

IBT 432 Aplikasi Bioinformatika

Presentasi Mahasiswa

Riza Arief Putranto

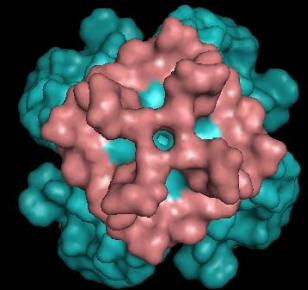
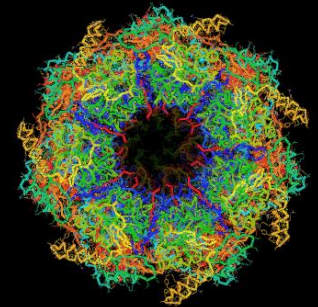
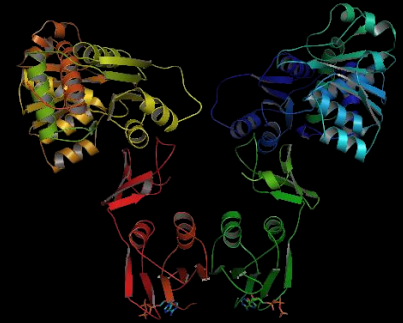
Rencana Perkuliahan

- ~~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

Follow the instruction carefully

1. Fetch these three pdb proteins and open it in the PyMol
 - **1apx**
 - **1h7a**
 - **1c4z**
2. Find Catalytic site for each of these proteins
3. Annotate the catalytic site in the PyMol
 - Catalytic site on “**Show Surface**” and “**Red**” color
5. Save a “**Show Surface**” image of each of these proteins and in “**Grays**” color
6. Save a “**Show Cartoon**” image and close up
 - “**Label**” your residues of Catalytic site
 - “**Zoom**” of Catalytic site
6. Use the ppt template for presentation (look below)
7. Each group will present their results

Remember your slide must contain all three proteins with their Cartoon image and their Cartoon Catalytic site



Example: 1cev

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/. 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 the current CSA. The search interface has three input fields for PDB ID, UNIPROT ID, and EC Number, each with a "SEARCH CSA" button. Below the search interface, there is a section titled "A NEW VERSION OF THE CSA UPDATED 14th November 2013" with a bullet point providing a reference to the latest CSA paper. The page also includes a sidebar with links to CSA Home, Browse Lit Entries, Help & Documentation, Downloads, and Contact The Developers, and a "Latest EBI News" section.

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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"/>	SEARCH CSA
UNIPROT ID	<input type="text"/>	SEARCH CSA
EC Number	<input type="text"/>	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

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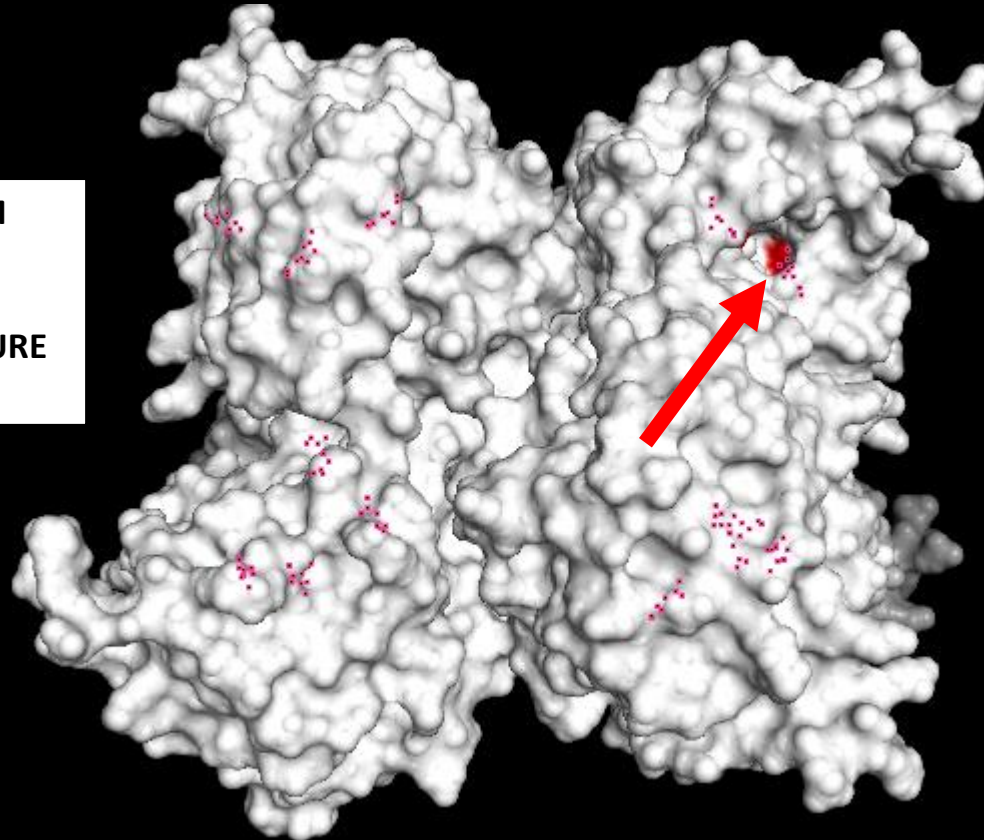
Presentasi Mahasiswa

