

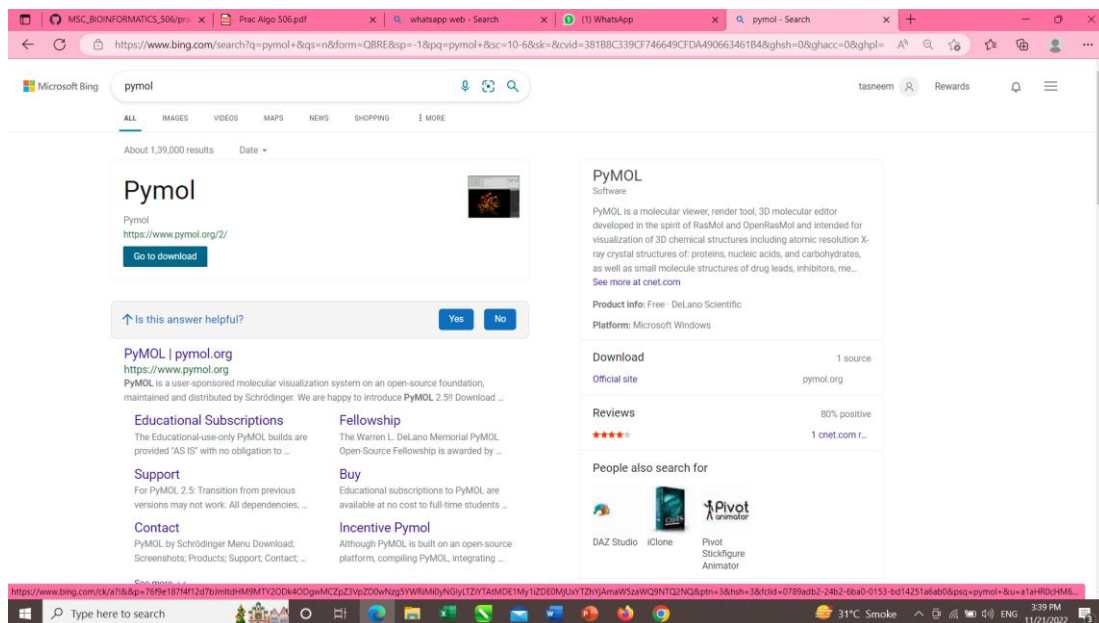
Topic: Retrieving 3D structure from PDB

Aim: Retrieving 3D structure from PDB.

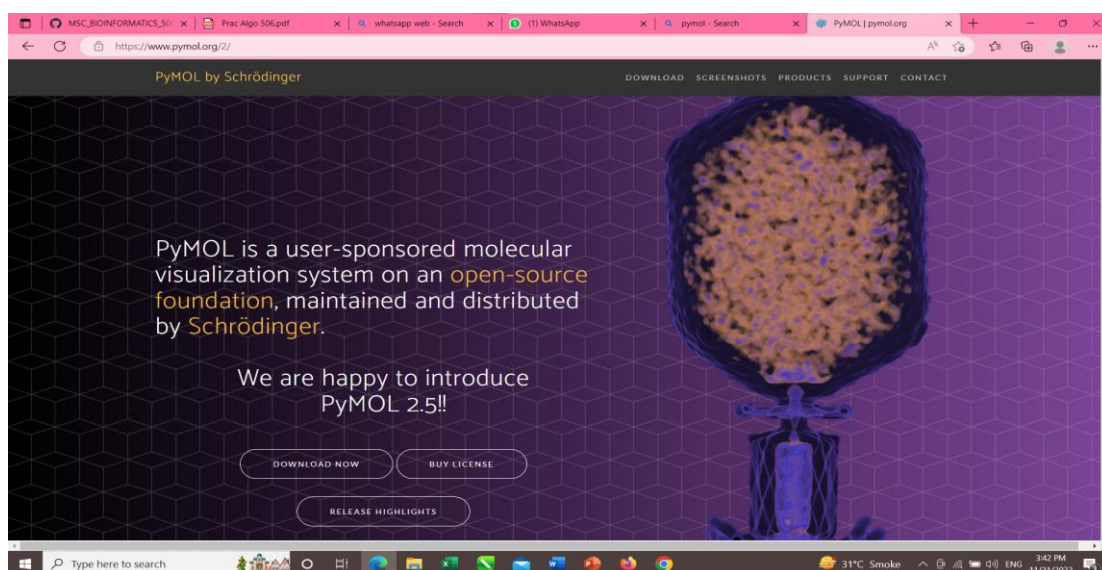
Steps: To perform the current practical, you'll be needing two things

