PyMol tutorial

Made with PyMol 1.7 educational
Feb. 2017
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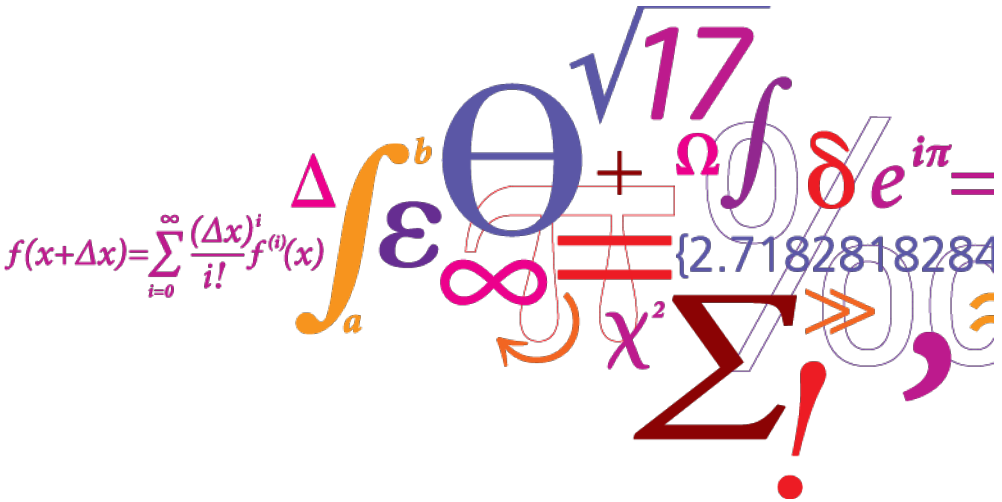
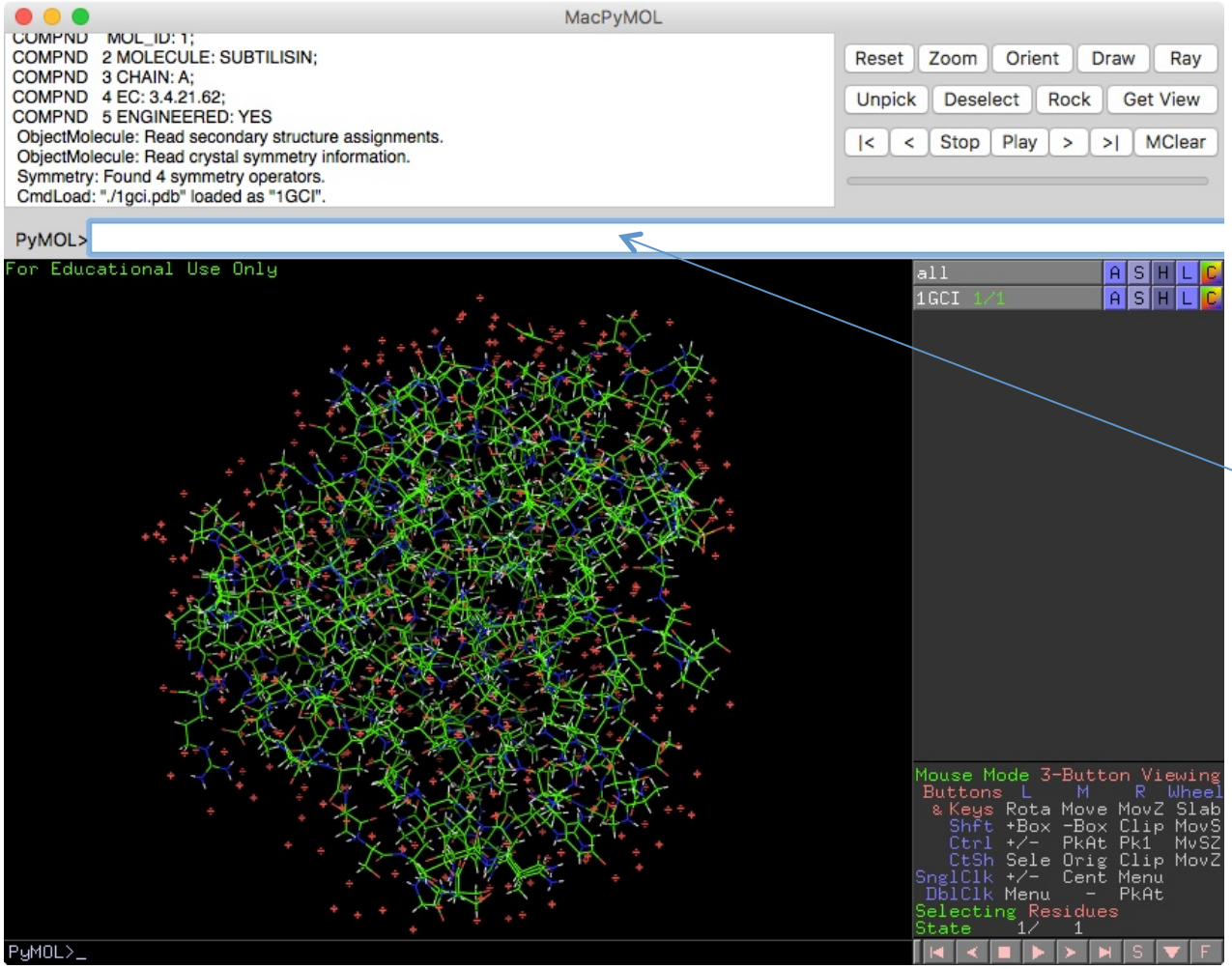


