

# IBT 432 Aplikasi Bioinformatika

## Praktik: Visualisasi protein modelling

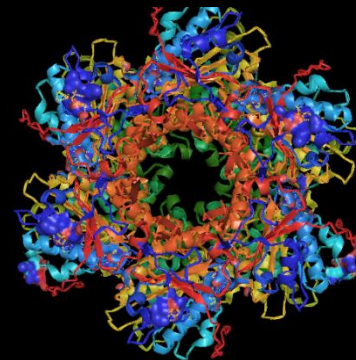
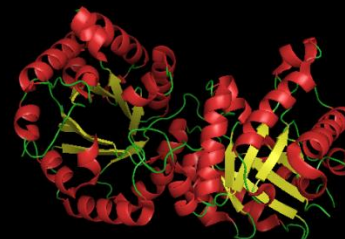
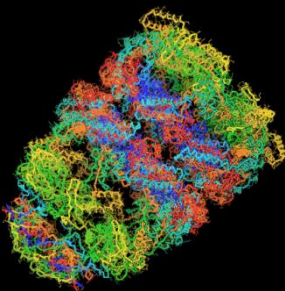
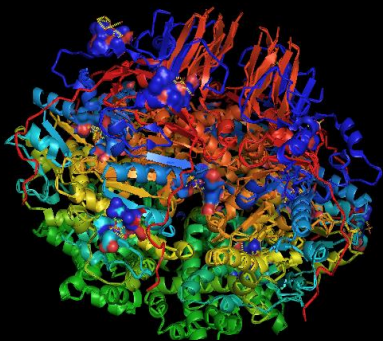
**Riza Arief Putranto**

# Rencana Perkuliahan

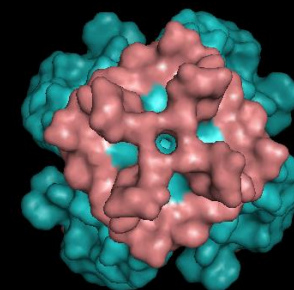
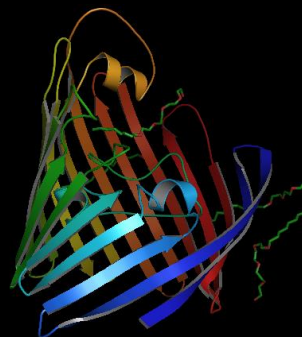
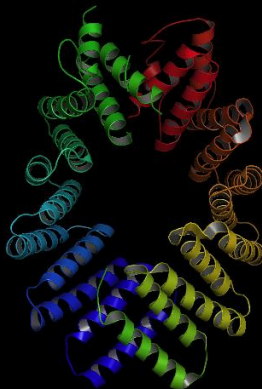
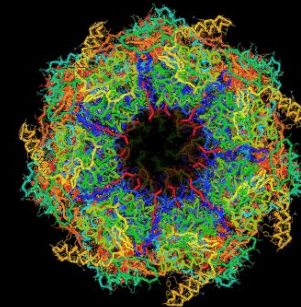
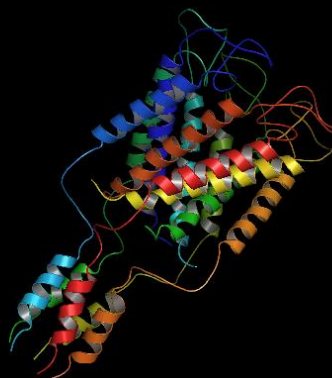
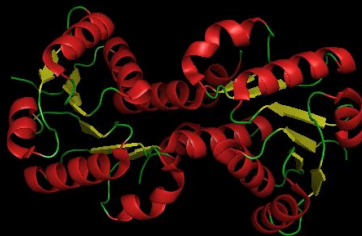
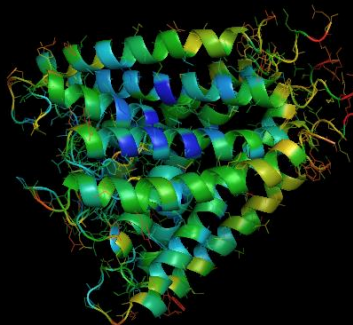
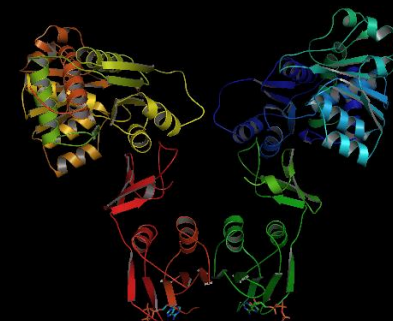
- ~~1. Kontrak belajar dan pengenalan bioinformatika aplikatif~~
- ~~2. Database sekuen dan analisis genomika~~
- ~~3. Anotasi sekuen ke genom – Praktik~~
- ~~4. Analisis komparasi genomika I~~
- ~~5. Analisis komparasi genomika II~~
- ~~6. Analisis komparasi genomika III~~
- ~~7. Analisis komparasi 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



