Universitas Esa Unggul

Smart, Creative and Entrepreneurial

IBT 432 Aplikasi Bioinformatika

Praktik: Visualisasi protein modelling

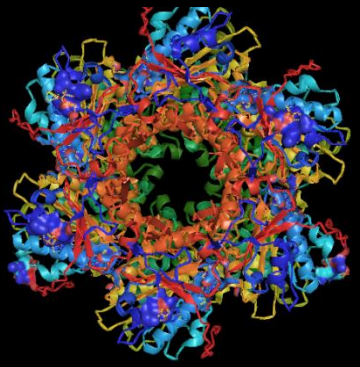
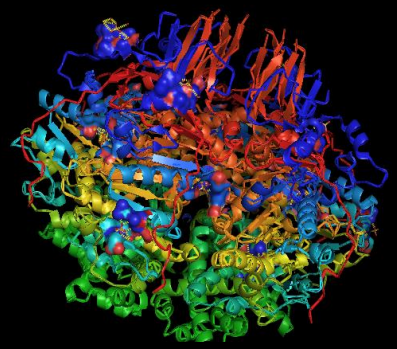
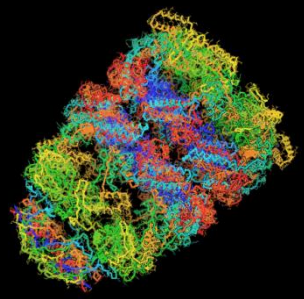
Riza Arief Putranto

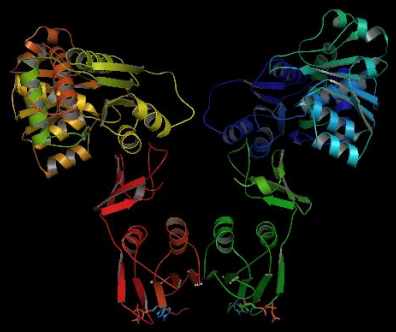
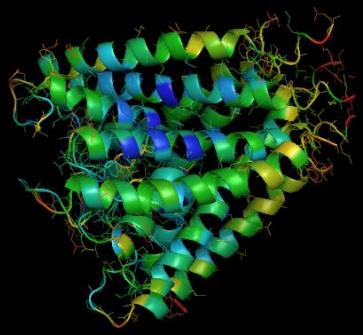
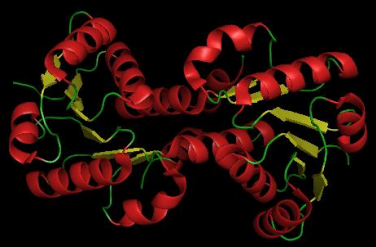
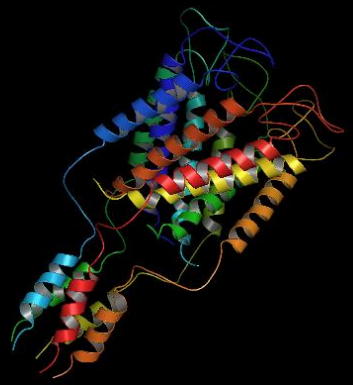
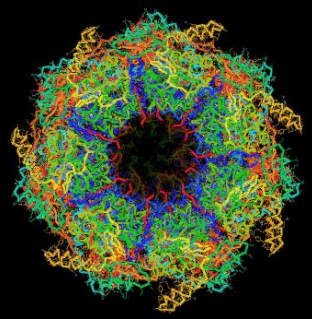
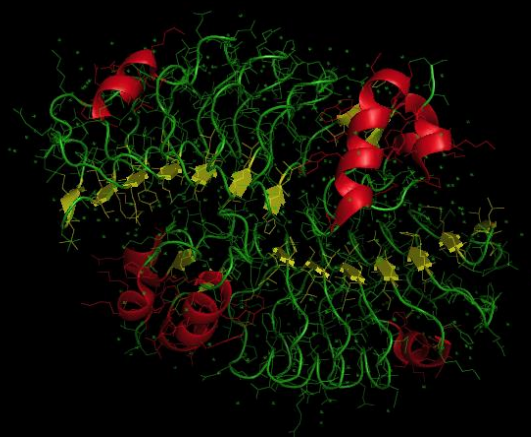
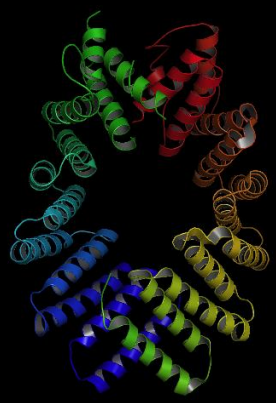
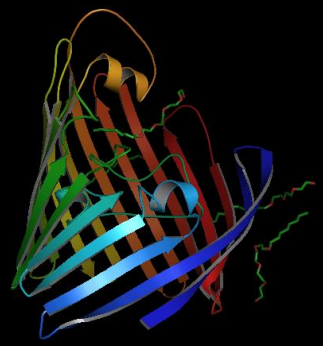
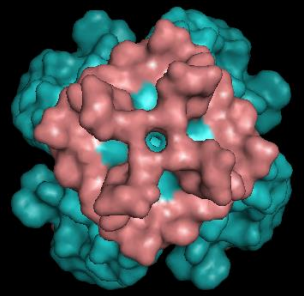
Rencana Perkuliahan

1. ~~Kontrak belajar dan pengenalan bioinformatika aplikatif~~
2. ~~Database sekuen dan analisis genomika~~
3. ~~Anotasi sekuen ke genom - Praktik~~
4. ~~Analisis komparasi genomika I~~
5. ~~Analisis komparasi genomika II~~
6. ~~Analisis komparasi genomika III~~
7. ~~Analisis komparasi genomika – Praktik~~
8. ~~Protein modelling I~~
9. ~~Protein modelling II~~
10. ~~Protein modelling III~~
11. ~~Protein modelling - Praktik~~
12. ~~Visualisasi protein modelling~~
13. Visualisasi protein modelling - Praktik
14. Presentasi mahasiswa