1. PyMOL (software)
 2. Protein in .pdb format
- Installing PyMOL Software

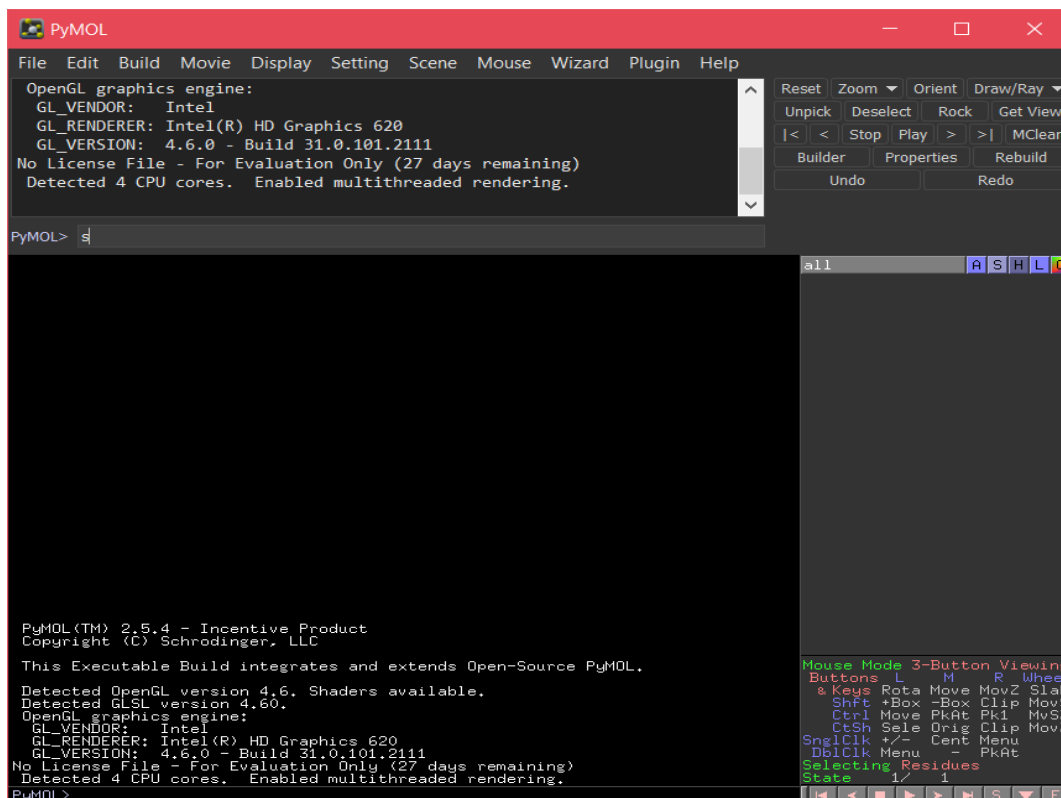
First, we need to install PyMOL. To do so open google and simply search PyMOL



