PyMOL Introduction

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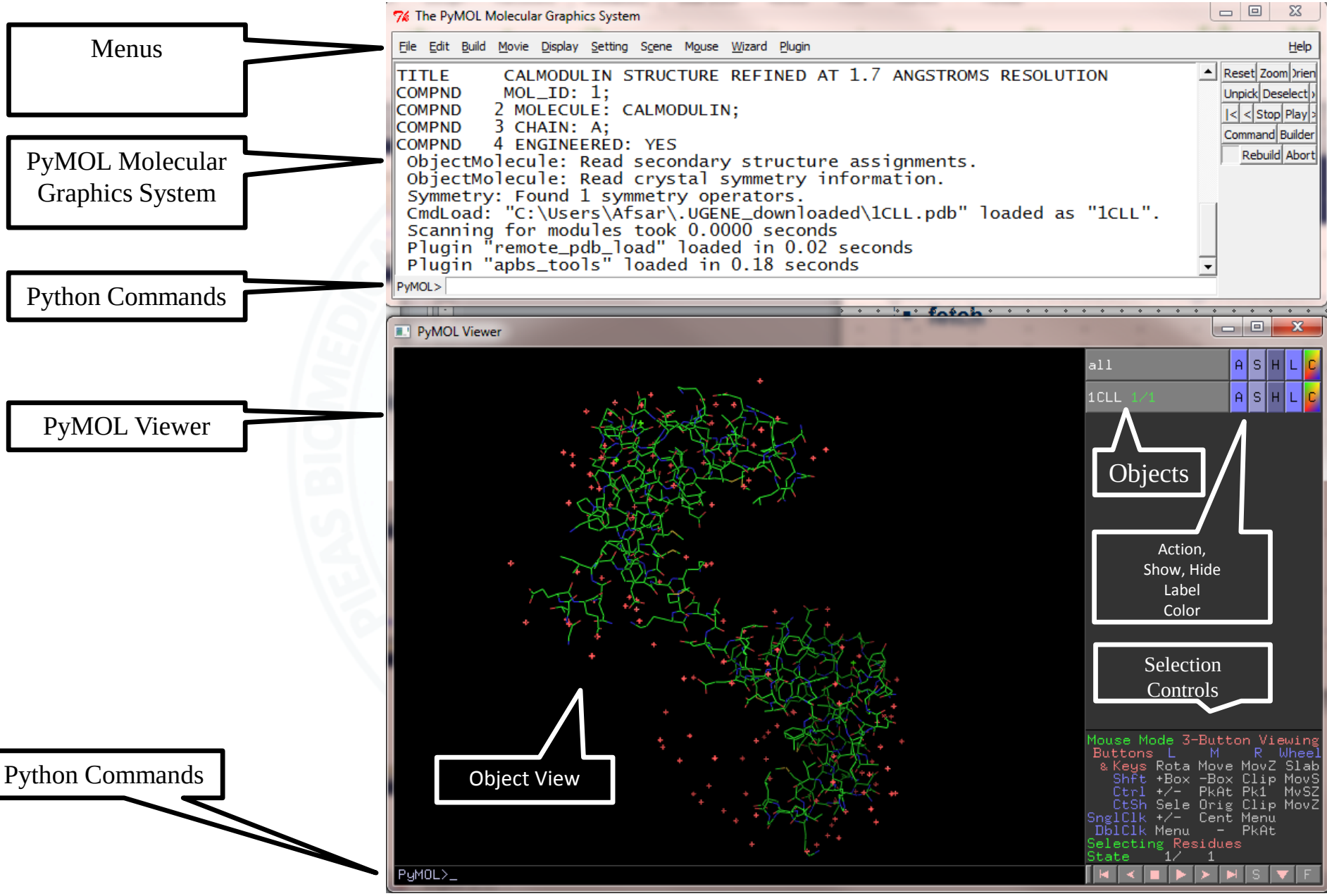
PyMOL

