

A Brief Introduction to Protein Visualization Using Protein Explorer (PE)

Opening the molecule in PE:

- obtain the PDB code for the molecule of interest (either from Protein Data Bank, the primary literature, or the 'Find Any Molecule's PDB ID code' link in PE)
- type the PDB code into the Find Any Molecule box in PE (human procathepsin B = **3PBH**)
- it will take a few moments for your computer to open PE and display the molecule
- toggle the spinning OFF and HIDE the water using the buttons (saves memory and runs faster)
- in the top left-hand window, choose "Explore More at *Features*" and then "Explore More with QuickViews!"

Three main ways to explore the molecule in PE:

- rotate the molecule by holding down and moving the mouse in the right window
- use the buttons and SELECT, DISPLAY, AND COLOR pull-down menus in the top left window
- use the command line in the bottom left window

Exploring the molecule:

basic information on the molecule: look in the lower left window for number of atoms selected (initially it's all of them), number of structural features (α -helices, β -sheets, turns, disulfide bridges, etc.), etc.

getting back to the starting view of the molecule: use pull-down menus to SELECT 'all', DISPLAY 'backbone', and COLOR 'Chain (PE)'.

highlighting structural features and amino/carboxy termini: short-cut= click the 2° button *OR* in top left window, use pull-down menus to SELECT 'all', DISPLAY 'cartoon', and COLOR 'structure'. Play around with different options in the pull-down menus. Use COLOR 'N→C Rainbow' to follow the peptide chain from amino (blue) to carboxy (red) terminus.

highlighting polarity and charge: in top left window, use the pull-down menus to SELECT 'all', DISPLAY 'spacefill', and COLOR 'polarity 2'. This shows hydrophobic groups in white and polar/charged groups in purple (explained in middle window). Try other COLOR selections.

cutting the molecule in half with Slab mode: to cut the molecule in half to see the center plane, click on the Slab button and slowly rotate the molecule with the mouse. (This is especially useful when polarity/charge is displayed as you can demonstrate how most internal groups are nonpolar/hydrophobic and external, water-accessible groups are polar/charged.)

highlighting specific amino acids: first go back to the starting view of the molecule (see above). In the command line of the bottom left window, use the following text format to select specific amino acids: **select Cys29** <enter> (this text will select cysteine number 29, but any three-letter amino acid code followed by the residue number will work). Next use the pull-down menus to DISPLAY 'spacefill' and COLOR 'Element (CPK)'. Do the same to select the other active site residue of cathepsin B, His199.

role of the propeptide in blocking the active site: with Cys29 and His199 highlighted (see above), use the pull-down menus to SELECT 'all', DISPLAY 'spacefill'. Note how active site is blocked so no substrate can enter. To highlight the propeptide only, use the command line: **select atomno>=1 and atomno<=644**. Use the pull-down menus to color it a new color (e.g. red). Play around with various DISPLAY options.