DTU Bioinformatics
Department of Bio and Health Informatics

Loading a structure "fetch 1GCI"



Structure: 1GCI (PDB)

0.78Å structure of Savinase

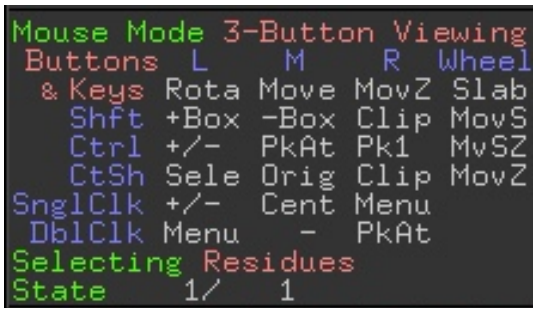
Two ways:

- Write "**fetch 1GCI**" in the command field
- Download .PDB file from pdb.org and use the File->Open menu

TASKS

- Load in the 1GCI structure

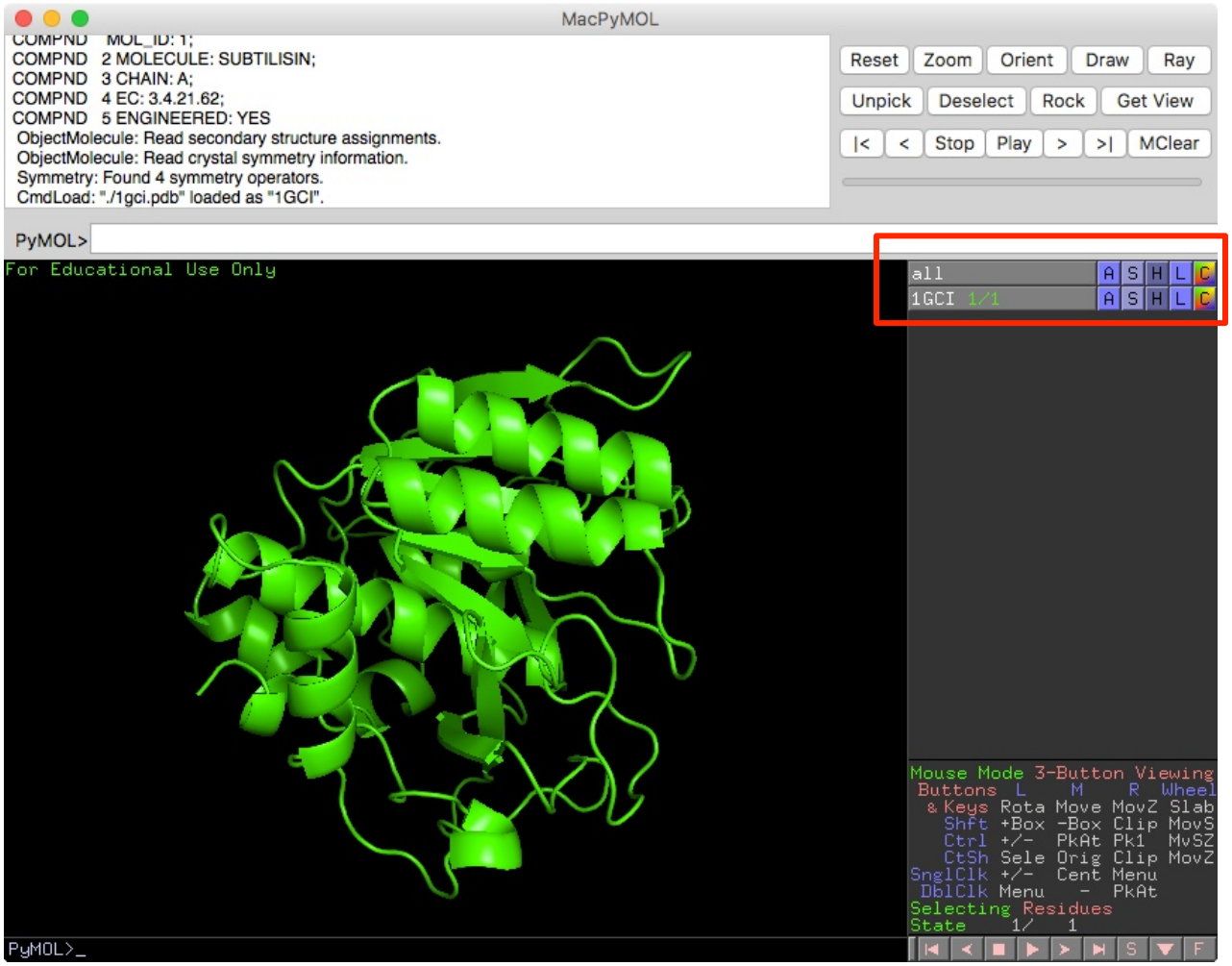
- Play around with the interface – learn how to rotate and zoom the structure:
  - Rotate: Click and hold left mouse button and move around
  - Zoom:
    - 1) Right click + move up/down (a bit slow)
    - 2) Shift + control + scroll wheel
    - 3) Shift + control + two finger drag on mouse pad