12as



# Open Catalytic Site Atlas:

<http://www.ebi.ac.uk/thornton-srv/databases/CSA/>

The screenshot shows a web browser window with the URL [www.ebi.ac.uk/thornton-srv/databases/CSA/](http://www.ebi.ac.uk/thornton-srv/databases/CSA/). The page header includes the EMBL-EBI logo and navigation links for Databases, Tools, Research, Training, Industry, About, and Help. A search bar is present with the text "Enter Text Here" and a "Find" button. The main content area features a notice about a new version of CSA (M-CSA) and a search interface for PDB ID, UNIPROT ID, and EC Number. The search interface consists of a table with three rows and two columns: the first column contains the input field and the second column contains the "SEARCH CSA" button.

EMBL-EBI  **Find** [Terms of Use](#) [Privacy](#) [Cookies](#)

Databases Tools Research Training Industry About US Help Site Index

EBI > Thornton Group > CSA

## Catalytic Site Atlas

A new version of CSA is available [here](#). M-CSA (Mechanism and Catalytic Site Atlas) is a database of enzyme reaction mechanisms that combines CSA and MACiE (Mechanism, Annotation and Classification in Enzymes).

The information contained in this webpage is no longer being updated. If there is any functionality in this website that you still use, but that is not available in M-CSA, please [contact us](#).

Enter a PDB code, UniProtKB code or EC number in one of the boxes Below to obtain catalytic residue details from the CSA.

Search The CSA	
PDB ID	<input type="text"/> <input type="button" value="SEARCH CSA"/>
UNIPROT ID	<input type="text"/> <input type="button" value="SEARCH CSA"/>
EC Number	<input type="text"/> <input type="button" value="SEARCH CSA"/>

**A NEW VERSION OF THE CSA UPDATED 14th November 2013**

- To reference the CSA please use the latest CSA paper  
Furnham N, Holliday GL, de Beer TA, Jacobsen JO, Pearson WR, Thornton JM. The Catalytic Site Atlas 2.0: cataloging catalytic sites and residues identified in enzymes. Nucleic Acids Res. 2014 Jan;42(Database issue):D485-9. PubMed PMID: 24319146.

### Introduction

The Catalytic Site Atlas (CSA) is a database documenting enzyme active sites and catalytic residues in enzymes of 3D structure. We defined a classification of catalytic residues which includes only those residues thought to be directly involved in some aspect of the reaction catalysed by an enzyme. The CSA contains 2 types of entry:

- Original hand-annotated entries, derived from the primary literature. References for these entries are given.
- Homologous entries, found by sequence comparison methods to one of the original entries. The equivalent residues, which align in sequence to the catalytic residues found in the original entry are documented.

<https://www.ebi.ac.uk/Information/>     . number. Accessing via PDB ID takes you straight to the CSA entry for that PDB, while accessing via UniProtKB ID or E.C. number gives a list of all PDB codes for

18:08  
14-Dec-18

# Look for ActiveSite

PyMOL Educational | Webmail - Main | Google Agenda - d | (2) WhatsApp | Test de vitesse Inte | Catalytic Site Atlas | Catalytic Site Atlas

Non sécurisé | www.ebi.ac.uk/thornton-srv/databases/CSA/SearchResults.php?PDBID=12as&SUBMIT\_PDB=SEARCH

Gmail - Boîte de réce | Webmail - RPN | Webmail - PPBBI | Google Agenda | Facebook | Twitter / Accueil | Welcome! | LinkedIn | Riza Arief Putranto | Riza-Arief Putranto - | Google Maps

the ammonia molecule, which acts as a nucleophile to attack the carbonyl group (attached to the phosphate) of the L-aspartate in an addition reaction. Arg100 and Gln116 stabilise the intermediates formed. The tetrahedral intermediate collapses to reform the carbonyl, cleaving the P-O bond and liberating AMP and the L-asparagine. Asp46 donates its proton back to the free AMP. Arg100 and Gln116 stabilise the intermediates formed. An Mg(II) ion is also believed to be involved in catalysis, stabilising negative charges along with Arg100 and Gln116 in each transition state or intermediate, but this is not present in the crystal structure.

Reaction

**Catalytic Sites for 12as**

Annotated By Reference To The Literature - Site 1 (Perform <a href="#">Site Search</a> )							
Residue	Chain	Number	JniProtKB Number	Functional Part	Function	Target	Description
Asp	A	46	06	macie:sideChain			Deprotonates the ammonia molecule to activate it as a nucleophile, and donates the proton back to AMP. Also stabilises the positive charge on the substrate nitrogen during the transition state.
Gln	A	116	16	macie:sideChain			The NH2 group forms part of oxyanion hole to stabilise the negative charge on oxygen during the transition state. The oxygen of Gln116 also stabilises the positive charge on the substrate nitrogen during the transition state.
Arg	A	100	00	macie:sideChain			Forms part of oxyanion hole to stabilise the negative charge on substrate oxygen during the transition state.

