



Working with protein structures

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PyMOL – A Molecular Graphics Program

- ▶ A molecular visualization program for small molecules and proteins
- ▶ One quarter of published images of 3D protein structures are produced with PyMOL
- ▶ Features:
 - Rendering of 3D images of proteins
 - Structural alignment
 - The computation of structural similarity scores
 - Visualization of features about proteins
 - Extendable with Python

Our goals today

- ▶ Structure manipulation in Pymol
- ▶ Selection
- ▶ Different structure models
- ▶ Rendering
- ▶ Superposition
- ▶ Output

Download and visualize a structure

- ▶ Download the protein HIV protease from the RCSB Protein Data Bank (PDB) (pdb and fasta file)
- ▶ Each protein has a unique 4-charcted alphanumeric identifier (PDB ID)
- ▶ The PDB ID of HIV protease is 1FB7
- ▶ Open the pdb file in a text editor and try to understand ist elements

Visualising

- ▶ Open pymol and load the structure

```
load 1fb7.pdb
```

- ▶ Try
- ▶ Rotating the camera (Left Button)
- ▶ Zooming in and out (Right Button)
- ▶ Moving in the XY plane (Middle Button)
- ▶ Setting origin of rotation (Ctr-Shift)

Visualizing 2

- ▶ Use the buttons to the right of the pannel to look at all the representations of the proteins
- ▶ Use the buttons to the right of the pannel to color the protein from the N terminal to the C terminal
- ▶ Use the buttons below to view and select part of the structure
- ▶ Identify the secondary structure in the structure
- ▶ Why do the secondary structure appear in the structure

Hide all

Show lines, (name c+n+ca)

Making selections

- ▶ Select selection-name, selection expression

```
Select alpha, name ca and chain A and resi  
86:94
```

```
Label (alpha), "%s-%s" % (resn, resi)
```

- ▶ To unlabel

```
label
```

Two chain protein

Download and load 1ZIK

Hide all

Show lines, (1ZIK and name c+ca+n)

Color cyan, 1ZIK and chain A

Color red, 1ZIK and chain B

Show cartoon, 1ZIK

Hide lines, 1ZIK

Back to HIV PR

Hide all

Show cartoon, 1fb7

Color purple, ss h

Color yellow, ss s

Color green, ss ""

Rendering

Show surface, 1fb7

Set transparency=0.7

Bg_colr white

Ray 800

Png 1fb7

Comparing proteins

```
fetch 1hhp  
fetch 1hvr  
select 1hvrA, chain A and 1hvr  
hide all  
show cartoon, 1hhp or 1hvrA  
align 1hhp, 1hvrA
```

- ▶ Compare the sequences
super 1hhp, 1hvrA
- ▶ Compare the sequences
deselect
- ▶ What is the difference between super and align
- ▶ Why are these two proteins similar

-
- ▶ <http://www.protein.osaka-u.ac.jp/rcsfp/supracryst/suzuki/jpxtal/Katsutani/en/hydrophobicity.php>
 - ▶ Run the script
 - ▶ Change the script to:
 - color glycines in red and the rest of the structure in blue
 - Show the cartoon
 - ▶ What did you discover

Fold.it

- ▶ Download foldit
- ▶ Play

▶ **References:**

- ▶ **PyMol Wiki (tutorials, scripts,...):** http://www.pymolwiki.org/index.php/Main_Page
- ▶ PyMol user manual: <http://pymol.sourceforge.net/newman/user/toc.html>
- ▶ PyMol CheatSheet: <http://pymolwiki.org/images/7/77/PymolRef.pdf>
- ▶ Official Pymol Website: <http://www.pymol.org>
- ▶ **HowTo Linux Build:** http://www.pymolwiki.org/index.php/Linux_Install
- ▶ **Unofficial Pymol binaries for Windows:** <http://www.lfd.uci.edu/~gohlke/pythonlibs/#pymol>
- ▶ HowTo Windows Build: http://www.pymolwiki.org/index.php/Windows_Install
- ▶ Macromolecular visualization laboratory: http://www.chem.ucsb.edu/~kalju/chem110L/public/tutorial/task3_v8.html
- ▶ Molecular surface- structure-based drug design: <http://www.netsci.org/Science/Compchem/feature14i.html>