- Background info:
  - The structure is of the Novozymes peptidase "Savinase" that we have worked with before

  - PDB link: http://www.rcsb.org/pdb/explore/explore.do?pdbId=1GCI
  - UniProt link: http://www.uniprot.org/uniprot/P29600

Working with the structure



A = Action

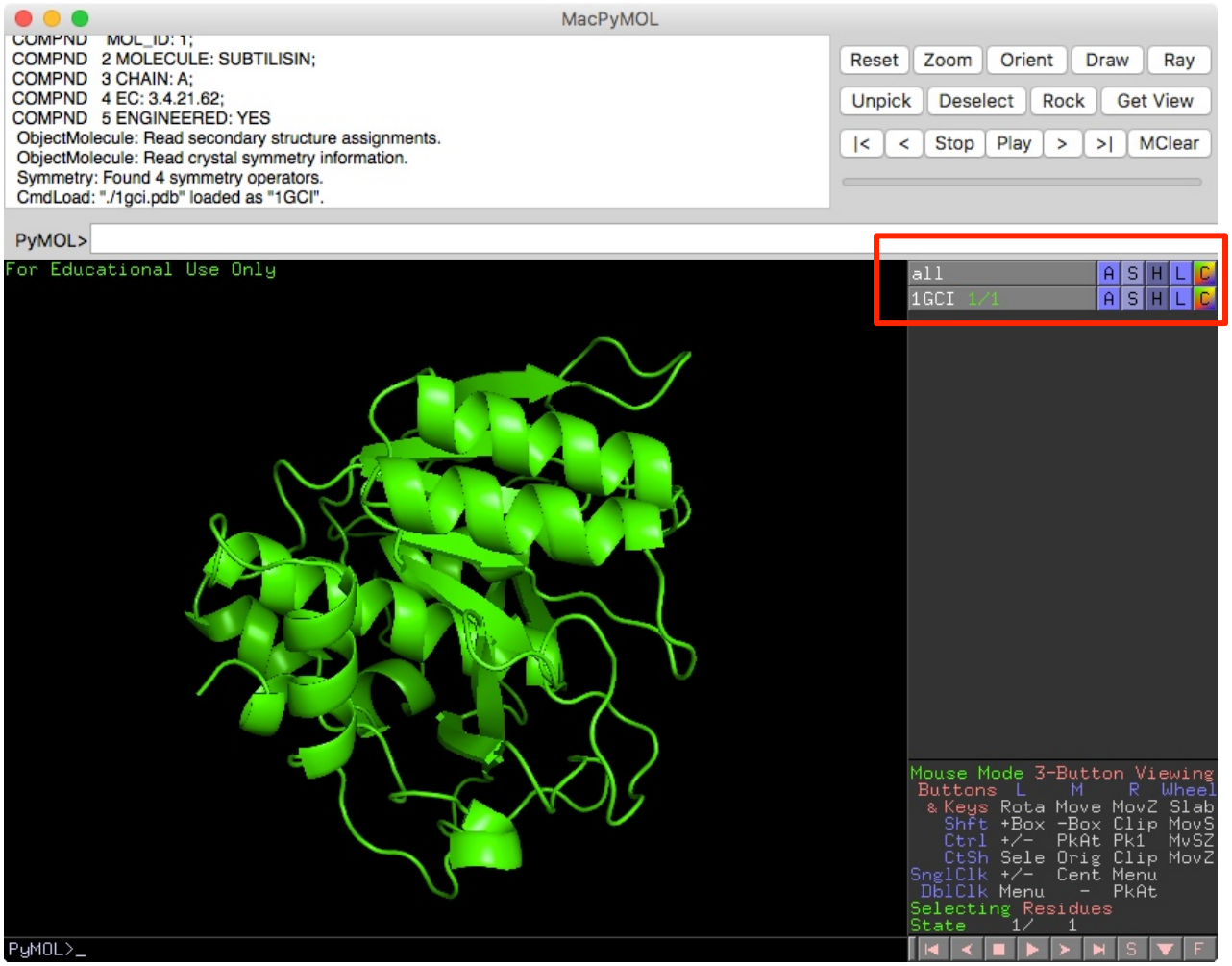
S = Show