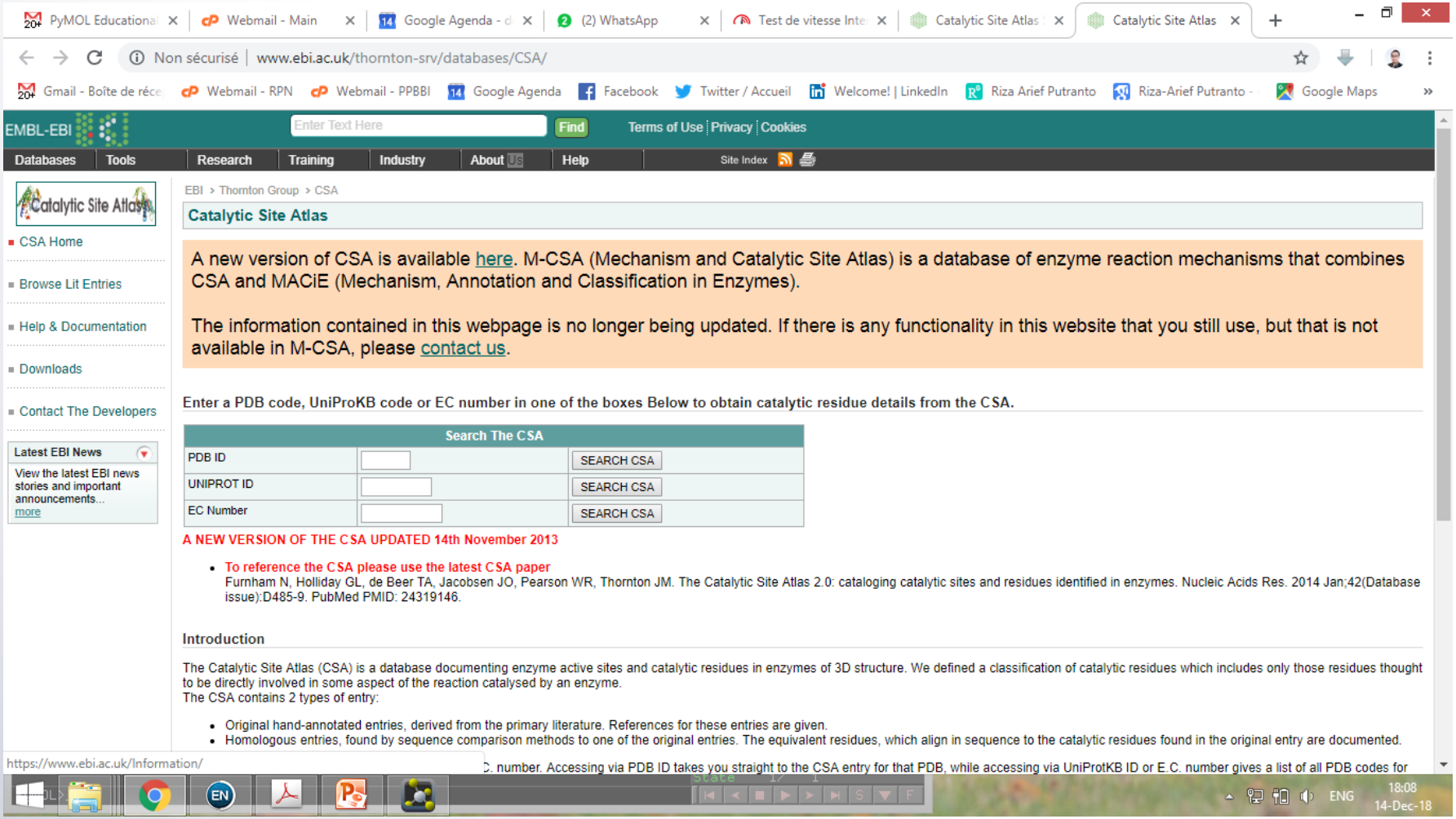
Use the three PDBs below and find each of them, their active site

