An Introduction to Protein Structure Viewers

George Bell, Ph.D.
Bioinformatics and Research Computing

Hot Topics – March 2009

Outline

- Why protein structure viewers?
- Web tools
- Stand-alone tools
- Generating figures
- Swiss-PdbViewer demo
- See http://iona.wi.mit.edu/bio/education/hottopics.html for all Hot Topics slides and information

Why protein structure viewers?

- Get a general understanding about structure/function relationships of your favorite protein
- Explain the biochemistry of YFP
- Map mutations to structure
- Compare structure/function relationships between related proteins
- Spice up your presentations

Protein structure repositories

- Protein Data Bank (PDB; www.rcsb.org) of the Research Collaboratory for Structural Bioinformatics (RCSB)
- PDBe and PDBj
- Molecular Modeling Database (MMDB) at NCBI
  http://www.ncbi.nlm.nih.gov/Structure/MMDB/mmdb.shtml
- Most structures determined by X-ray crystallography or NMR-spectroscopy

Web tools and applets

Web tools and applets

- WebMol
- Jmol
- KiNG
- PDB Protein Workshop
- FirstGlance (using Jmol)
- Cn3D (NCBI; standalone too)

Stand-alone tools

- Swiss-PdbViewer (DeepView; spdbv.vital-it.ch)
- Jmol (jmol.sourceforge.net)
- RasMol (www.rasmol.org)
- Cn3D (NCBI)
- PyMol (http://pymol.sourceforge.net)
- Chimera (UCSF)

Choosing a tool

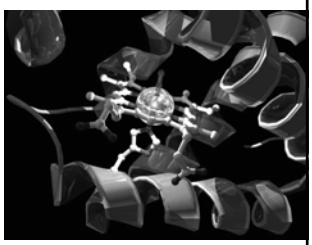
- What do you want to do?
- What have you used before?
- Graphical interface?
- Scripting capabilities?
- Customizable to your needs?
- Output figure options?

Swiss-PdbViewer

- All operating systems
- Nice graphical interface
- Scripting language
- Multiple structures at once
- Can produce great figures together with POV-Ray software
- Good tutorials

High-quality figures with POV-Ray

- Swiss-PdbViewer can save images as
  - PNG image format
  - a "Pov-Ray scene"
- Pov-Ray =
- Persistence of Vision Raytracer:
  - "a high-quality, totally free tool for creating stunning three-dimensional graphics"

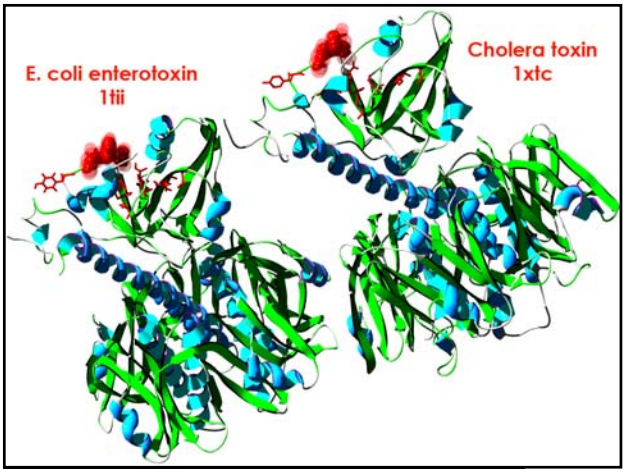


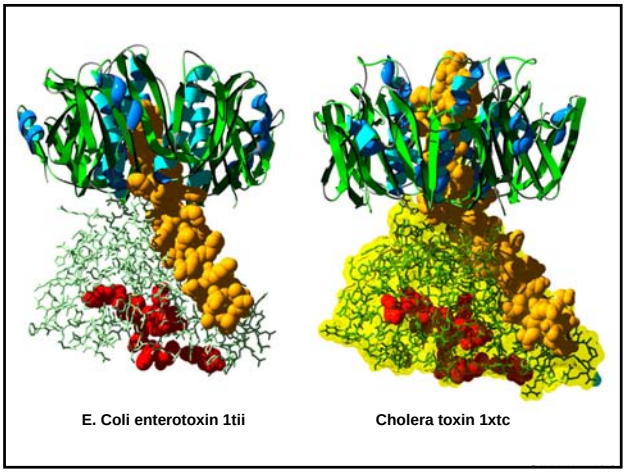
Swiss-PdbViewer – more info

- Site: http://spdbv.vital-it.ch/
- Manual:
  http://spdbv.vital-it.ch/Swiss-PdbViewerManualv3.7.pdf
- Tutorials
  - SPDBV:
    - http://spdbv.vital-it.ch/TheMolecularLevel/SPVTut/index.html
    - http://spdbv.vital-it.ch/main_tut.html
  - Babraham Bioinformatics:
    - http://www.bioinformatics.bbsrc.ac.uk/training.html#deepview
- POV-Ray (for best images):
  - http://www.povray.org/