H = Hide

L = Label

C = Color

Working with the structure



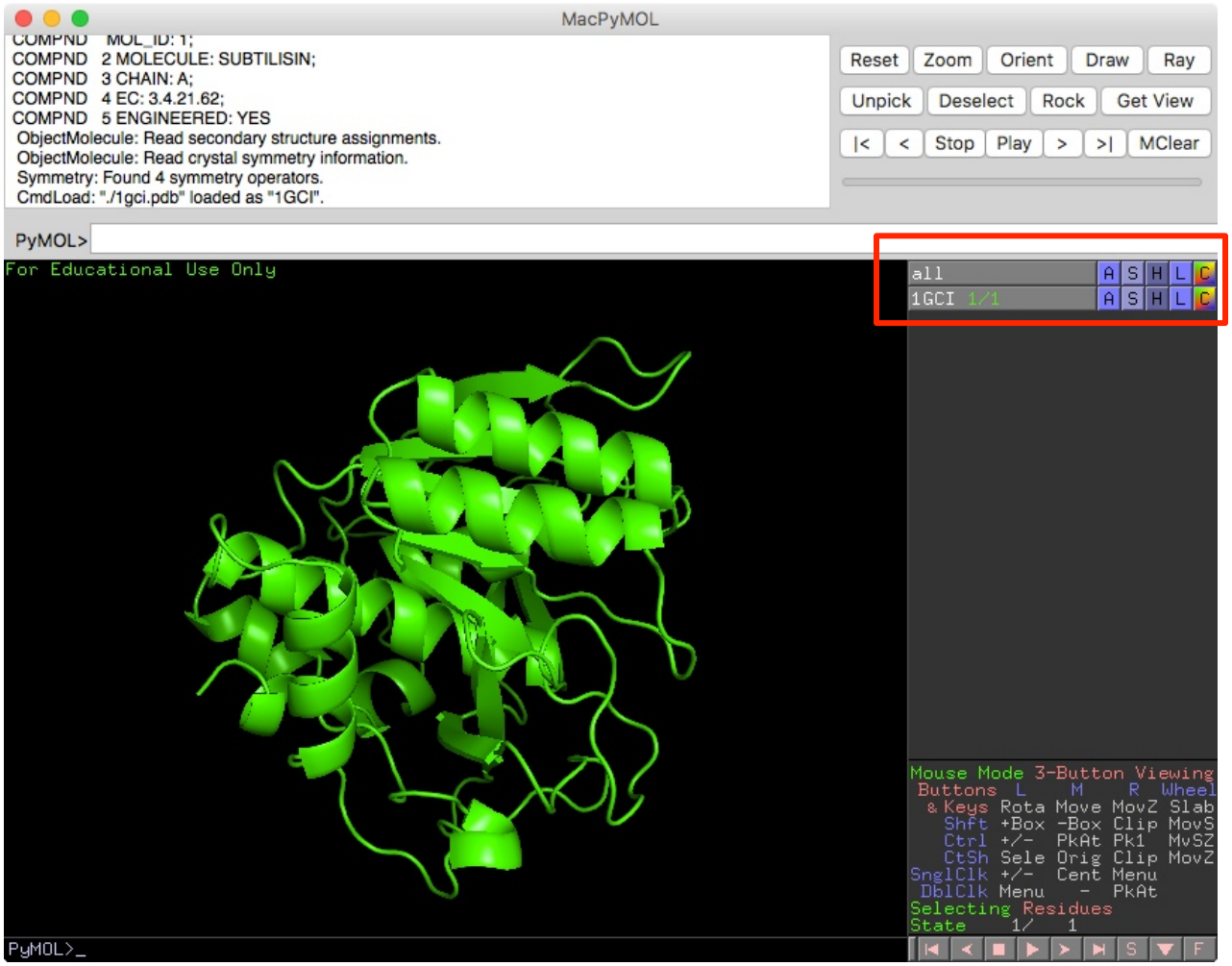
List of things to manipulate

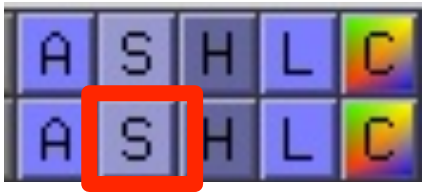
"all": shortcut to ALL objects

1GCI: the structure we have loaded

Multiple structures, peptide chains and selections can be in play, as we shall see later.