- 12as
- 2wfh
- 3ceq

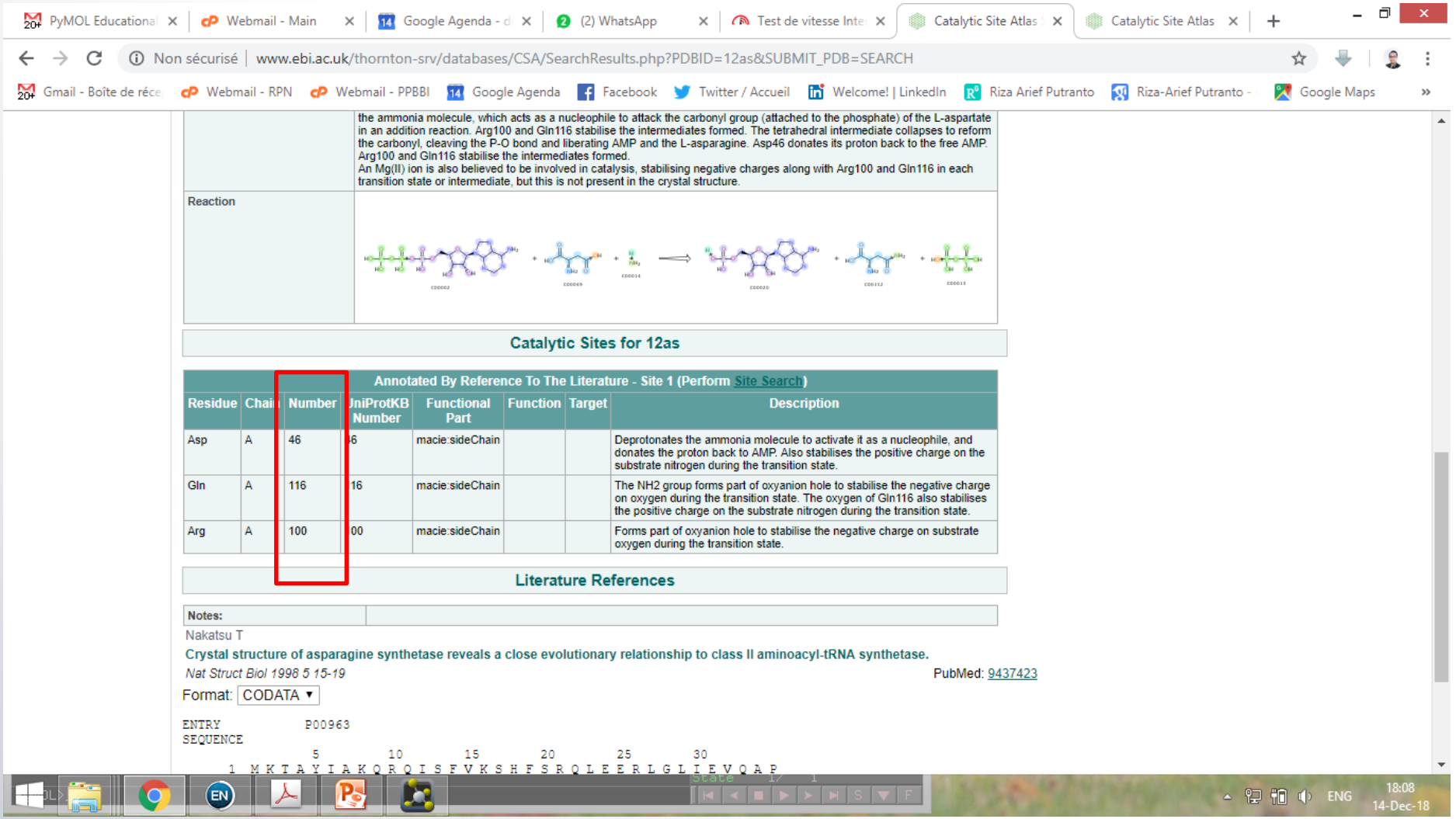




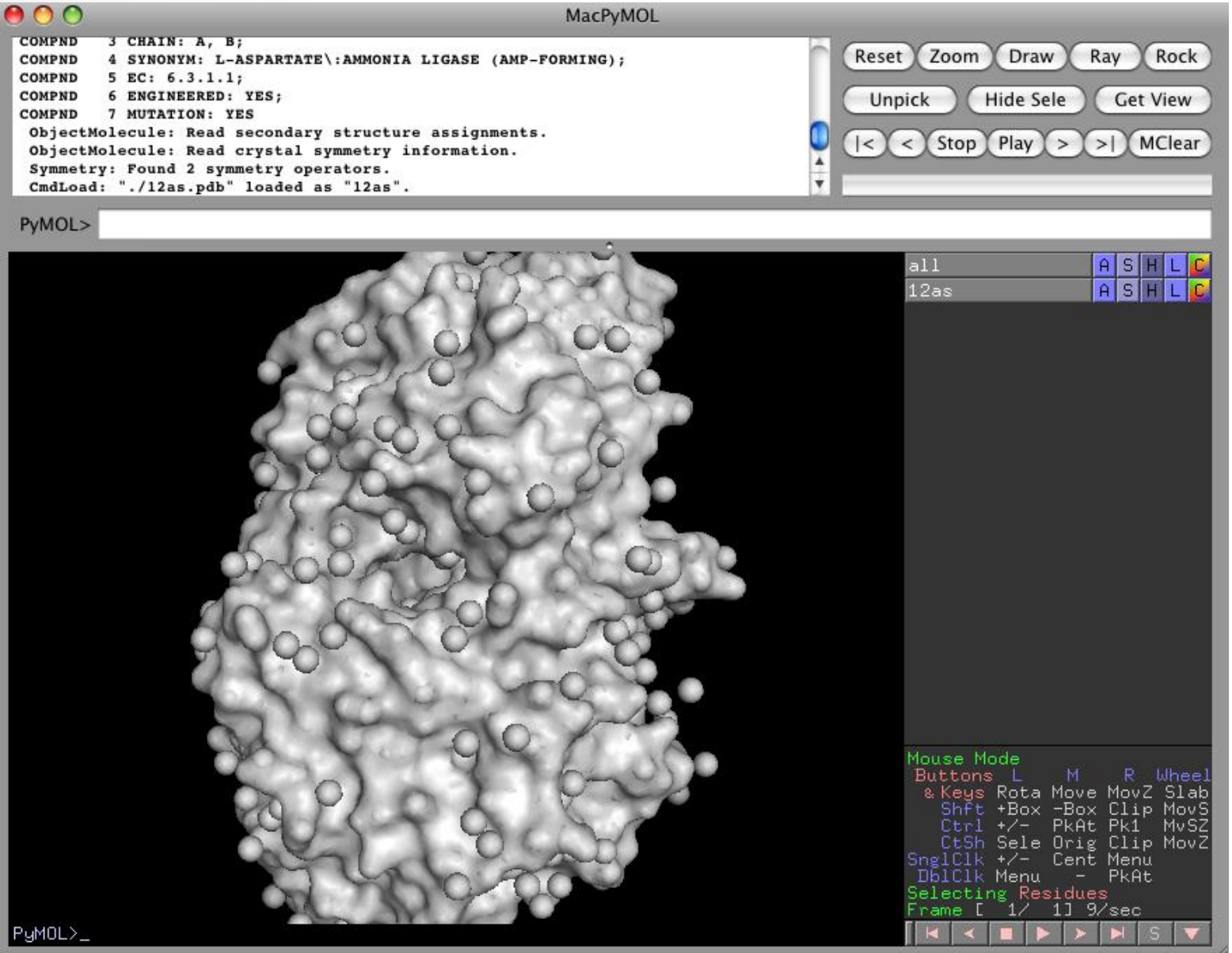
Open Catalytic Site Atlas:
http://www.ebi.ac.uk/thornton-srv/databases/CSA/