Open the first link and click Download Now

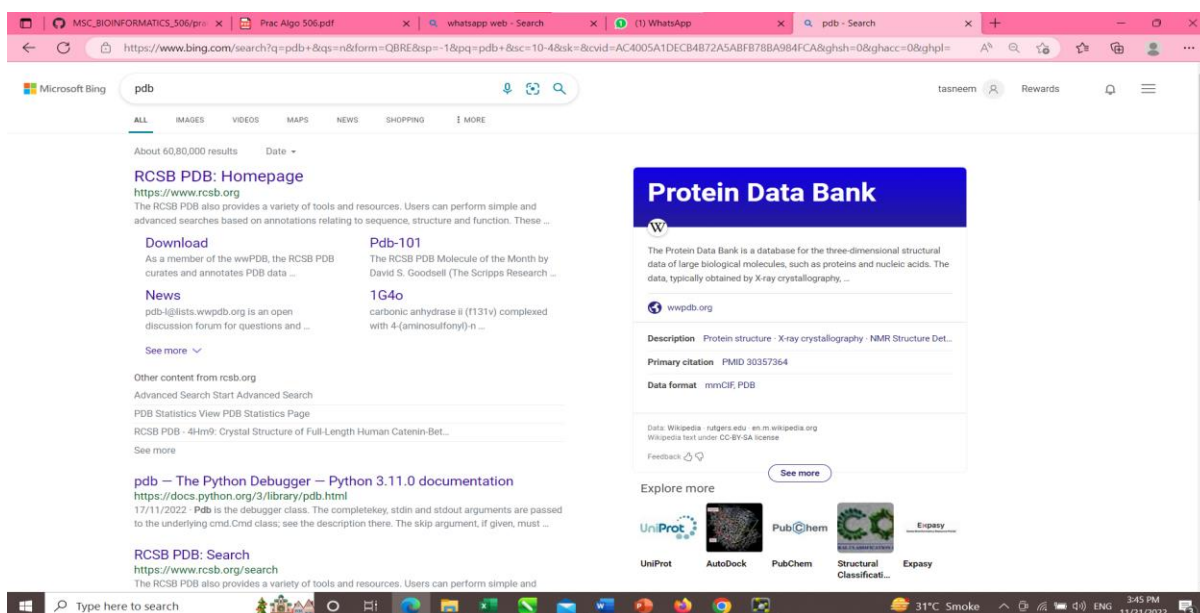


- When done downloading install the software.
- This is how the interface of the software looks like.