Styles





Setting visual style to "Cartoon"

1) Apply new style on top of old:

Press "S" -> Cartoon

2) Apply new style **replacing** the old style:

"S" -> Show AS -> Cartoon

TASKS

- Play around with the visual styles

- Make sure you understand the difference between the two ways of working:
  - S -> something
  - S -> as -> something

- In the end set the style to "Cartoon" **and make sure that is the only style used**.

Colors

Coloring the structure

1) Select any individual color for everything

2) Select a coloring scheme based e.g. on secondary structure

TASKS

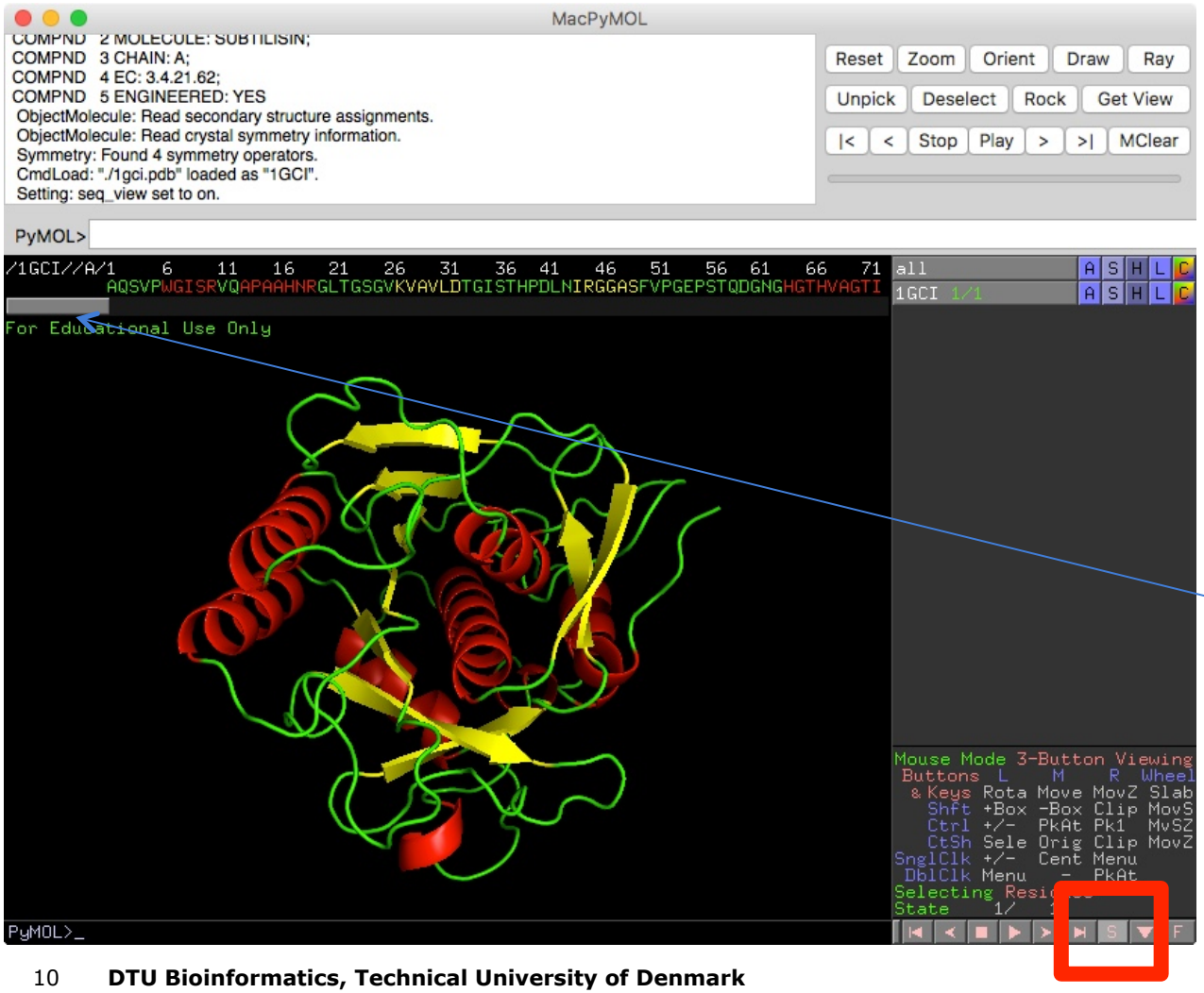
- Play around with the coloring menu and figure out how to change the color of the entire structure (red, green, blue etc.)

