Today, April 12, 2016:

Protein Data Bank (PDB)

- 1971: 7 structures
- Thursday Nov 8, 2015: 113,494 structures.

Today, April 12, 2016: 117,651

Overview of:

- Protein Data Bank Coordinates
- PyMOL interface
- Hands-on!
**Functional Biological Unit**

**Example 1:** *2biw*  
APOCAROTENOID CLEAVAGE OXYGENASE

**Example 2:** *1DUD*  
Escherichia coli dUTPase in complex with a substrate analogue (dUDP).

**Example 3:** *1AYM*  
HUMAN RHINOVIRUS 16 COAT PROTEIN AT HIGH RESOLUTION
Getting PDB file into PyMOL

```
fetch 2biw, type=pdb2
```

Graphics representations

Action Show Hide Label Color)

```text
lines sticks spheres surface
mesh dots ribbon cartoon
```

Mouse selection

Mouse Rotations

The power of “Settings”
Wizards

Specific functions are handled by calling on wizards.

Today we shall visit 2 wizards:
- **Measurement Wizard** (to draw a distance line between atoms)
- **Mutagenesis Wizard** (to mutate an amino acid side chain)

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**Scenes Export Movie**

- Example F1-F5 –

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**Where to get PyMOL**

Campus software library: [software.wisc.edu](http://software.wisc.edu)

PyMOL

- Linux - PyMOL v1.7 for Linux (glibc 2.3.4+) 32-bit - 68MB file
- Linux - PyMOL v1.7 for Linux (glibc 2.4+) 64-bit - 114MB file
- Macintosh - PyMOL v1.7 for Mac OS X (Intel only) 64-bit - 96MB file
- Windows - PyMOL v1.7 for Windows 32-bit - 79MB file
- Windows - AvPymol v1.7 for Windows 32-bit - 97MB file
- Windows - AvPymol v1.7 for Windows 64-bit - 100MB file

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**Where to get help:**

PyMOL Wiki: [pymolwiki.org](http://pymolwiki.org)

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Today

PyMol Exercises - start on page - 51-
- end on page - 115 -
Today’s protein 2BIW

Carotenoid Oxygenase

- Lignostilbene-alpha, beta-dioxygenase (retinal-forming oxygenase)

A

B

Before we start with PyMol – 2biw: carotenoid oxygenase

Table of Contents

1. Carotenoid Oxygenase enzyme

2. Oxygenase enzyme

3. PyMol – 2biw: carotenoid oxygenase

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