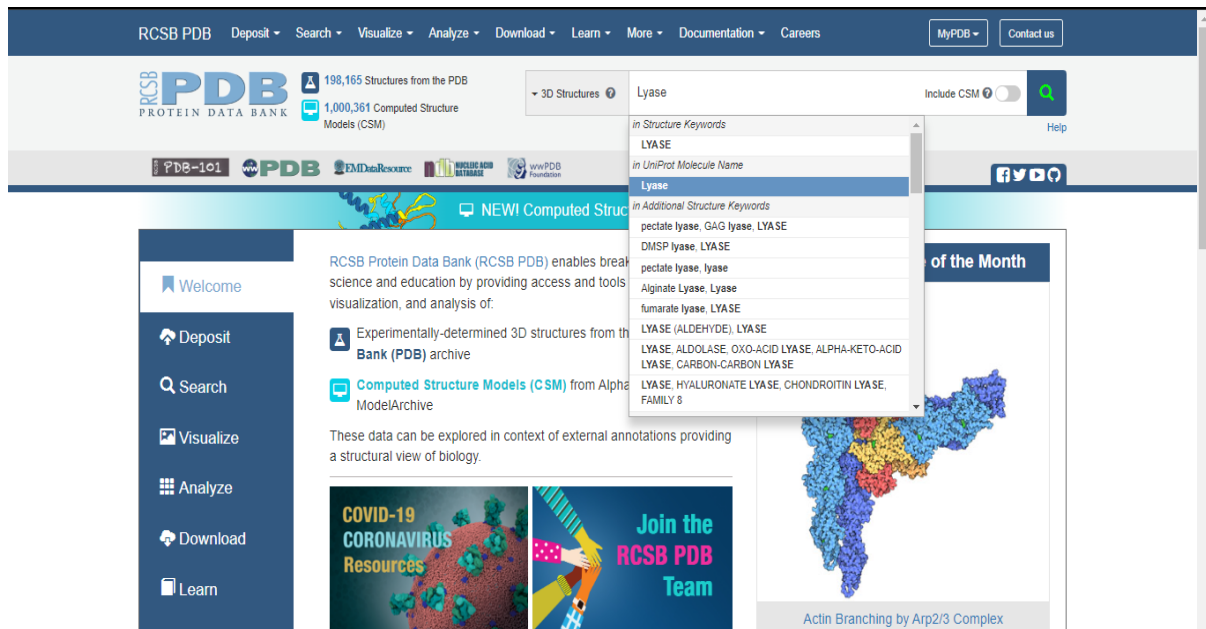


- Downloading Protein in .pdb format

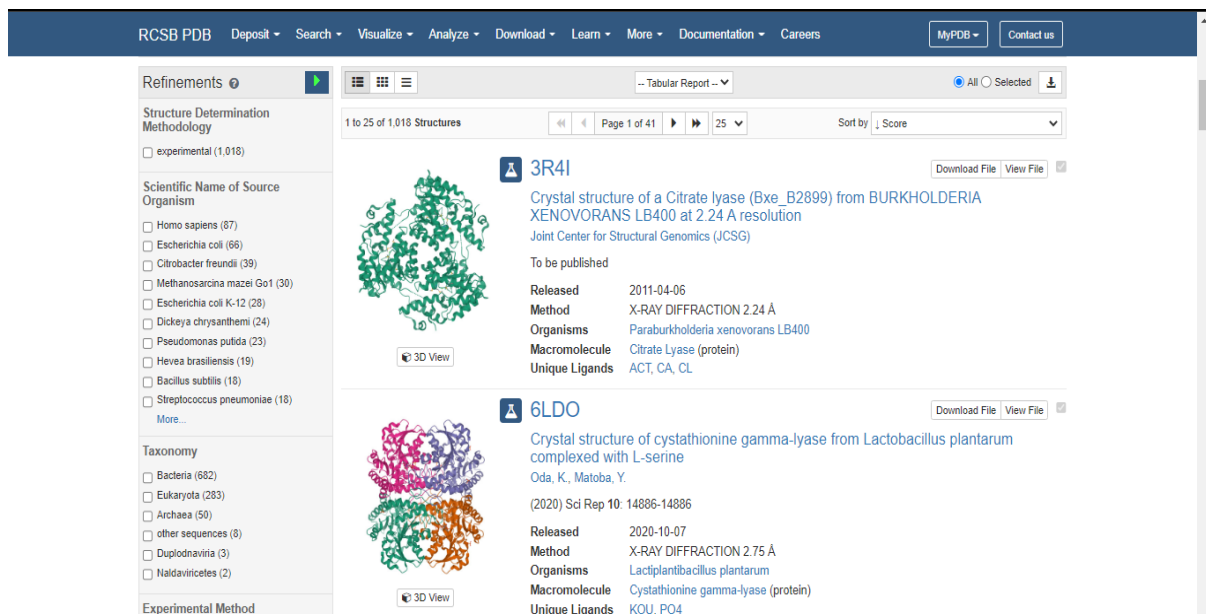
To download Protein open, google and search pdb or simply visit <https://www.rcsb.org/>



- Open the first link named “RCSB PDB: Homepage”
- On the search bar search for “Lyase”



- You'll see all the proteins listed below like this



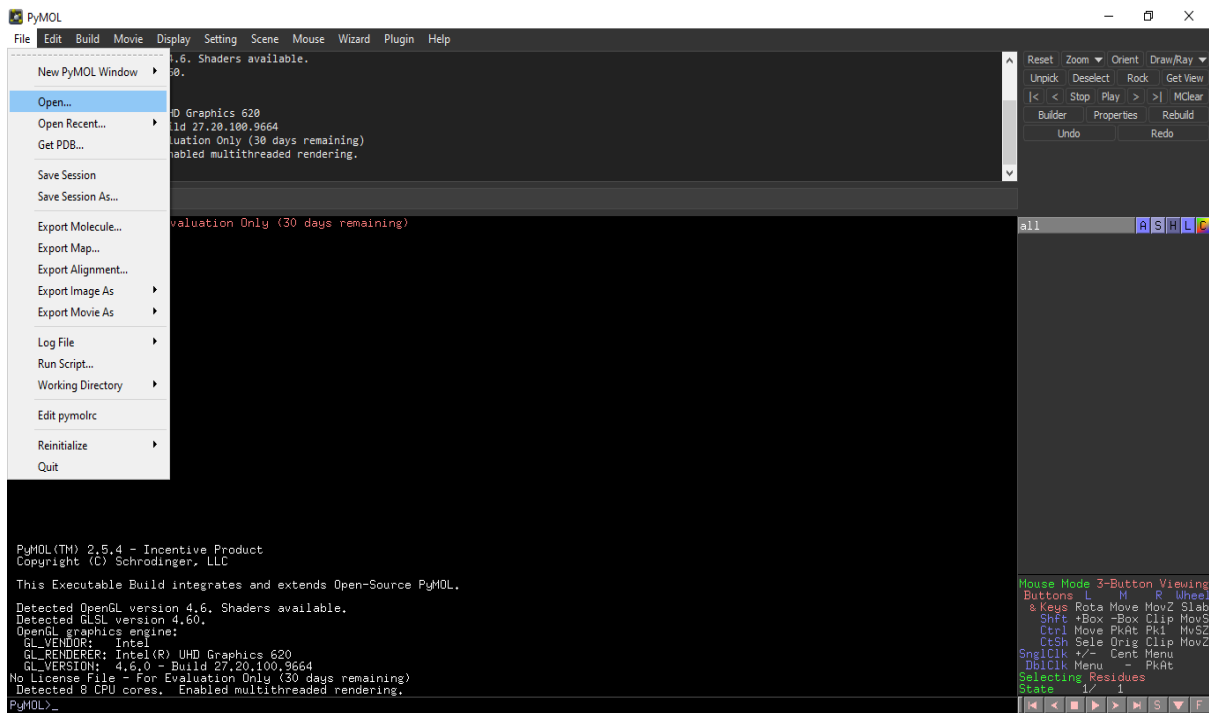
- Scroll down until you find “6LE4” and open it or you can directly search for “6LE4”

