

Insight II Tutorial: Basic Commands

Before we begin

First, you should make a separate file in your home directory for your Insight work.

mkdir insight (or whatever you want to call it)

Having done that, move into that directory

cd insight

Now, the command to run Insight is as follows:

Insight-II

After entering this command, you should be given a prompt window that asks for the path you want to use as your default for saving work done in Insight. It lists your home directory, something like:

/gt/usr3/<user_name>/

where <user_name> is whatever user name you were assigned when you registered. You cannot leave this as the path because you cannot save to your home directory. Therefore, at this prompt type:

/gt/usr3/<user_name>/insight/

This sets your new directory (folder) as the default and Insight should load. You are all set! Enjoy the tutorial.

1) **Download the trypsin PDB file**

Go to the web site <http://www.rcsb.org/pdb> and download the structure for trypsin (2PTC). Please be sure to put it into a folder in your directory. Also check the file to make sure it is saved in the correct format (Unix). Insight II cannot open files not stored in this format.

2) **Opening a PDB file using Insight II**

Within Insight II look at the bar that runs horizontally across the screen. One of the categories is called *Molecules*, click on it.

A column of choices will run down the screen, click on the first choice, *Get*. This will open a window.

Under the *Get Molecule* window, select *PDB*.

Under the *Files* window, navigate until you find the PDB file you just downloaded and select it. The name of the file will appear in the *Get Molecule* window under the *Mol File Name*. Hit *Execute*.

A sticks representation of the molecule should appear. Hit *cancel* to close the *Get Molecule* window. You must hit *cancel* to close most windows or they will remain open.

3) Playing with the three button mouse

The buttons on the mouse represents a plethora of different commands. Holding down the third button (third button from the left) rotates the molecule in the direction of the mouse. Holding down the second button (Second button from left or center button) translates the molecule in the direction of the mouse. Holding down the second and third buttons zooms the molecule. Holding down the first and third button spins the molecule around the determined center of the molecule. These commands are important for moving a molecule into a desired position or view. The first button selects atoms. Holding the mouse down will draw a box and all atoms in that box will be selected. A simple click will only select the atom at the cursor. Play with the mouse until you have mastered all of the commands.

4) Controlling the Depth perception

On the vertical tool bar is an icon that is white and has a face on the right and a black quadrilateral on the left, click it. A window called *SideView* will open. In this window is your molecule and two white lines. Select the line to the right and move it around. Notice how the object in the screen changes. Moving the two lines optimizes the view for the molecule. Set up the lines to allow you the best image of the molecule.

5) Displaying the molecule: Simple Representations

The default representation for display in Insight II is sticks, but there are other representations. Select *Molecule* from the horizontal menu bar and from that list select *Render*. (*The shortcut for this is in the vertical toolbar, select the box with the green ball and sticks*).

Two windows will pop up. Under *Render Style* are four choices for Render, these are the basic renderings for a structure. The size of the rendering is controlled in the box(es) below the large, white box for *Molecule Specs*. Each rendering has a different set of control. Go through all four to see the different controls. Once you have selected a *Render Style* and qualities for that render, hit *execute*. Go through all the different *Render Styles* and get a feel for them.

6) Displaying the Molecule: Secondary Structure

Lets start by looking at the secondary structure by using ribbons to trace out the protein backbone. Please make sure that the molecule is in a stick rendering, so we can see the changes.

Insight II Tutorial: Basic Commands

Select *Molecule* from the horizontal command bar and then *Ribbon*. Two windows should open up, *Ribbon Molecule* and *Parameters*.

For starters, just hit the Execute button. The backbone of the structure should change from a stick representation to a rectangular ribbons representation. The representation can be changed to Lines or Oval under the Ribbons style selection. The quality of the representation can be controlled under the Ribbon resolution selections. It is best to use medium and low resolution until a figure quality image is desired. High resolution slows the computer speed and makes movements choppy and difficult to work with.

Yet another way to do this is with the *SecondaryRender* command under the *Molecule* selection. Selecting this will again open two windows, *SecondaryRender Molecule* and *Parameters*. Once again hit *Execute*.

This representation of the molecule is more like a cartoon. Sheets are flat yellow arrows and helices are red cylinders. Notice that the previous ribbons representation is still present. Insight II allows a multitude of representations and they must be specifically turned off or they will remain displayed. This is helpful in making figures that have combinations of different representations of different regions. Lets delete the SecondaryRender by selecting the *delete* option and hitting *Execute*. Go back to the *Molecule/Ribbons* and delete that representation.

7) **How to color your molecule**

Go to *Molecule* and then select *Color*. (There is a shortcut for this on the vertical tool bar, look for the four-colored box (blue, green, yellow, red).)

Once again two windows will appear. Go to the *Atom_Set* and click on it. A list of choices will appear. This list includes groups of atoms in your molecule. This is how you can control which atoms get colored. There is another way to control the atom set, but that will be covered in another tutorial. For now just select *Specified*.

Below that is another list, click on *Color Methods*. Here is a list of a few choices of coloring schemes, choose *By_Atom*. This will color trypsin by the atom type. Hit *Execute*.

In this scheme carbons are green, oxygens are red, nitrogens are blue, and sulfur is yellow. This is a common default coloring scheme. You may choose to color the entire molecule one color, let's try that. Click on *Color Method* and select *Specification*.

Insight II Tutorial: Basic Commands

Click on the light blue box below Color. A color window will appear. You may choose a color from the checkerboard on the left or use the slide bars to tweak a desired color in the right window. Pick a color or create one and then hit *Execute*.

8) **How to modify the display: Controlling what you see**

It is possible to control what gets displayed. Previously I showed you how to display the molecule in different representations. I also mentioned to remove the representation, how to go back and delete them. There is another way to control what gets displayed, in case you don't wish to permanently delete a representation (like the method mentioned before). Under *Molecule*, select *Display*. (The shortcut for this is in the vertical tool bar, look for the box that says *on/off*.)

These windows can control what gets displayed using the *On/Off/Only* commands. Select *Off* for now, under *Atom Set* select *Sidechains* and then hit *Execute*.

Notice that the sidechains in the trypsin molecule are gone. They can be turned back on selecting *On* and *Sidechains*. This display can turn on and off all representations that can be done with Insight II. This is useful when you want to quickly move back and forth between different representations of a molecule.

9) **How to save your work: PDB file**

It is important to be able to save a PDB file of the structure that you have created. In our case we have done nothing to modify the structure, but we are going to save it anyways. First you will need to select *File* from the horizontal bar and then select *Export*. Two windows will appear.

Under *Put_File_Type* select PDB. This is the format of the file we wish to save. Take note that there are other formats in which to save a structure, which are used by different programs. Now click in the Mol File name box and type in a file name. (Example Trypsin.pdb, make sure it ends with PDB). Hit *Execute*. The file has been saved in the directory you specified.

11) How to save your work: Insight II folders

It is also possible to save all the work you have done on the molecule, so you can come back at a latter date and finish the work that has been started. Select *File* and then select *Save_Folder*.

Under Save Object, leave the *, that indicates that all work will be saved. Now click on the Folder Name. Now, on the right (Under Files) select the folder in which to save your work or type the path in the Folder Name box. After which give the file a name (Example Work). The file will be found in the folder you saved it in and it will be called work.psv. You can open the folder by selecting *File* and *restore folder*. Just navigate to find the file and then hit *Execute*.

11) How to delete your molecule to start over

Finally, there is a command that allows the molecule to be removed. Under the horizontal tool bar, select *Object* and then *Delete*. In the parameters box will be a list of all the object(s), just select them (it) and hit *execute*.