**Literature References**

Notes:

Nakatsu T  
**Crystal structure of asparagine synthetase reveals a close evolutionary relationship to class II aminoacyl-tRNA synthetase.**  
*Nat Struct Biol* 1996 5 15-19 PubMed: [9437423](#)

Format:

ENTRY P00963  
 SEQUENCE

1 M K T A Y I A K Q R I S F V K S H F S R Q L E E R L G L I E V Q A P

# Look for ActiveSite

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".
```

PyMOL>

all A S H L C  
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 ] 9/sec

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

```

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".

```

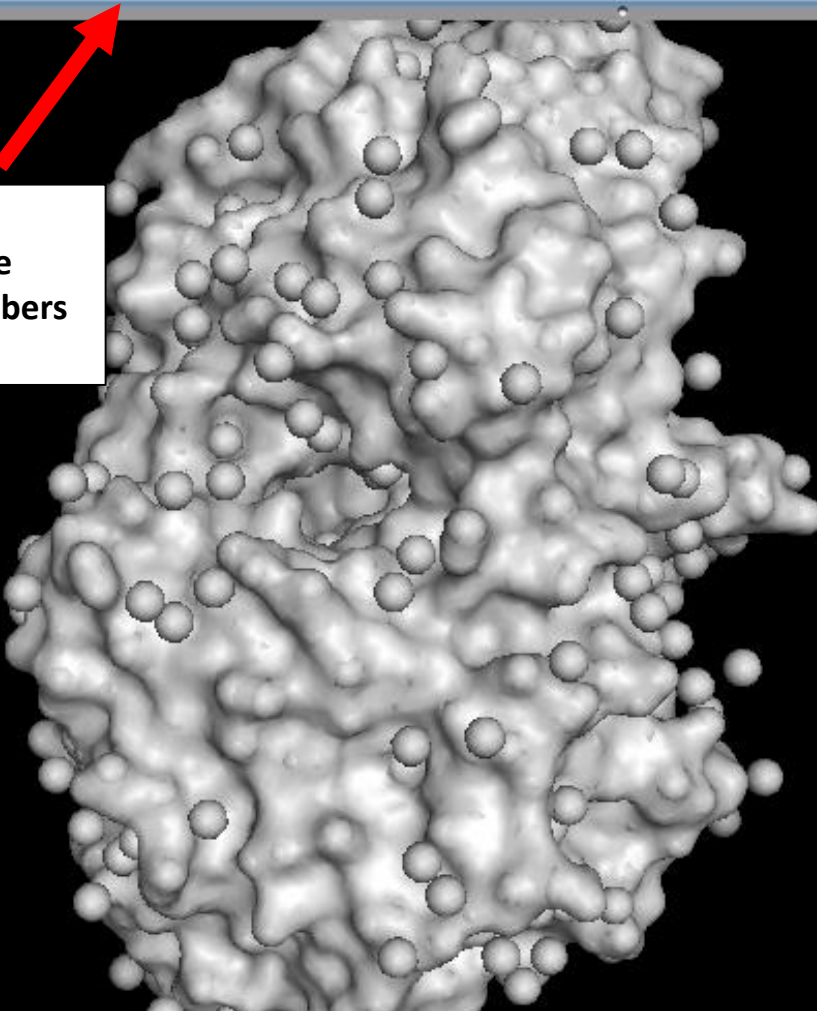
Reset Zoom Draw Ray Rock

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	A	S	H	L	C
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	
Db1Clk	Menu	-	PkAt	

Selecting Residues

Frame [ 1 / 11 ] 0/sec

PyMOL>\_

```

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.