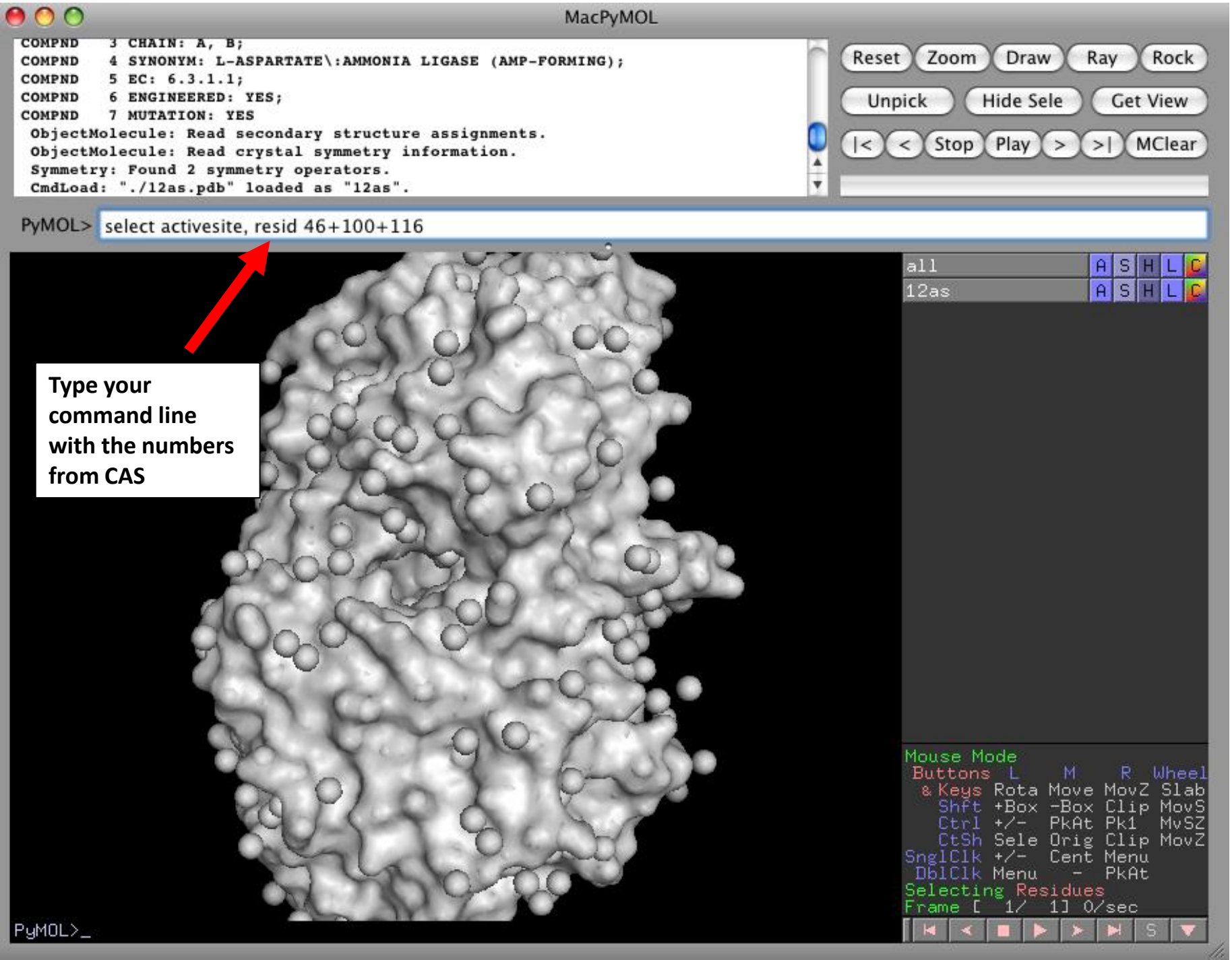
Look for ActiveSite

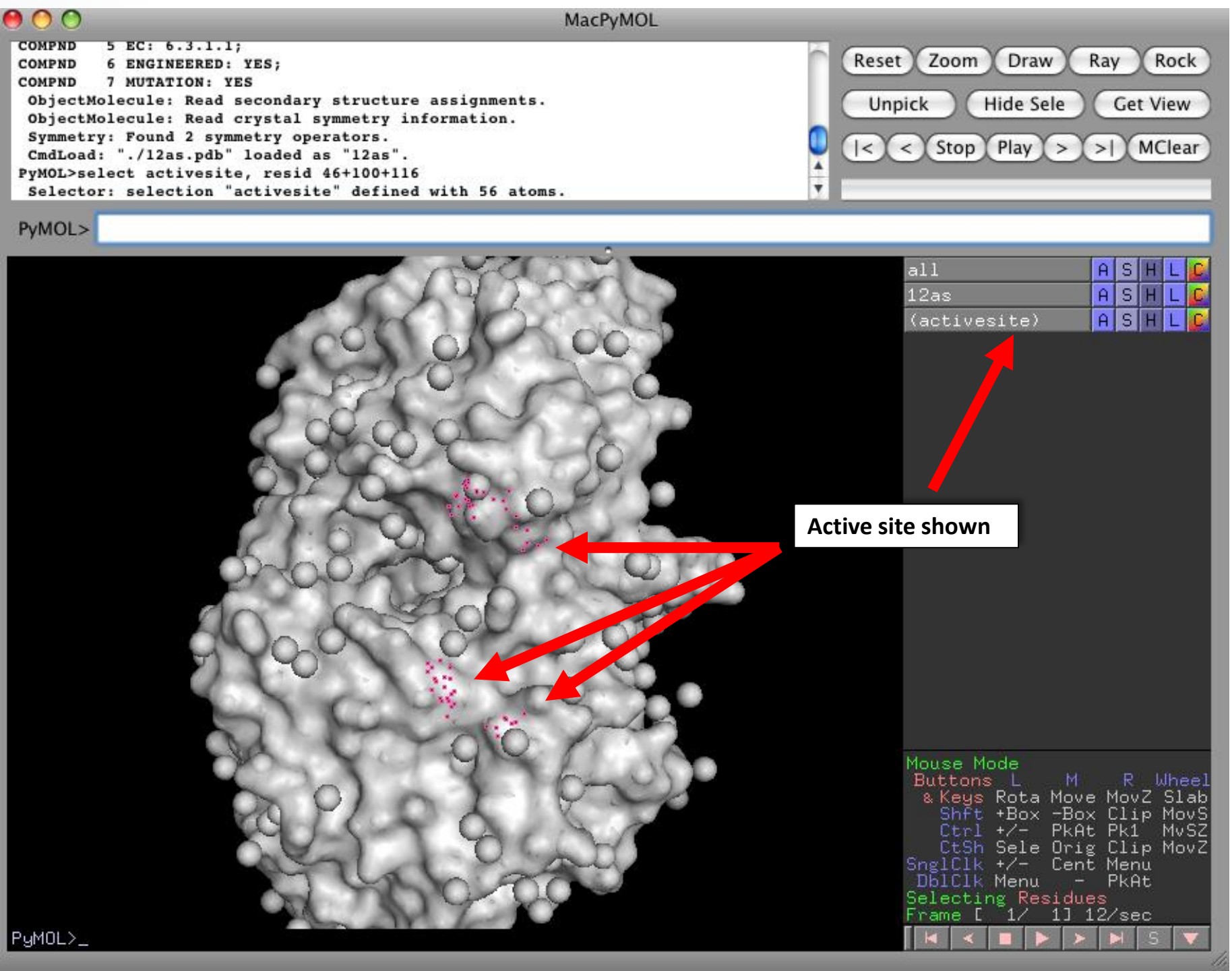


Look for ActiveSite



1. Hide everything
2. Show spheres
3. Show surface
4. Color grays


MacPyMOL
COMPND 3 CHAIN: A, B;
COMPND 4 SYNONYM: L-ASPARTATE\:AMMONIA LIGASE (AMP-FORMING);
COMPND 5 EC: 6.3.1.1;
COMPND 6 ENGINEERED: YES;
COMPND 7 MUTATION: YES
ObjectMolecule: Read secondary structure assignments.
ObjectMolecule: Read crystal symmetry information.
Symmetry: Found 2 symmetry operators.
CmdLoad: "./12as.pdb" loaded as "12as".
Reset
Zoom
Draw
Ray
Rock
Unpick
Hide Sele
Get View
|<
<
Stop
Play
>
>|
MClear
PyMOL>
select activesite, resid 46+100+116
Type your command line with the numbers from CAS
all
12as
A S H L C
Mouse Mode
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
Frame [1/ 1] 0/sec
PyMOL>_