Swiss-PdbViewer demo

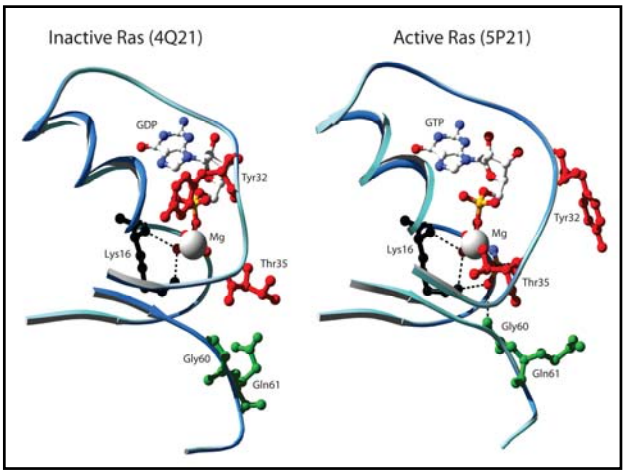
- Compare the cholera (1xtc) and E. coli (1tii) toxins
- Highlight the active sites
- Optimize the structure representation
- Create a nice figure using POV-Ray software

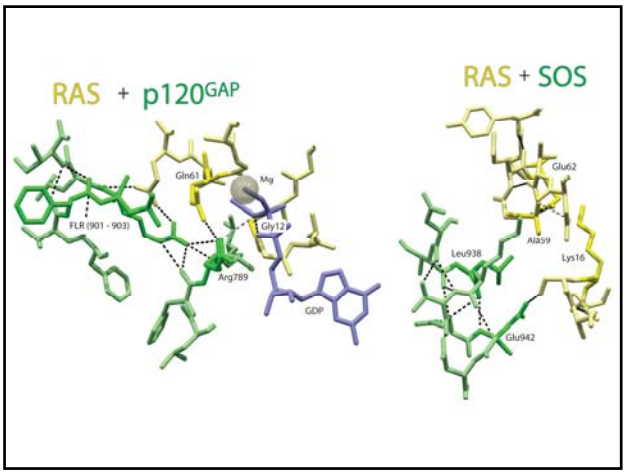




E. Coli enterotoxin 1tii

Cholera toxin 1xtc





Protein Structure Viewers
Hot Topics – March 2009

Swiss-PdbViewer demo

1. Open (or import) cholera toxin (1xtc) PDB file.

2. Browse main interface
    Rotate, translate zoom
    Display ➔ Render in Solid 3D
    Wind (windows) ➔ Control Panel, Alignment

3. Select by chain or atoms, and/or using Select menu

4. Browse Control Panel
    Chain, secondary structure, group, show (ball and stick), side (chain), label, surface (::v), ribbon, color, backbone/side chain/etc.

5. Preferences (Prefs) menu

6. Change 5 chains of ring (DEFGH) into ribbons
    Prefs ➔ colors

7. Change chain C to orange space-filled

8. Make molecular surface of chains AC
    Prefs ➔ Surfaces
        Check “Ignore Selected Residues”
        Transparency (1 - 100) ➔ 90
    Tools ➔ Compute Molecular Surface

9. Select active site residues and show as red space-filled atoms

10. Save layer (File ➔)

11. Save Pov-Ray Scene (File ➔)

12. Open (or import) E. coli enterotoxin (1tii) PDB file.

13. Browse new display options:
    Control Panel ➔ pull-down menu for structure selection
        Visible? Can move?

14. Fit ➔ Iterative Magic Fit (and then separate)

15. Select active residues and change to space-filling
    Look at Alignment

10. Save Project (File ➔)

11. Save Pov-Ray Scene (File ➔)

12. Go to POV-Ray (or open *.pov file) and Run, generating image of desired size.