Kelompok I: Nathan, Lifda, Stevina

Kelompok II: Anita, Dessy, Tazkia

Example: 1cev – Whole protein image

ARGINASE FROM
BACILLUS
CALDOVELOX,
NATIVE STRUCTURE
AT PH 5.6



Whole protein

1. Show Surface
2. Color Grays – White

Catalytic site

1. Show Surface
2. Color Red

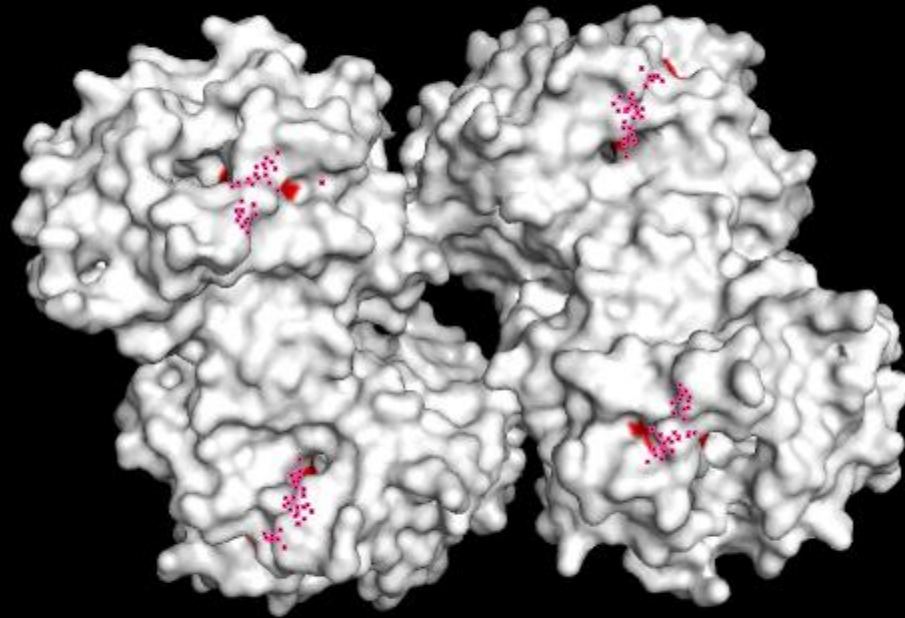
Example: 1cev – Zoom Catalytic site



Catalytic pocket at Asp 126 and Glu 271