- PyMOL
  - Free *for academic use (http://pymol.org/edu/?q=educational/)
  - Tool for molecular visualization

http://www.pymolwiki.org/index.php/Practical_Pymol_for_Beginners

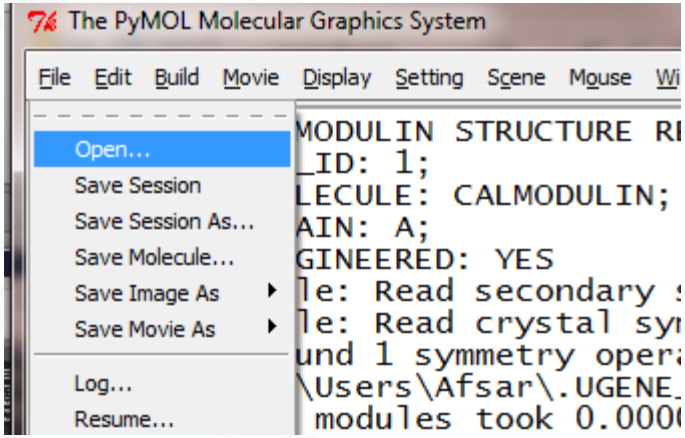

Menus
PyMOL Molecular Graphics System
Python Commands
PyMOL Viewer
Python Commands
The PyMOL Molecular Graphics System
File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help
TITLE CALMODULIN STRUCTURE REFINED AT 1.7 ANGSTROMS RESOLUTION
COMPND MOL_ID: 1;
COMPND 2 MOLECULE: CALMODULIN;
COMPND 3 CHAIN: A;
COMPND 4 ENGINEERED: YES
ObjectMolecule: Read secondary structure assignments.
ObjectMolecule: Read crystal symmetry information.
Symmetry: Found 1 symmetry operators.
CmdLoad: "C:\Users\Afsar\.UGENE_downloaded\1CLL.pdb" loaded as "1CLL".
Scanning for modules took 0.0000 seconds
Plugin "remote_pdb_load" loaded in 0.02 seconds
Plugin "apbs_tools" loaded in 0.18 seconds
PyMOL>
Reset Zoom Orien
Unpick Deselect
Stop Play
Command Builder
Rebuild Abort
PyMOL Viewer
all
1CLL 1/1
Objects
Action, Show, Hide Label Color
Selection Controls
Object View
Mouse Mode 3-Button Viewing
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shft +Box -Box Clip MovS
Ctrl +/- PkAt Pk1 MvSZ
CtSh Sele Orig Clip MovZ
SnglClk +/- Cent Menu
DblClk Menu - PkAt
Selecting Residues
State 1/ 1
PyMOL>_

Visualization types

- Types:
  - Lines
  - Sticks
  - Cartoon
  - Space-fill
  - Surface
- How are secodnary structures assigned?
  - DSSP
  - STRIDE (http://en.wikipedia.org/wiki/STRIDE_%28protein%29)