MacPyMOL
COMPND 5 EC: 6.3.1.1;
COMPND 6 ENGINEERED: YES;
COMPND 7 MUTATION: YES
ObjectMolecule: Read secondary structure assignments.
ObjectMolecule: Read crystal symmetry information.
Symmetry: Found 2 symmetry operators.
CmdLoad: "./12as.pdb" loaded as "12as".
PyMOL>select activesite, resid 46+100+116
Selector: selection "activesite" defined with 56 atoms.
Reset
Zoom
Draw
Ray
Rock
Unpick
Hide Sele
Get View
|<
<
Stop
Play
>
>|
MClear
PyMOL>
all
12as
(activesite)
Active site shown
Mouse Mode
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
Frame [1/ 1] 12/sec
PyMOL>_

MacPyMOL

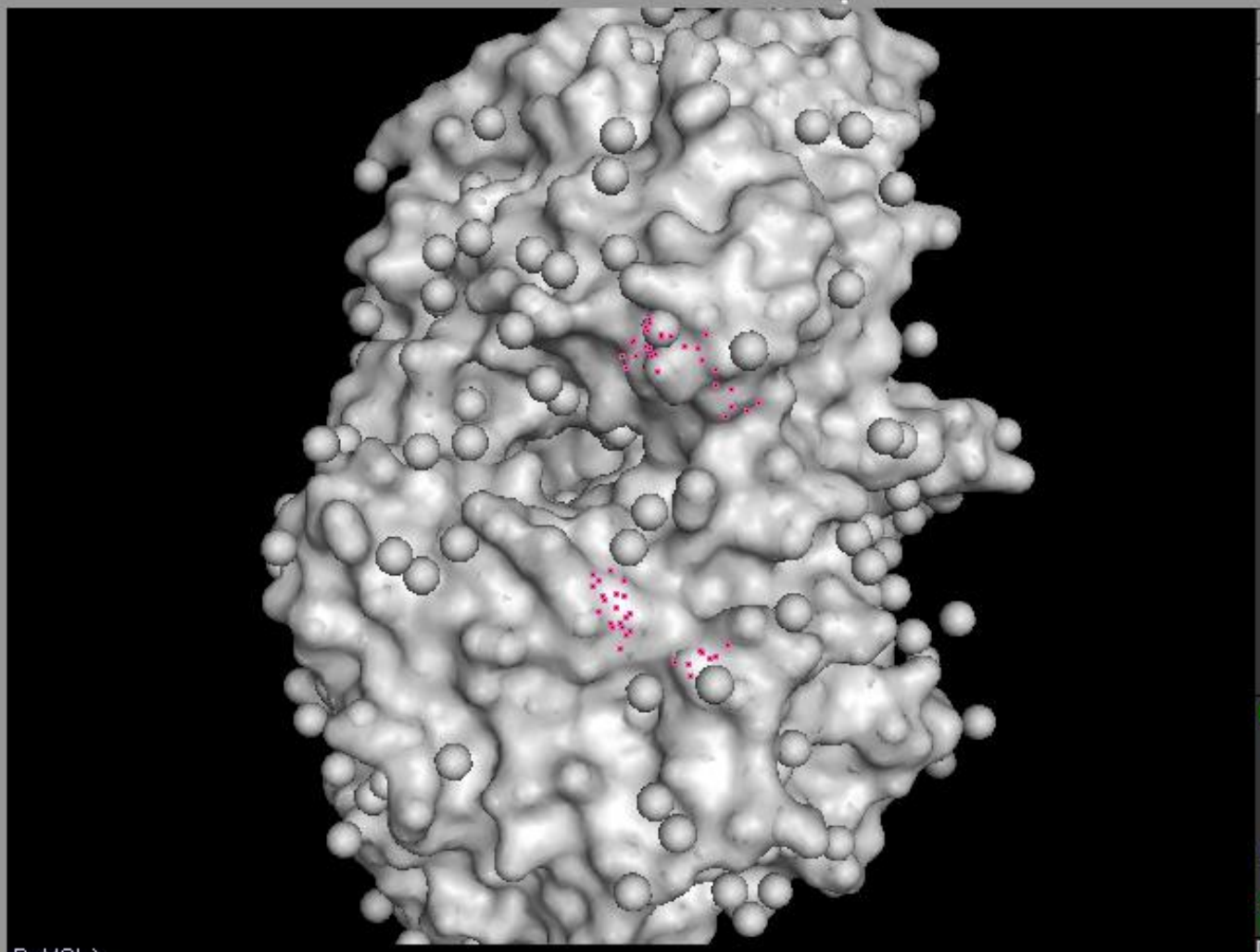
```
COMPND    5 EC: 6.3.1.1;
COMPND    6 ENGINEERED: YES;
COMPND    7 MUTATION: YES
 ObjectMolecule: Read secondary structure assignments.
 ObjectMolecule: Read crystal symmetry information.
 Symmetry: Found 2 symmetry operators.
 CmdLoad: "./12as.pdb" loaded as "12as".
PyMOL>select activesite, resid 46+100+116
 Selector: selection "activesite" defined with 56 atoms.
```

Reset Zoom Draw Ray Rock

Unpick Hide Sele Get View

|< < Stop Play > >| MClear

PyMOL>



all A S H L C

12as A S H L C

(activesite)

Color:
by element
by chain
by ss
spectrum

Reds
red
tv_red
raspberry
darksalmon
salmon
deepsalmon
warmpink
firebrick
ruby
chocolate
brown