1apx– Whole protein image

CRYSTAL STRUCTURE
OF RECOMBINANT
ASCORBATE
PEROXIDASE



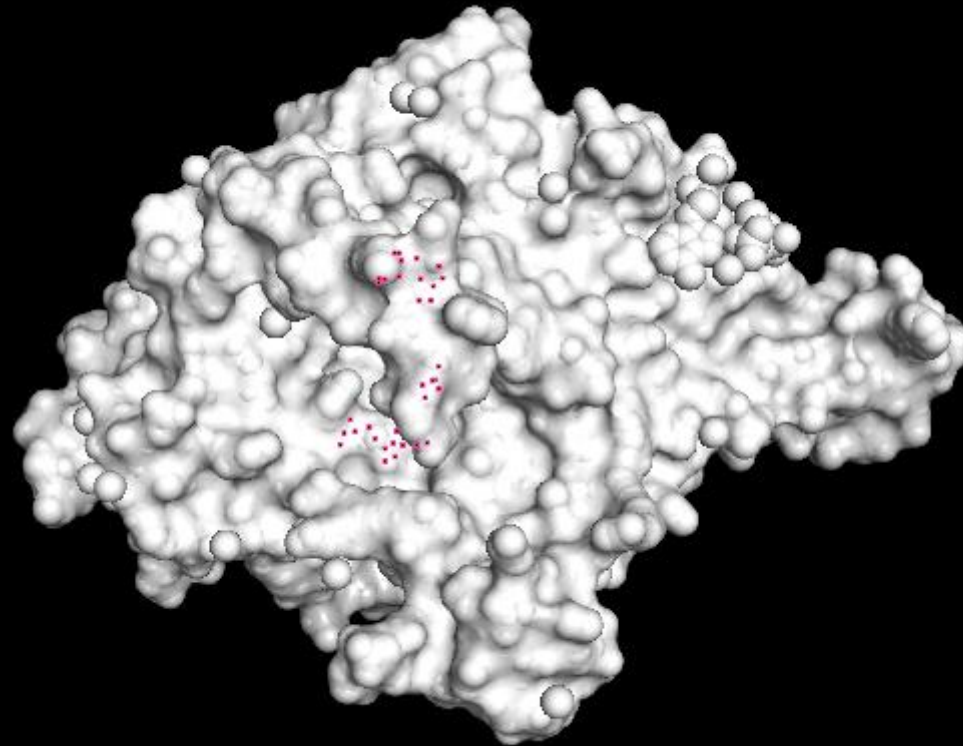
1apx – Zoom Catalytic site



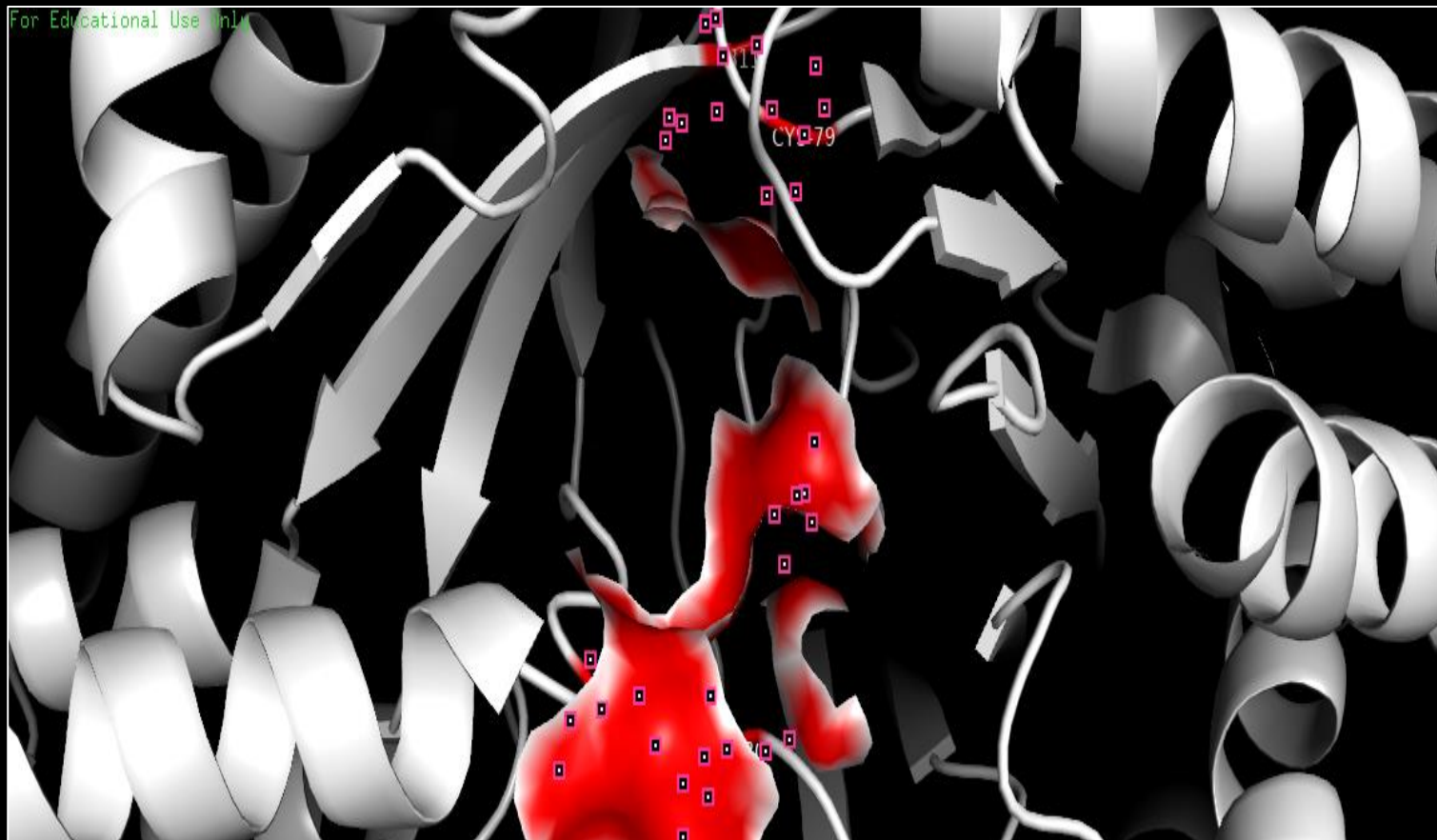
Arg 38, His 42, Asn 71

1h7a – Whole protein image

**Structural basis for
allosteric substrate
specificity regulation
in class III
ribonucleotide
reductases: NRDD in
complex with dATP**