Commands

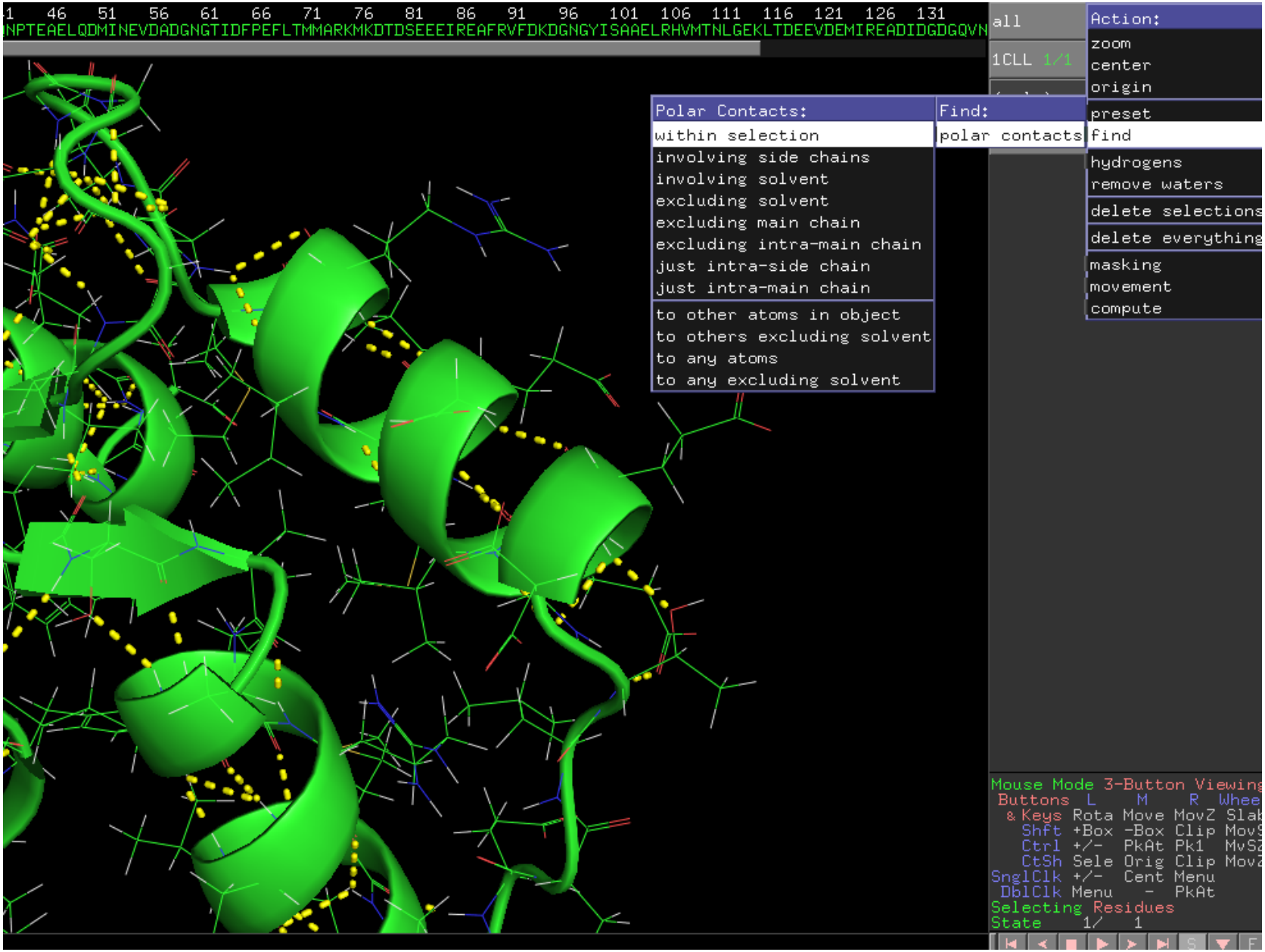
- Fetch
- Open



- Using Mouse
  - Hold Left Click and rotate
  - Hold Right Click and zoom in and out
  - Left Click for selection
  - Right Click for Menu
  - Middle Click and hold to move
  - Roll to change the z-min and z-max of the view window

PyMOL

- Actions
  - Center
  - Hydrogens
  - Remove Waters
  - Deleting
- Show
  - As – lines, sticks, ribbon, cartoon, dots, spheres, mesh and surface
- Hide
  - Everything or certain views
- Label
  - Hide – label
- Color
  - Spectrum or in certain ways



Polar contacts

PyMOL Visualization Exercise

- Load 1CLL
- Visualize 1CLL
  - Show the structure as a cartoon
  - Hide lines
  - Try Action-> Presets (Ligand, technical, b-value)
  - Get rid of Water-atoms
  - Show the Calcium ions as spheres
  - Show lines
  - Show hydrogens
  - Find polar contacts of the calcium ions
  - Select all atoms in an alpha helix and show the hydrogen bonds between them
  - Do the same for a beta sheet
  - Show surface
  - Show Binding sites of EOH

Saving views

- You can save sessions
- You can also create images
  - R click “ray”
  - Display -> Background -> White
  - File -> Save Image As ->…

Using PyMOL for analysis

- View Binding Site of Calcium
- EOH

MORE HELP ON PYMOL

- You can even do programming in Python for visualization
  - VIDEOS!

http://www.pymolwiki.org/index.php/Main_Page

http://www.protein.osaka-u.ac.jp/rcsfp/supracryst/suzuki/jpxtal/Katsutani/en/index.php

Structural Alignment

- Types
  - Global
  - Local
  - Multiple structure alignment
- RMSD
- Methods
  - DALI
  - FSSP
  - ProBiS
  - PyMol

tp://en.wikipedia.org/wiki/Structural_alignment

PyMOL Visualization Assignment

- Load 1CFD & 1DMO
  - Is it showing hydrogens?
- Align the two structures
  - http://www.pymolwiki.org/index.php/Align
  - http://pldserver1.biochem.queensu.ca/~rlc/work/teaching/BCHM823/pymol/alignment/

http://pymol.sourceforge.net/newman/user/toc.html

End of Lecture

It is the true nature of mankind to learn from mistakes, not from example.

Fred Hoyle (lived 1915), British astronomer, mathematician, and writer.
Into Deepest Space (1975).