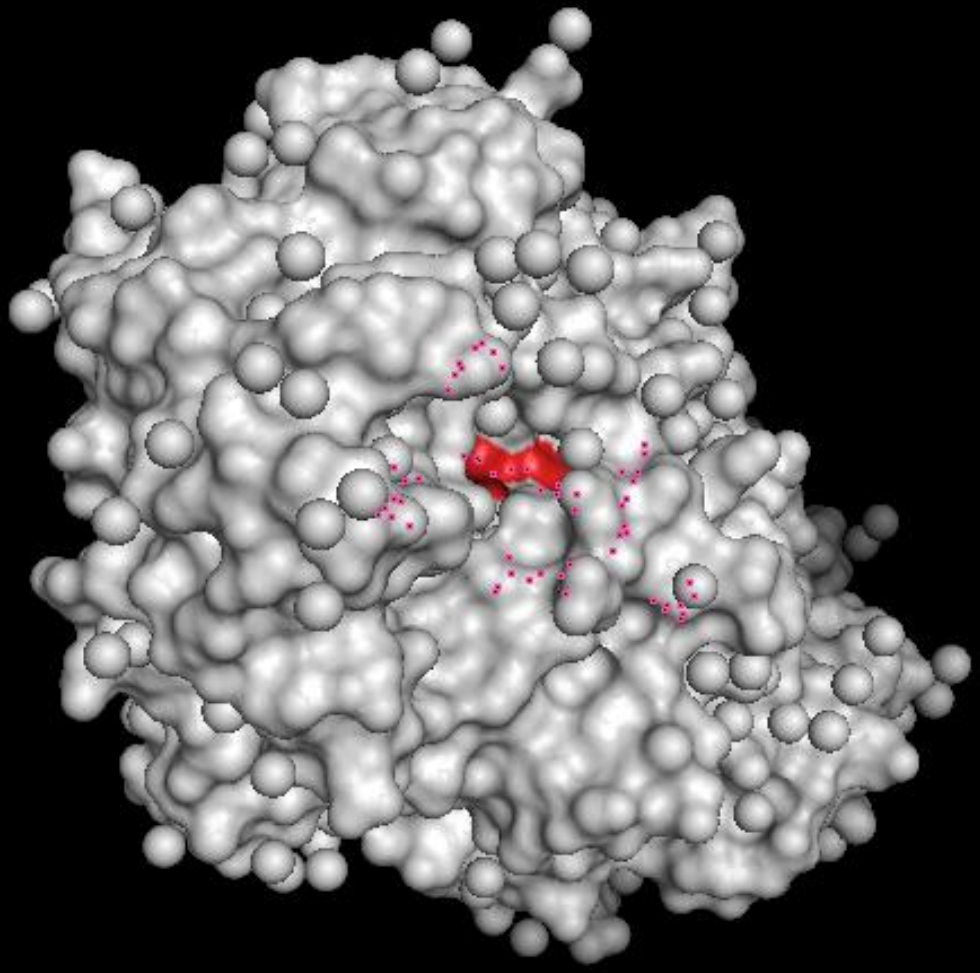
auto
reds
greens
blues
yellows
magentas
cyans
oranges
tints
grays

Mouse Mode
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
Frame [1/ 1] 3/sec