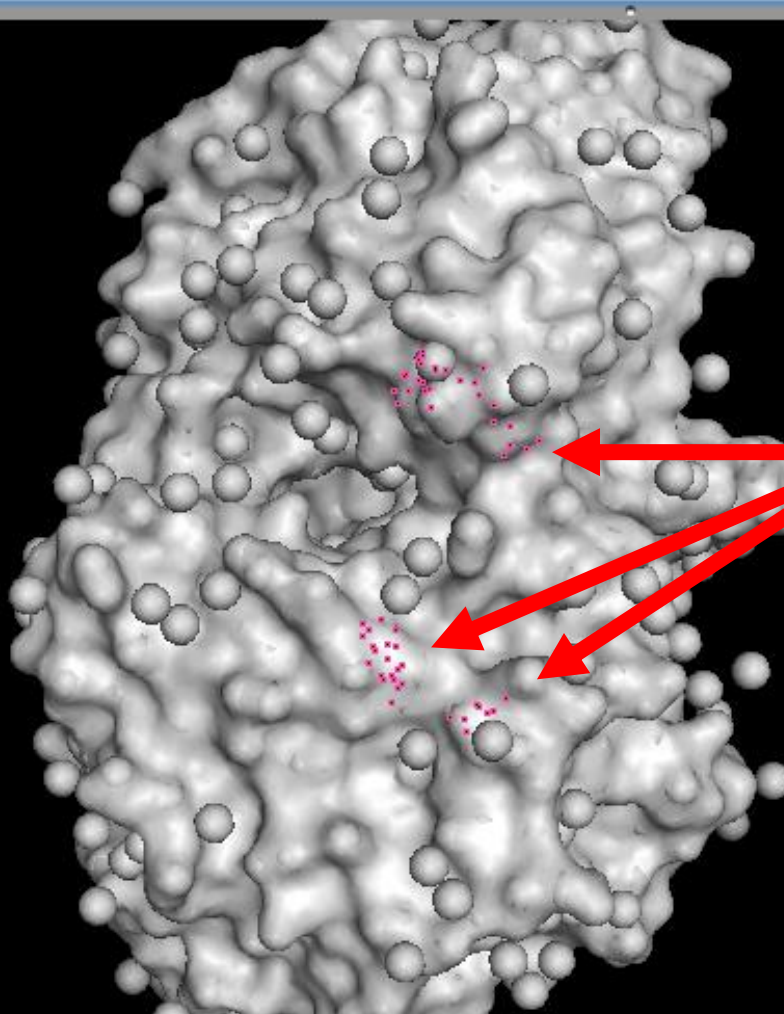
```

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)	A	S	H	L	C

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	
Db1Clk	Menu	-	PKAt	

Selecting Residues

Frame [ 1 / 1 ] 12/sec

PyMOL>\_



Reset Zoom Draw Ray Rock

Unpick Hide Sele Get View

|&lt; &lt; Stop Play &gt; &gt;| MClear

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.

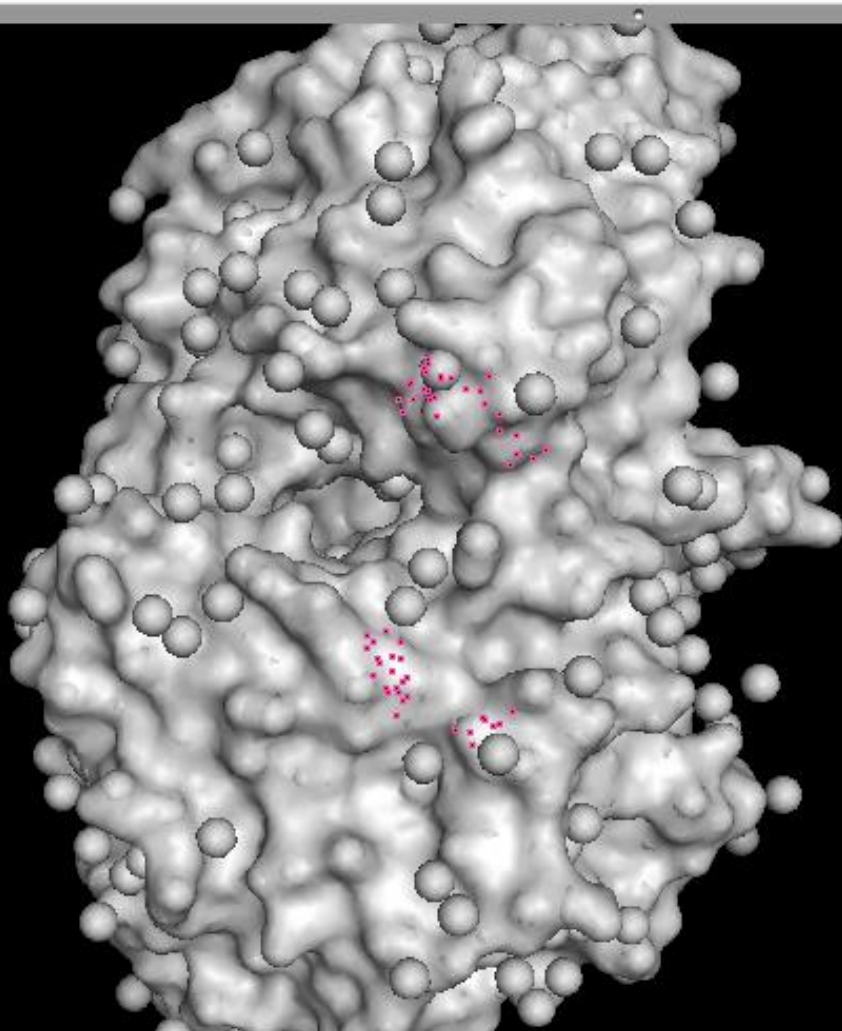