- Next, figure out how to color according to the secondary structure, and select a scheme that will high-light 1) alpha helices 2) beta-strand 3) turns

- Rotate the structure to make it easier to see the different kinds of secondary structure

- *… we'll return to coloring, after we have learned how to select subsets of the structure …*

Amino acid sequence



View sequence by:

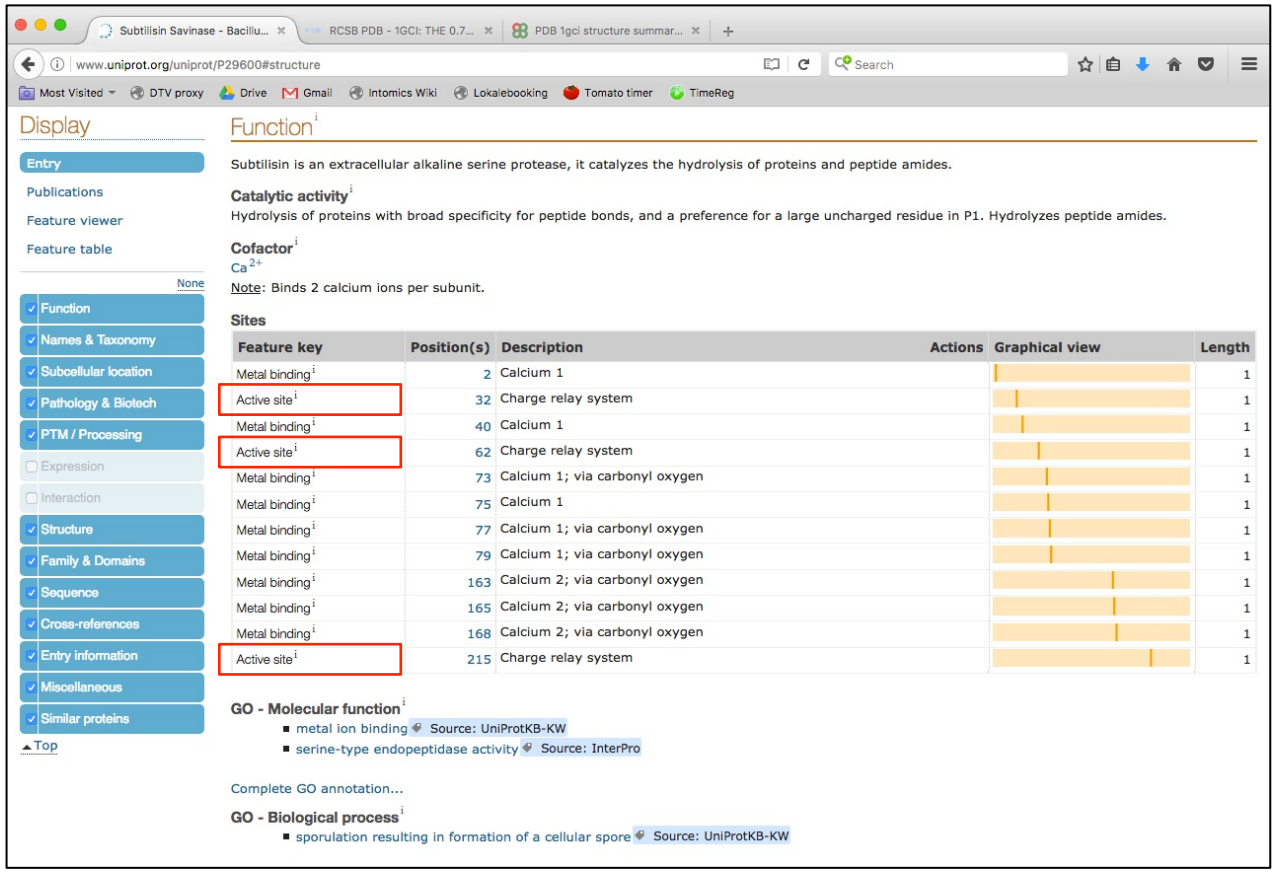
1) Pressing the "S" button in the lower right hand corner

