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PYMOL tutorial

http://www.pymol.org/ download Pymol

1) Double-click on the PyMol icon to launch the software.

   File → Open → Path of your PDB (2WLY.pdb)

   Or

   Pymol command line write → fetch 2WLY.pdb enter

2) Representation of the molecule

   Wireframe to cartoon representation

   Click → Show (S)→ Cartoon

   Click → Hide (H)→ lines

   Click → Color (S) →by SS → Helix sheet loop

   Click → Hide (H) → Waters

   Click → Show (S) → organic →spheres [display hetro atom (e.g. cofactor ,ligand) in the file]

   Left mouse click sphere→ sele →label (L)→ residues

3) Display sequence

   External GUI → Display → Sequence

   Click on any amino acid residue of sequence → sele (right side) → L (Label) residue

4) Adding polar hydrogen on protein structure

   2WLY → Action (A) → hydrogen → add polar

5) Align two similar structures

   Open two structures 1WLY (already opened), on pymol command line type “fetch 1CTN.pdb”, → go to the structure (1CTN) you want to align → Action (A) → select align → to molecule → select → 2WLY.pdb

   Hide (H) everything → show(S) cartoon

   Display → sequence → view alignment

6) Display ligand and nearby residues at 5 Å region

   File → reinitialize → everything

   Pymol command line → fetch 1nh6.pdb

   Click → All → Hide (H) everything

   Display → sequence

Scroll at the end of sequence → select heteroatom (click NAG NAG NAG NAG NAG NAG) at the end of sequence

Click → sele → show → sticks

Click → sele → Action (A) → modify → expand → by 5 A, residues

Click → sele → show → line

Click → sele→ label → residues

Select heteroatom (NAG) → sele → modify → expand 4A → find → polar contacts → just intra side chain

or

Visualize polar contacts between ligand and protein

Click → Action (A) → Preset ligands

Click → Hide (H) → ribbon

Click → sele → label residues

7) Surface form of protein

All → Click Hide (H) → everything → All Show (S) → cartoon → Show (S) -→ Surface

Menu bar → Setting → Transparency → Surface → 20%

Display → Sequence → click NAG NAG NAG NAG NAG → sele → Show (S) → stick -→ click again sele (to deactivate sele)

8) Distance between two residues

fetch 1v5d.pdb → hide everything → show cartoon → Select residues 122 and 311 → show sticks

Measure the distance between the two residues

Wizard → measurement → click one atom from 122 residue then click one atom from 311 residues

9) Duplicate the object

Action → duplicate object → obj01 → action → rename object

10) Site directed mutagenesis

Open 1v5d.pdb→ hide everything→ select residue e.g 1v5d-GLU122

wizard mutagenesis → pymol right side click on no mutation → select the residue from box for mutation → display → sequence →click on residue 319

11) Separate complex pdb (1nh6.pdb) file into individual component

External Gui → Display → Sequence

Scroll at the end of sequence →select heteroatom (NAG) at the end of sequence

Click→sele→ Action→ extract object

13) Putting the ligand structure from one pdb file (1nh6.pdb) to another pdb file (1wly.pdb)

File → reinitialize → fetch 1nh6.pdb → fetch 1wly.pdb → 2wly → Action (A) → align 1nh6.pdb

Display Sequence -→ click on NAG NAG NAG NAG NAG → sele → Action (A) → copy to object 2wly (sequence of 2WLY copied NAG object appear

File → export molecule → selection 2wly → save → save as type → pdb

14) Creating picture for publication

File -→ reinitialize → fetch 1nh6.pdb

All→ Hide everything →show → cartoon → show organic spheres → click color (C) → by ss (helix, sheet, loop)

Display → sequence → scroll end of sequence → select NAG → sele → color(C) → by element

Show(S) → surface → external GUI → settings→ transparency → surface → 50%

External Gui→ Display Background → white

File → save image →png → enter name

15) Save pymol session file → save session as→ name of your file