Symmetry: Found 2 symmetry operators.

CmdLoad: "./12as.pdb" loaded as "12as".

PyMOL&gt;select activesite, resid 46+100+116

Selector: selection "activesite" defined with 56 atoms.

PyMOL&gt;



all	A S H L C
12as	A S H L C
(activesite)	Color:
	by element
	by chain
	by ss
	spectrum
Reds	auto
red	reds
tv_red	greens
raspberry	blues
darksalmon	yellows
salmon	magentas
deepsalmon	cyans
warmpink	oranges
firebrick	tints
ruby	grays
chocolate	
brown	

## 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	

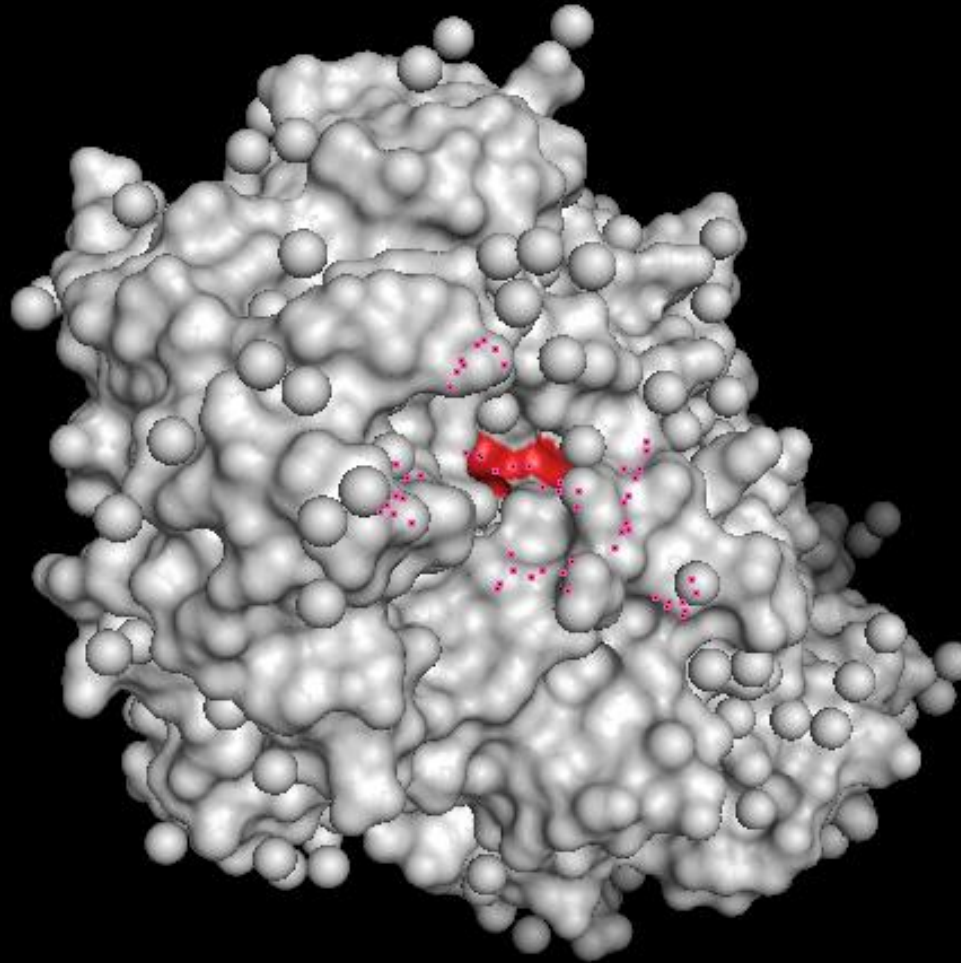
## Selecting Residues

Frame [ 1/ 1] 3/sec

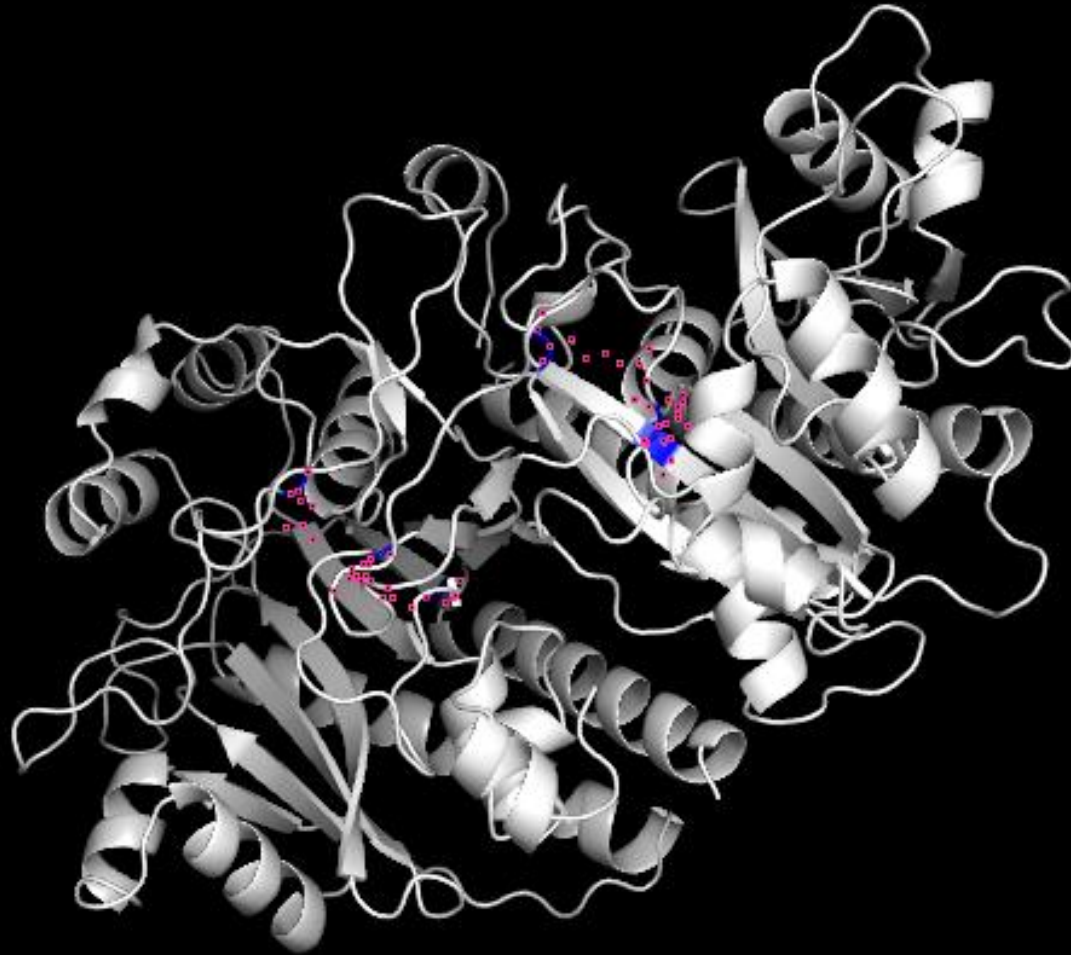
PyMOL&gt;\_

<	<	■	>	>	S	▼
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Active site is clearly in a cleft

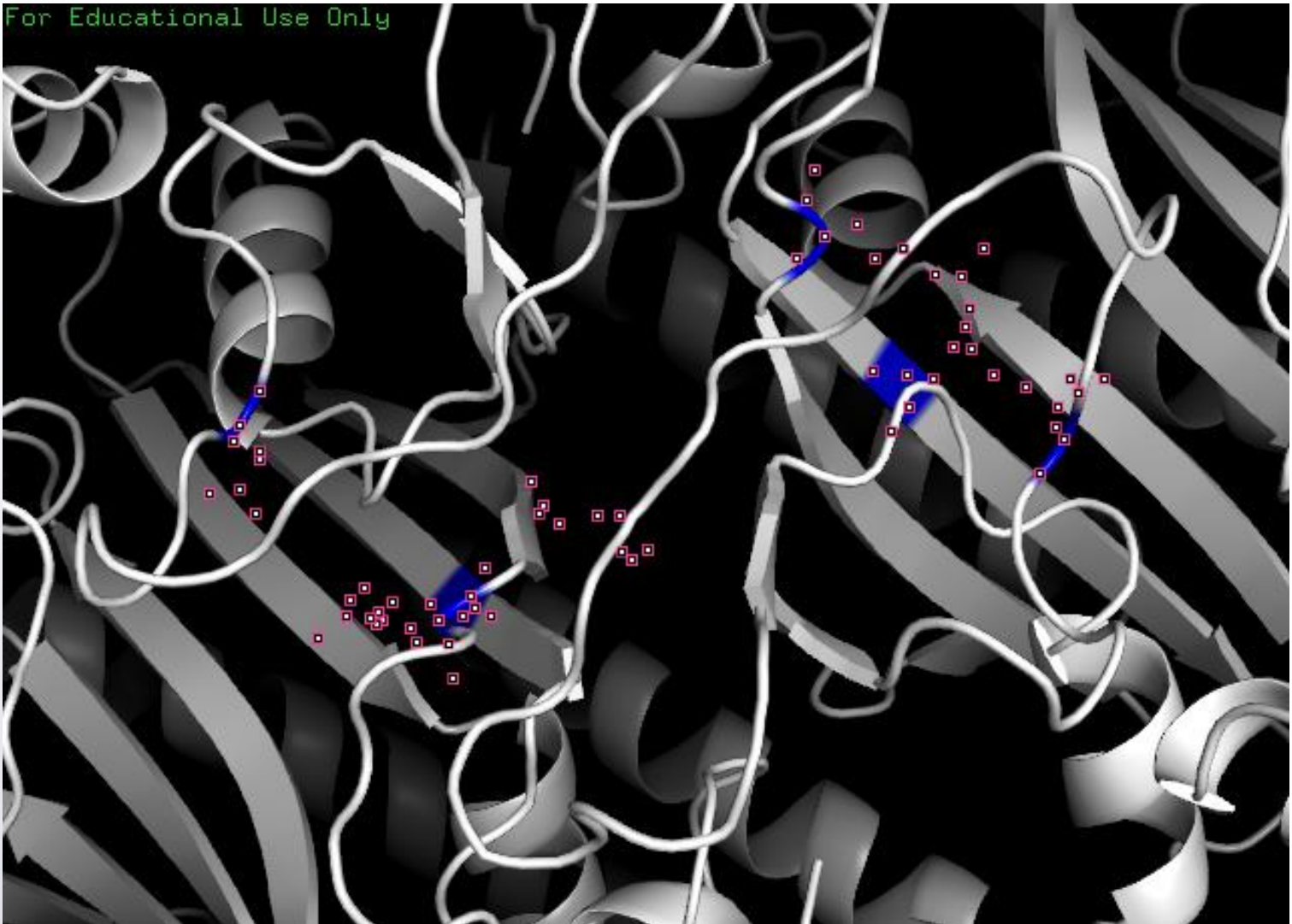