The screenshot shows the RCSB PDB website interface. On the left, there are search filters for X-RAY DIFFRACTION (1,007), ELECTRON MICROSCOPY (10), and SOLUTION NMR (1). Below these are filters for Polymer Entity Type (Protein, DNA, RNA), Refinement Resolution (Å), Release Date, and Enzyme Classification Name. The main content area displays three protein structures: 6LE4 (Crystal structure of cystathionine gamma-lyase from Lactobacillus plantarum), 1AOS (HUMAN ARGININOSUCCINATE LYASE), and 1AUW (H91N DELTA 2 CRYSTALLIN FROM DUCK). Each entry includes a 3D view button and download/view file options.

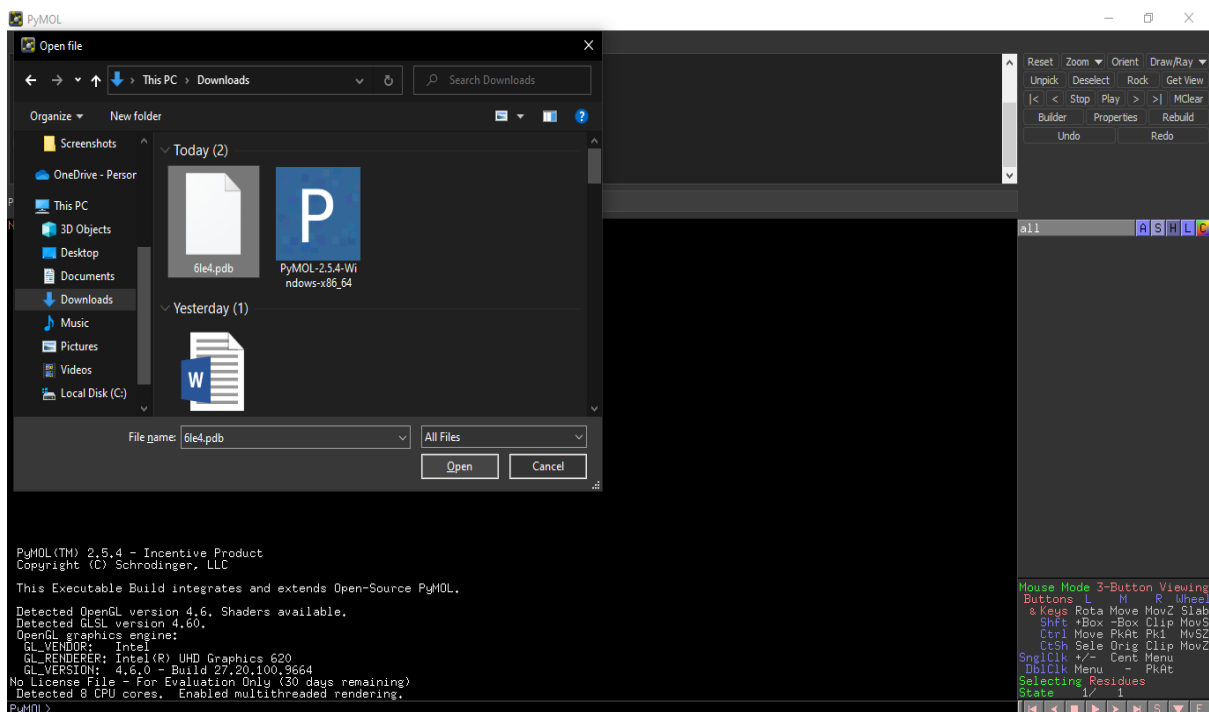
- On the right-hand side, you'll find the download option. Click on it and download as PDB format

This screenshot shows the detailed view of protein structure 6LE4 on the RCSB PDB website. The left sidebar contains a 3D view of the protein structure. The main content area displays the protein's name, PDB DOI, classification, organism, expression system, and deposition information. A 'Download Files' dropdown menu is open, showing various download options: FASTA Sequence, PDBx/mmCIF Format, PDBx/mmCIF Format (gz), PDB Format, PDB Format (gz), PDBML/XML Format (gz), Structure Factors (CIF), Structure Factors (CIF - gz), Validation Full PDF, Validation XML, and Biological Assembly 1 (CIF - gz). A 'Show all' button is visible at the bottom right of the dropdown menu.

- Now that protein is downloaded open PyMOL and on top left corner click File > open



- Now browse for the file you just downloaded (6le4.pdb)



- This is how the screen of imported file looks like