2) Menu: Display -> Sequence On

Scroll by dragging the bar

Select amino acids by clicking them

Active site

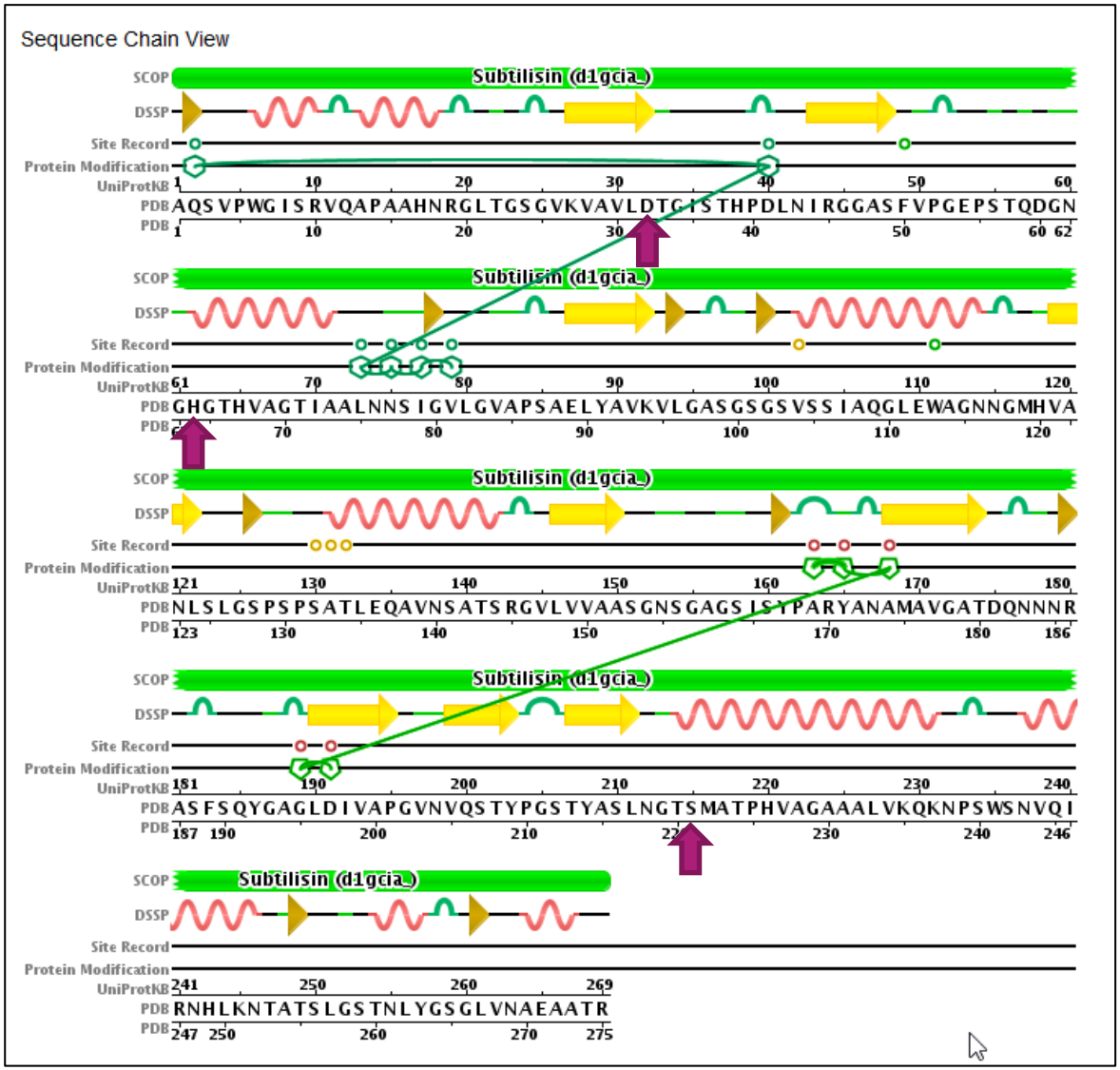


Active site consists of three amino acids

Easy to look up in UniProt

Active site according to UniProt: D32, H62, S215

PDB vs. UniProt numbering



PDB structures may choose to follow a different sequence numbering scheme than UniProt, **even if the sequence is identical!**

This is the case for Savinase, as seen in the figure, and we need to do **coordinate-mapping** of the active site information.

The three amino acids in the active site have been high-lighted.

TASKS

- Turn on sequence mode

- The ACTIVE SITE of the protein consists of (after coordinate mapping):
  - (D) Asp-32
  - (H) His-64
  - (S) Ser-221

- Play around with the sequence bar and figure out how to select these three amino acids (and only those)

Selection

Amino acid residues you click on (in both the sequence and in the actual structure) ends up in a special object named "(sele)".

As with any other object you can apply styles, colors etc. to this object.

That way it's possible to apply a different visualization to a subset of the structure.