**Switching to cartoon mode  
also switched active site residues to stick mode**



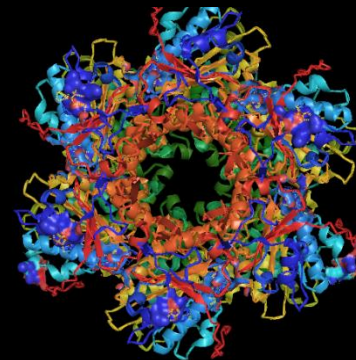
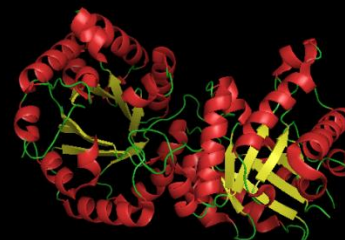
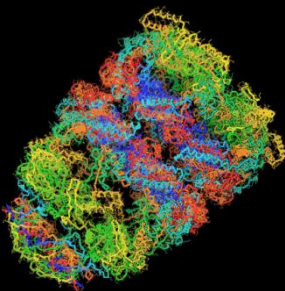
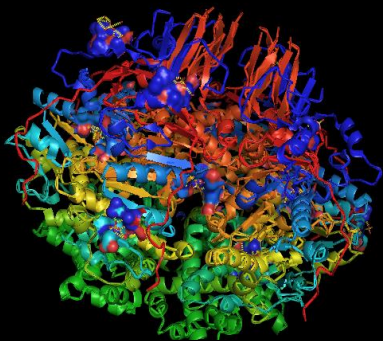
# Zooming in on the active site

For Educational Use Only

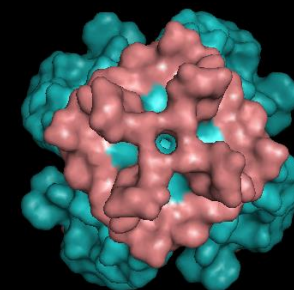
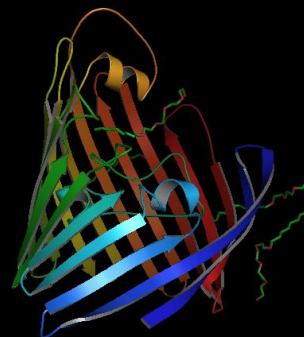
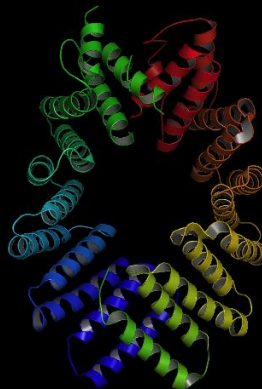