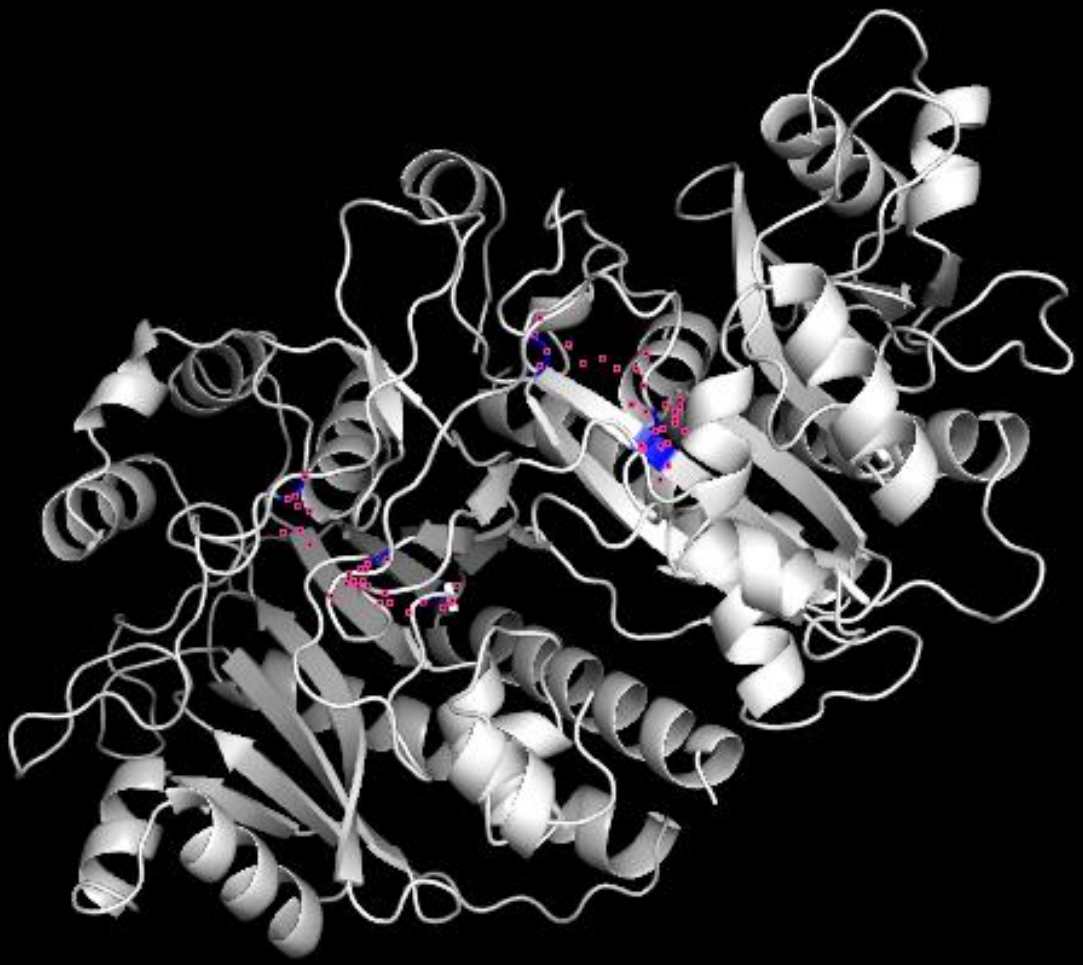
S

PyMOL>_

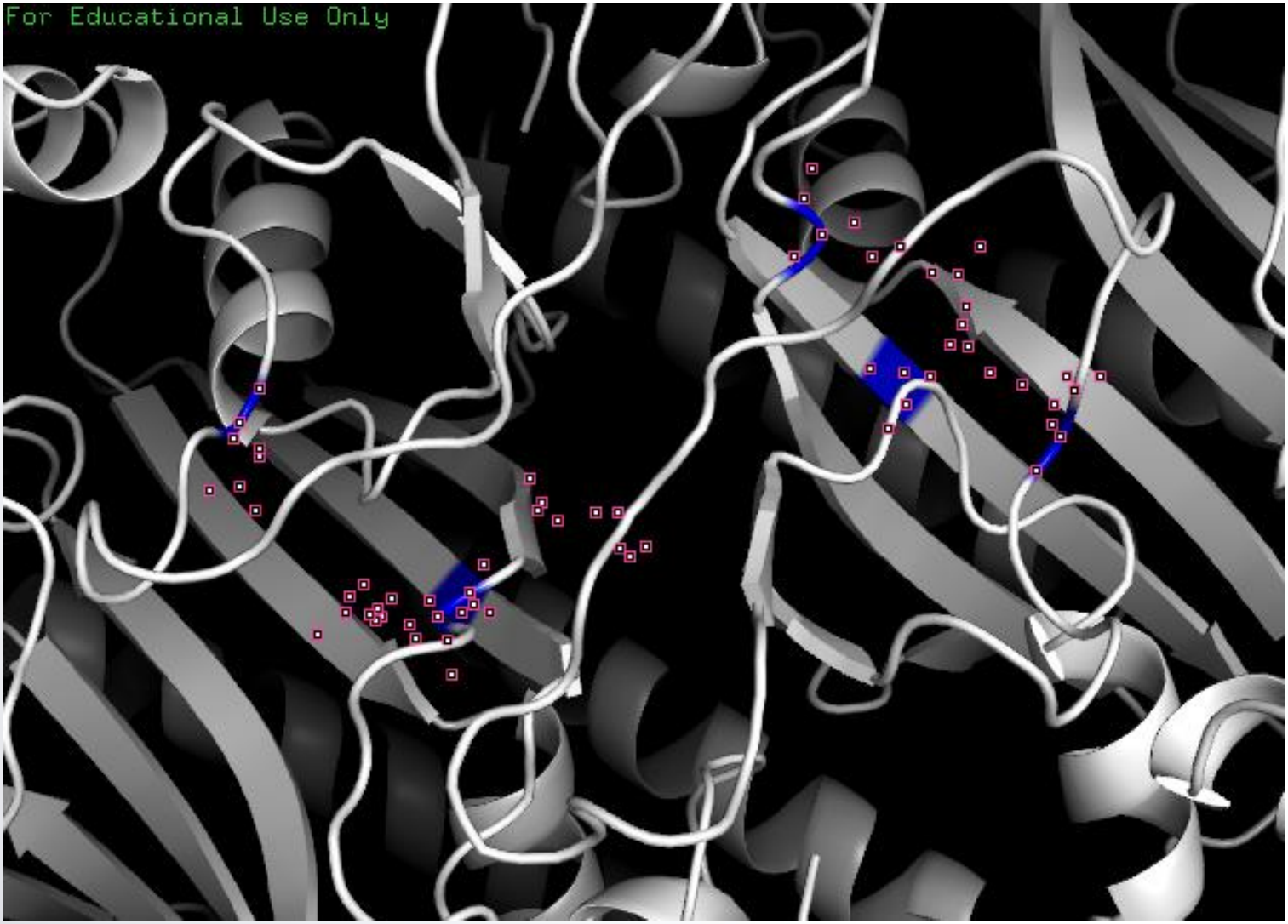
Active site is clearly in a cleft



Switching to cartoon mode
also switched active site residues to stick mode

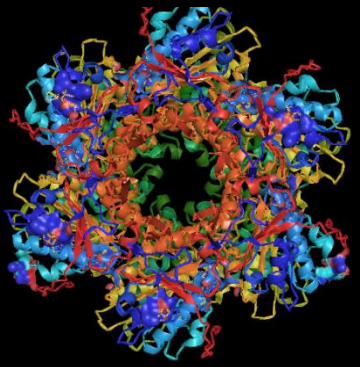


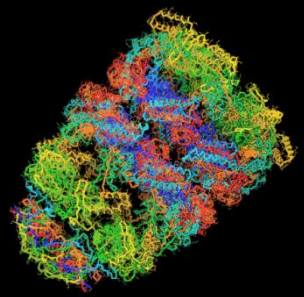
Zooming in on the active site

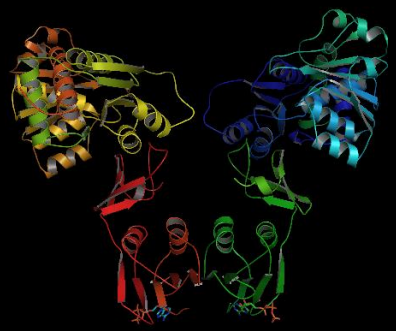
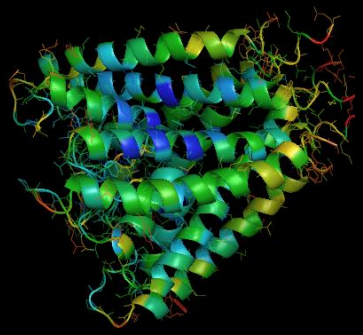
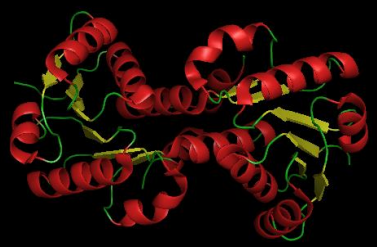
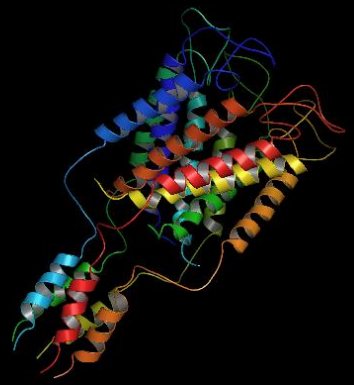
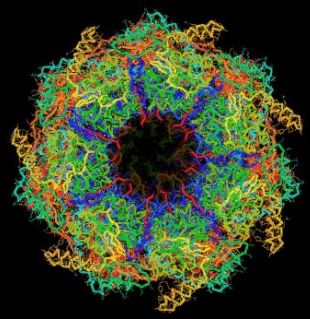
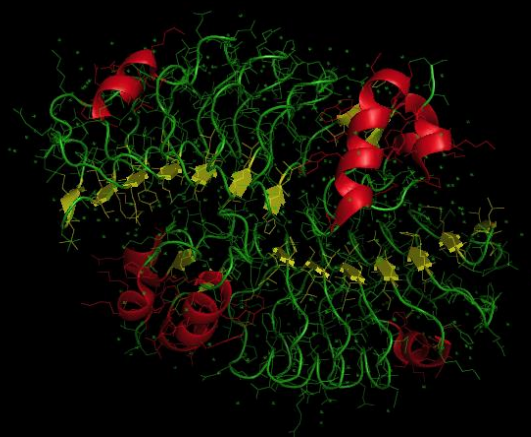
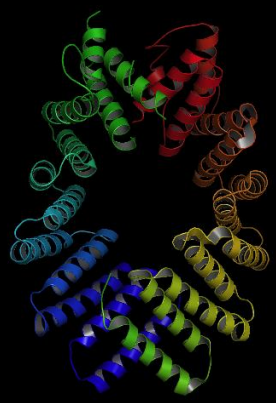