TASKS

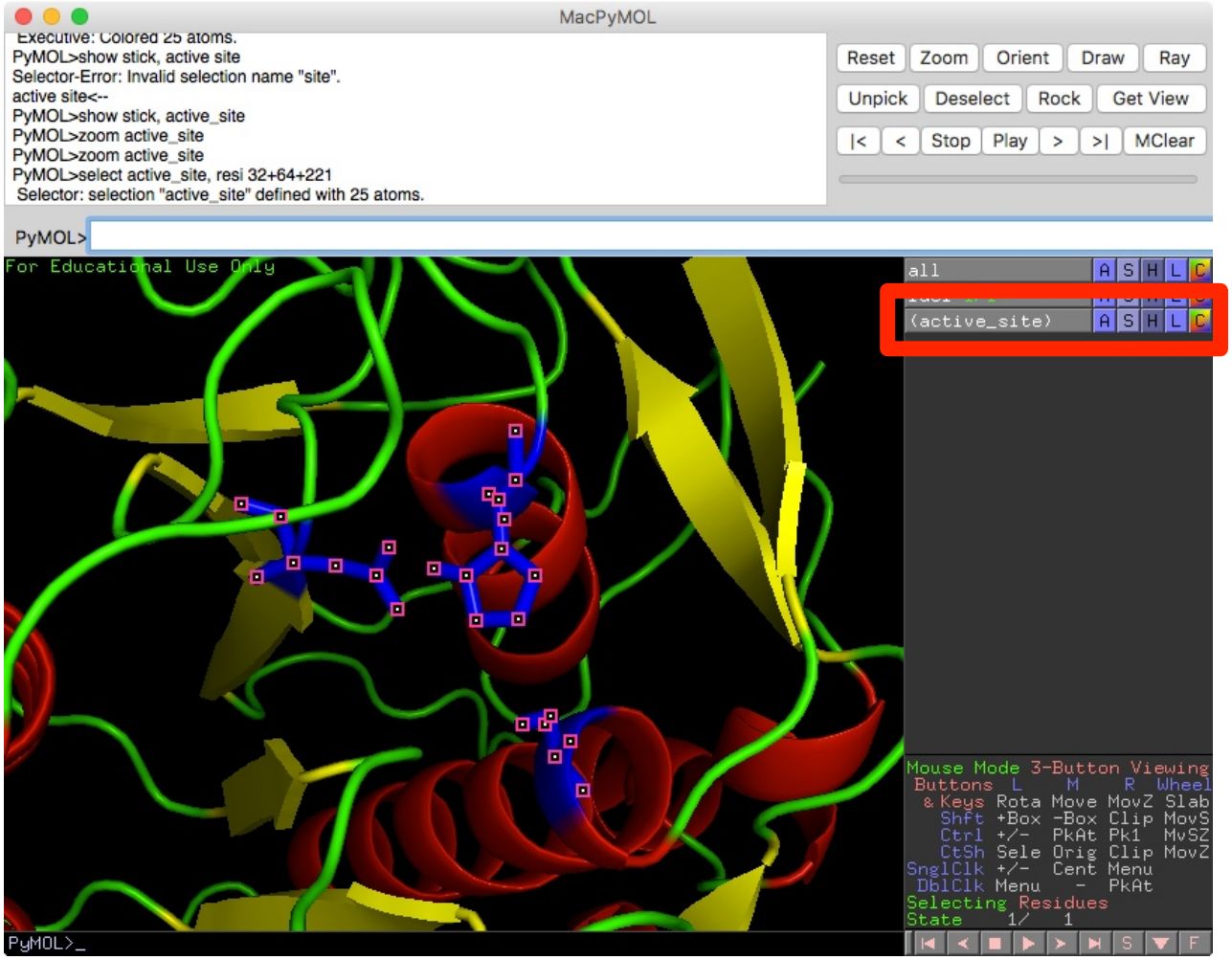
- Work with your selection to show the amino acids in the active site as:
  - "Sticks"
  - With a different color

- Figure out a way to maintain the "Cartoon" style of the backbone and have the sticks show as an additional feature

- If you mess up the visualization you can reset to where we were before by applying the following to the "**1GCI**" object:
  - Show -> As -> Cartoon
  - Color -> By ss -> (pick the first color scheme)

- Finally zoom in a bit so it's easier to see the three amino acids in the catalytic triad
  - Either use the mouse
  - Click "A" -> zoom
  - Or write "**zoom sele**" in the command field

Selection – commands, renaming



Selections can be renamed into something more useful by using the Action (A) button, and thus "saved for later use".

PyMol also makes it possible to specify selection ranges (and name) directly in the command field, as detailed on the next slide

TASK

- Play around with the selection command

- The general syntax for selecting individual amino acids is:
  - select resi 1 (Select only aa #1)
  - select resi 1-5 (Select the range 1-5)
  - select resi 1+5+10 (Select aa#1 and aa#5 and aa#10)

- Select the catalytic triad (D32, H64, S221)

- Rename your selection to something useful for late use:
  - Click “A” -> Rename selection

- You can also specify a name directly in the selection command:
  - select my_name, resi xx+yy+zz

In conclusion

- In this tutorial you have learned how to:
  - Load a structure into PyMol
  - Apply specific styles and colors
  - How to see the amino acid sequence behind the structure
  - How to select specific amino acids ranges in the structure
    - By clicking
    - By using commands
  - How to give those a different visual style + color
  - How to name selections for later use

- PyMol can do a lot of other things, and commands exists for automating the entire process of loading structures, selecting styles, colors, orientation, zooming and exporting the result as images.

- The tutorial has on purpose been kept simple and has only focused on working with amino acid selection – PyMol can do a lot of advanced stuff with atom level selection as well.

- Link to command overview:
  - http://pymol.sourceforge.net/newman/user/S0220commands.html