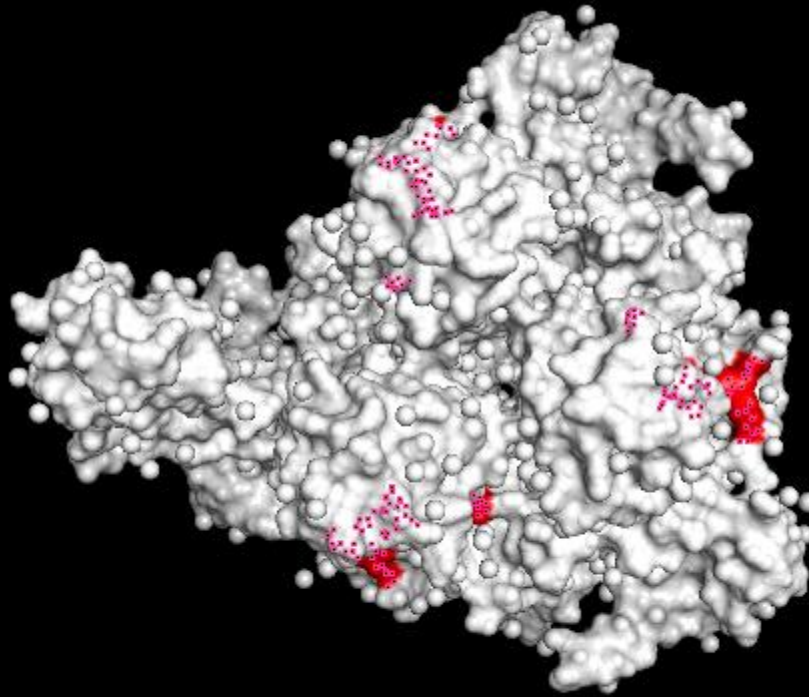
1h7a – Zoom Catalytic site



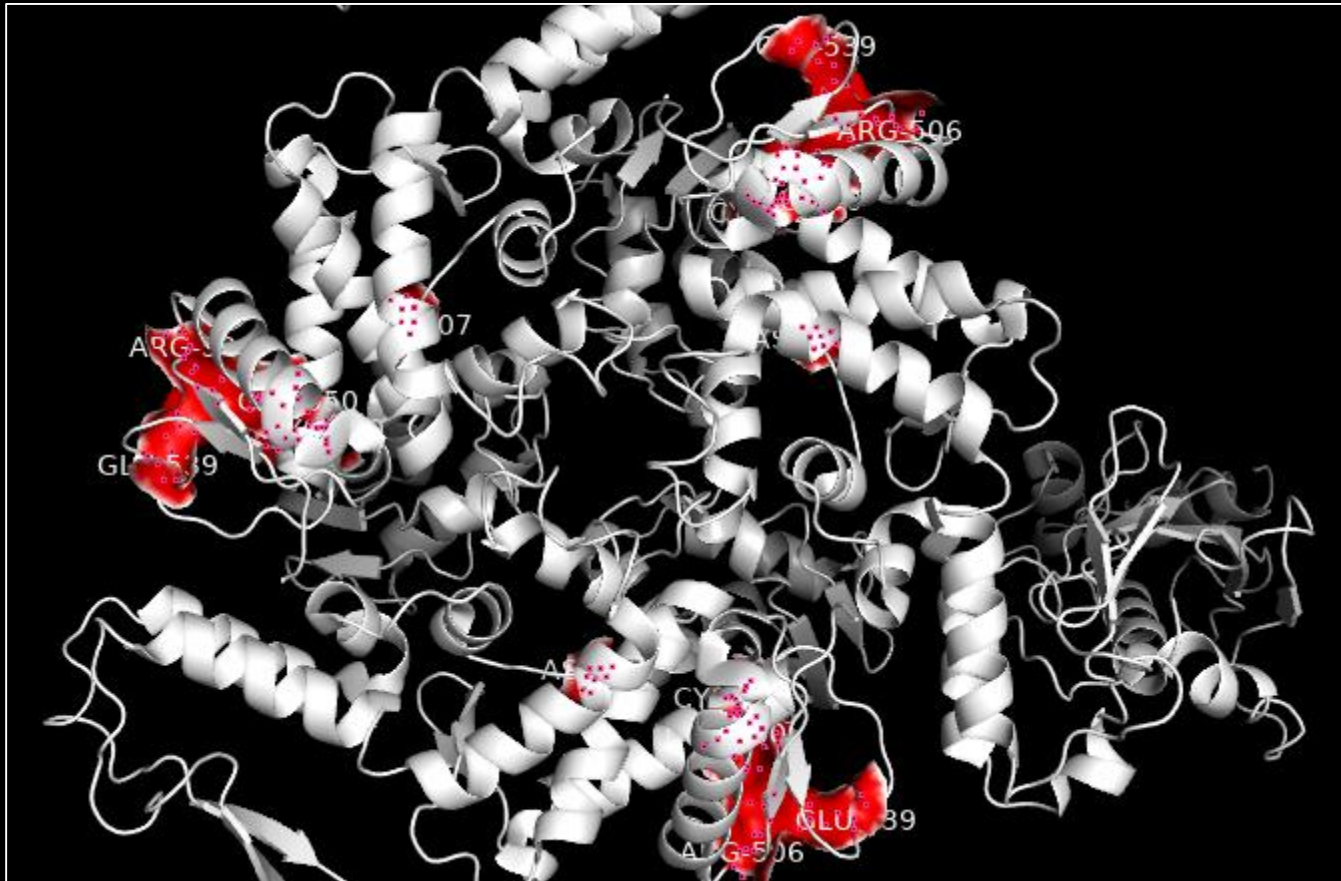
Asn 311, Ala 580, Cys 79, Cys 290, Glu 446

1c4z – Whole protein image

STRUCTURE OF AN
E6AP-UBCH7
COMPLEX: INSIGHTS
INTO THE
UBIQUITINATION
PATHWAY



1c4z – Zoom Catalytic site



Glu 550, Arg 506, Cys 820, His 818, Glu 539, Asp 607

It is the end of courses, you can
now get dizzy