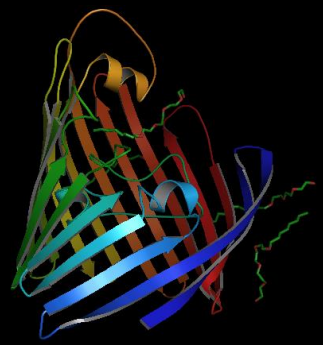
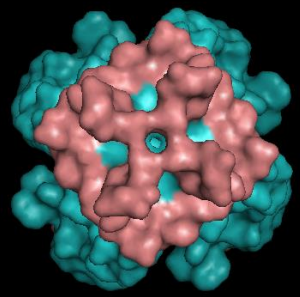


Do the same analysis for the next two PDBs

- ~~12as~~
- 2wfh
- 3ceq





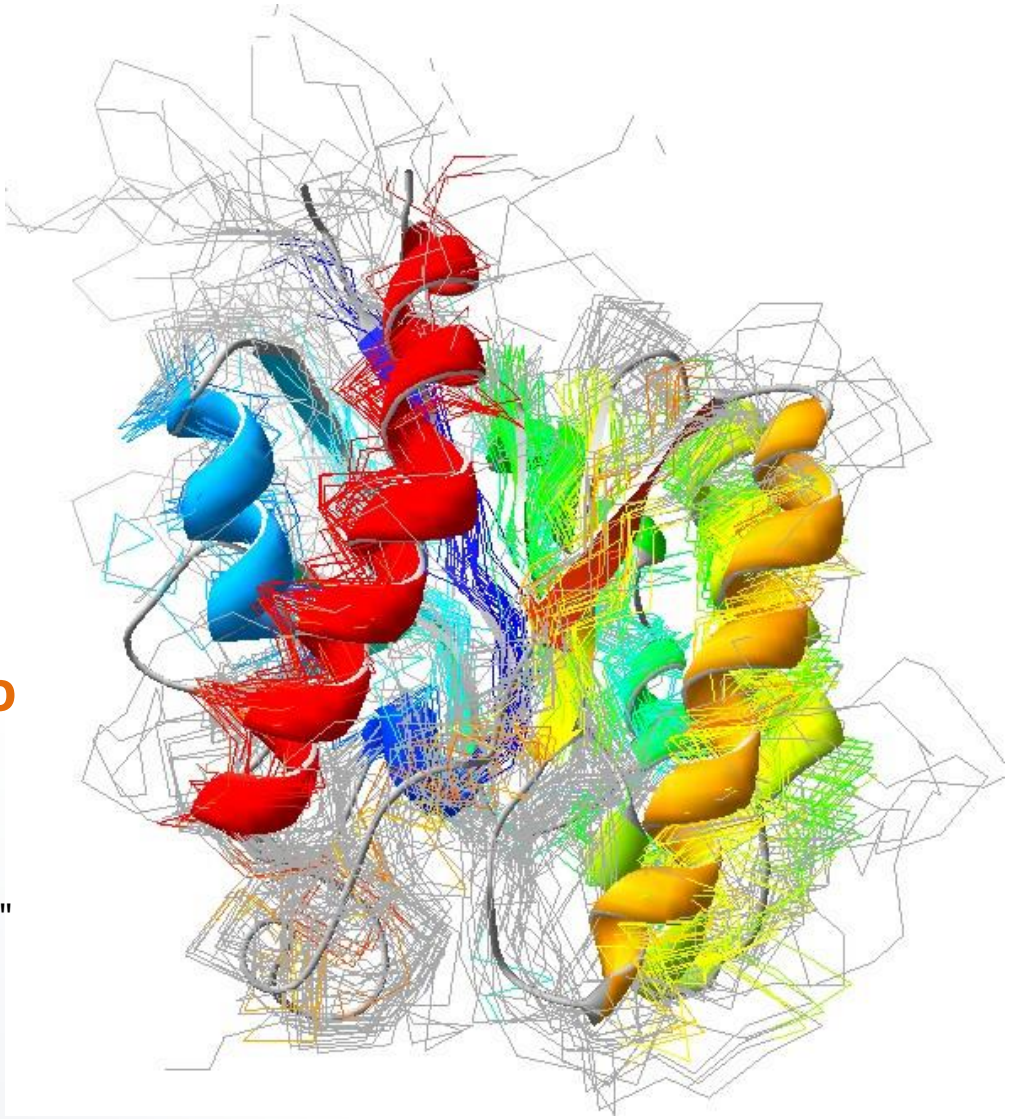










Paradox: modeling is not a real protein

Ceci n'est pas une protéine.

"... a model must be **wrong**, in some respects --- else it would be the thing itself. The trick is **to see** ... **where it is right**."

Henry A. Bent
"Uses (and Abuses) of Models in Teaching Chemistry,"
J. Chem. Ed. 1984 61, 774.



It was still the thirteenth course, don't get dizzy yet