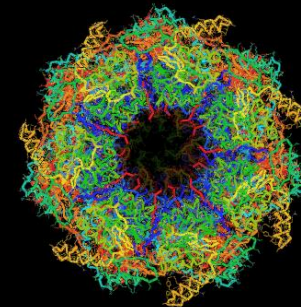
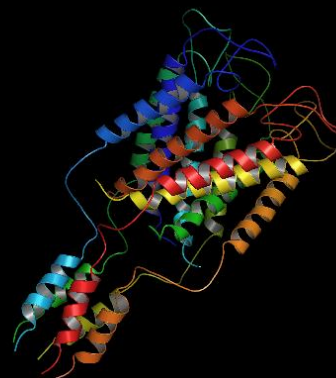
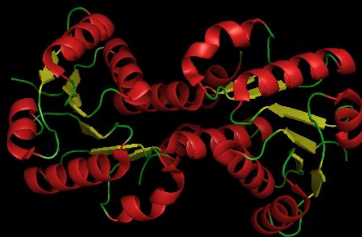
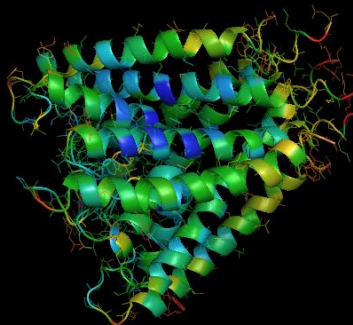
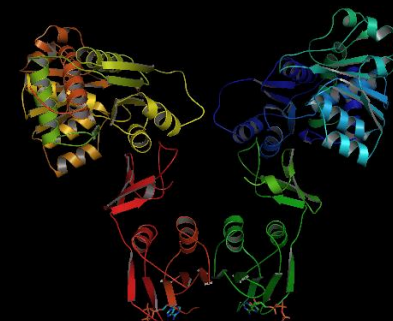


# Do the same analysis for the next two PDBs

- 12as
- 2wfh
- 3ceq



12as



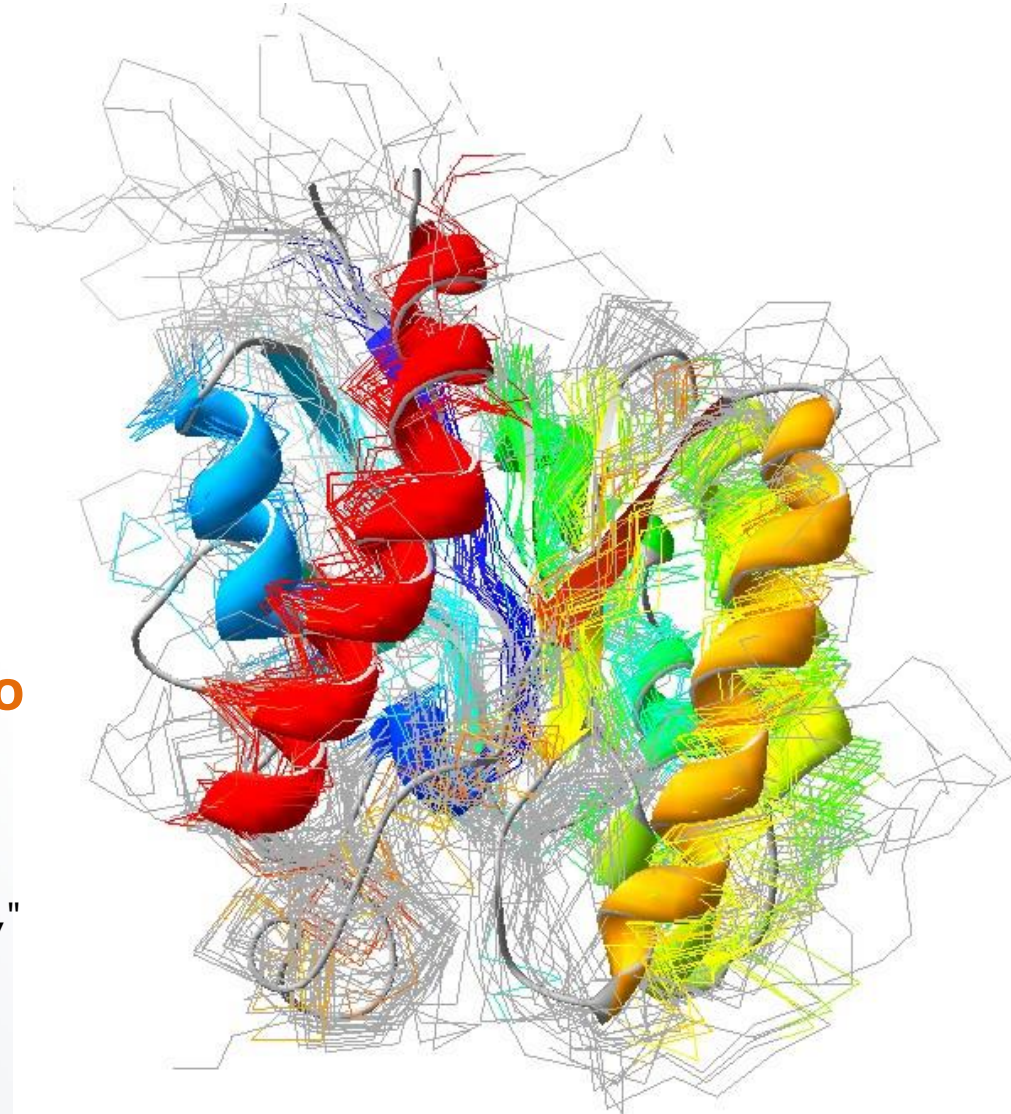
# Paradox: modeling is not a real protein

**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

