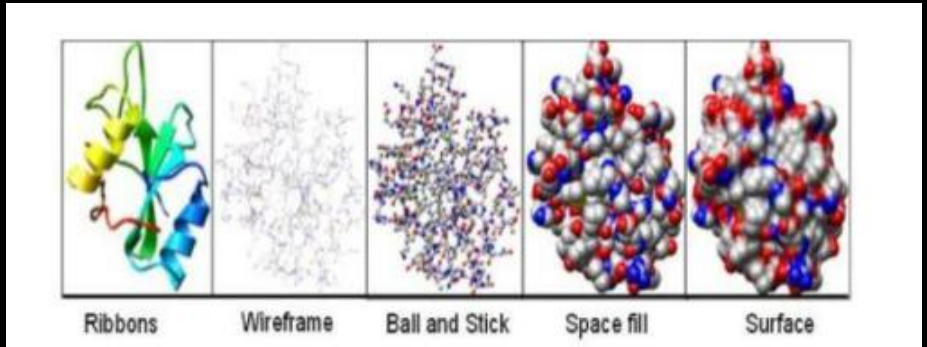
```
ATOM      1  N   SER A   1      21.389  25.406  -4.628  1.00 23.22      2TRX 152
ATOM      2  CA  SER A   1      21.628  26.691  -3.983  1.00 24.42      2TRX 153
ATOM      3  C   SER A   1      20.937  26.944  -2.679  1.00 24.21      2TRX 154
ATOM      4  O   SER A   1      21.072  28.079  -2.093  1.00 24.97      2TRX 155
ATOM      5  CB  SER A   1      21.117  27.770  -5.002  1.00 28.27      2TRX 156
ATOM      6  OG  SER A   1      22.276  27.925  -5.861  1.00 32.61      2TRX 157
ATOM      7  N   ASP A   2      20.173  26.028  -2.163  1.00 21.39      2TRX 158
ATOM      8  CA  ASP A   2      19.395  26.125  -0.949  1.00 21.57      2TRX 159
ATOM      9  C   ASP A   2      20.264  26.214   0.297  1.00 20.89      2TRX 160
ATOM     10  O   ASP A   2      19.760  26.575   1.371  1.00 21.49      2TRX 161
```

DISPLAY

☺ There are different ways of displaying coordinates.
☺ These include:-
#wireframe, sticks, spacefill, strands & cartoons.

☺ The initial image is shown as a „wire" model.

☺ In the last two styles, alpha helices are rendered as helical ribbons and beta structures as flat arrows pointing in the direction of the polypeptide chain.

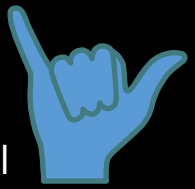


COLOUR

The atoms of the model can be coloured by the standard CPK (named after Corey, Pauling and Koltun)
To color by atom type : Colours/CPK

- ☺ Carbon: gray
- ☺ Hydrogen: white
- ☺ Oxygen: red
- ☺ Nitrogen: blue
- ☺ Sulfur: yellow
- ☺ Iron: yellow

COLOUR



The protein can be coloured based on polypeptide chains, the chemical property of the amino acids.

To color by the protein-secondary structure: Colours/Structure
-helices: magenta
-sheets: yellow
turns: pale blue
all other residues: white

The structure can be cut in the z-dimension

The left and right mouse buttons can be used to rotate the protein along the „x” and „y” axes.

RASMOL FEATURES

♥The ability to automatically mark non bonded atoms in wireframe and stick displays

♥The ability to report coordinates.

♥Additions to the list of pre-defined colours.

♥Updating the picture title with the PDB ID code and EXPDTA information, so models will be clearly distinguished from experimental data.

♥Correction of coordinate handling for Mol2 and XYZ coordinates

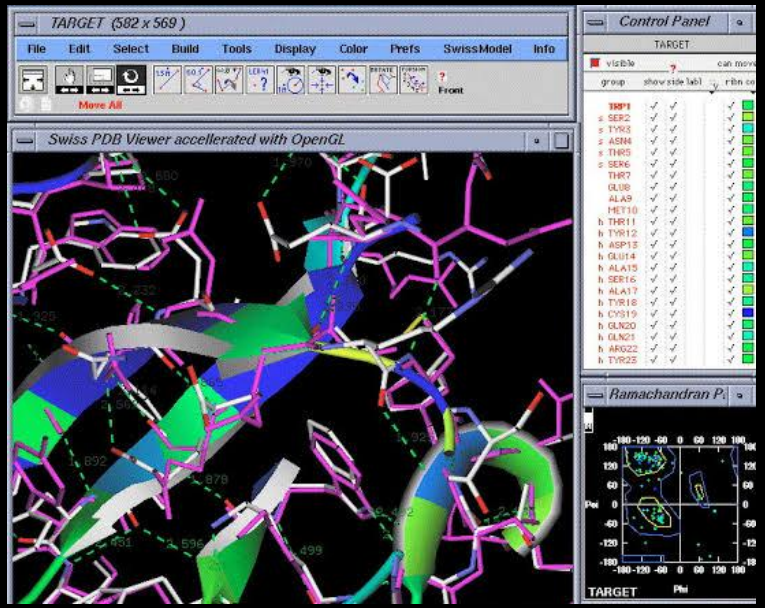
♥Improved accuracy of coordinates in pseudo-PDB output.

RASMOL FEATURES

♥Alternate conformers and multiple NMR models may be specially coloured and identified in atom labels.

♥Different parts of the molecule may be represented and coloured independently of the rest of the molecule or displayed in several representations simultaneously.

♥This software is freely available.Download link: http://www.openrasmol.org/#Software



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- HTTPS://WWW.GOOGLE.COM/URL?SA=T&SOURCE=WEB&RCT=J&URL=HTTPS://PROSITE.EXPASY.ORG/&VED=2AHUKEWIK7OG4H-Z9AHWXS2WGHWPWCAWQFNOECAUQAQ&USG=AOVVAW2YSYV7B25SZFM7D4PADBFC


THANK YOU