

# ICM-Browser & ActiveICM Graphical User Interface Guide v.3.7-2a

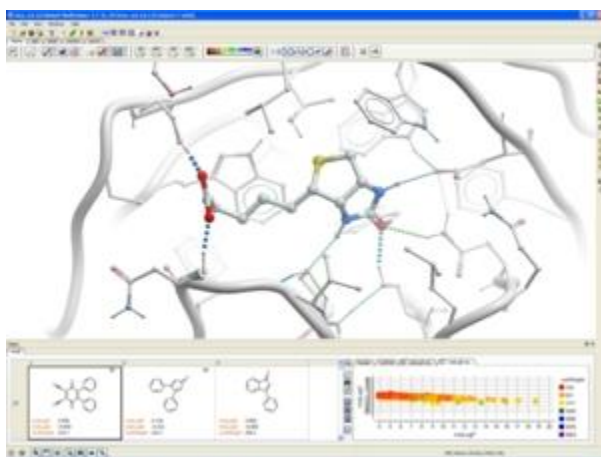
by Ruben Abagyan, Andrew Orry, Eugene Raush, and Maxim Totrov  
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Oct 28 2010 Feedback.

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## 1 Introduction

**Note:** Click **Next** (top right hand corner) to navigate through this chapter. Headings are listed on the left hand side (web version) or by clicking the **Contents** button on the left-hand-side of the help window in the graphical user interface.



Welcome to the ICM-Browser and ActiveICM manual. ICM-Browser provides a biologist or a chemist with direct access to the treasures of structural biology and protein families. It reads a variety of file formats directly from the database web-sites including: PDB, chemical, electron density maps, sequence and alignment files. ICM-Browser provides a rich professional molecular graphics environment with powerful representations of proteins, DNA and RNA, and multiple sequence alignments. With the free ActiveICM plugin you can save fully interactive 3D files to display on the web or in Windows PowerPoint. You can also add and optimize hydrogens to PDB files, display hydrogen bonds, and display transparent ligand binding pocket property surfaces as well as other molecule surfaces.

## Features

Please visit our [product web page](#) for all the ICM-Browser features.

## Download

Please follow the links below to download the software.

<b>Getting Started:</b> Download and Install ICM-Browser and ActiveICM.	
Download ICM-Browser Distribution.	<a href="#">Download</a>
Install ICM-Browser Instructions.	<a href="#">Windows</a> <a href="#">Linux</a> <a href="#">Mac</a>
Download ActiveICM Distribution.	<a href="#">Download</a>
Install ActiveICM.	<a href="#">Windows</a> <a href="#">Linux</a> <a href="#">Mac</a>

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## 2 How To Guides and Videos

**Note:** Click **Next** (top right hand corner) to navigate through this chapter or use the links below. Headings are listed on the left hand side (web version) or by clicking the **Contents** button on the left-hand-side of the help window in the graphical user interface.

[ICM-Browser How To Guide](#)

[ActiveICM How To Guide - Create 3D Molecular Documents for the Web and PowerPoint](#)

### 2.1 ICM-Browser How To Guide

For instructions on how to use ICM-Browser to make fully-interactive 3D slides and publish them in PowerPoint and the web please see the [ActiveICM User Guide](#). ActiveICM is a free plugin for Windows PowerPoint and web browsers. Other related tutorials include:

- [Graphical Display: Molecule Representation, Coloring, Labeling and Annotation](#)
- [Graphical Selections Tutorial](#)
- [Generating Fully Interactive Slides for PowerPoint and the Web Tutorial](#)

## 2.1.1 Download and Install ICM-Browser

<b>Getting Started: Download and Install ICM-Browser and ActiveICM.</b>	
Download ICM-Browser Distribution.	Download
Install ICM-Browser Instructions.	Windows Linux Mac
Download ActiveICM Distribution.	Download
Install ActiveICM.	Windows Linux Mac

## 2.1.2 How to use the Graphical Display

<b>How to use the Graphical Display</b>	
How to load a PDB structure.	HTML GUI Manual
How to Move a Structure in the Graphical Display.	HTML GUI Manual
How to use the Graphics window controls.	HTML GUI Manual
How to Make Selections.	HTML GUI Manual
How to Change the Selection Level and Mode.	HTML GUI Manual
How to Check What is Selected.	HTML GUI Manual
How to use the ICM Workspace Panel	HTML GUI Manual
How to Display a Molecule.	HTML GUI Manual
How to Change Protein Representation.	HTML GUI Manual
How to remove chain breaks (dotted lines).	HTML GUI Manual

How to Color.	HTML GUI Manual
How to Display a Binding Pocket Surface	HTML GUI Manual
How to (Un)Display Hydrogens.	HTML GUI Manual
How to Save an ICM Object.	HTML GUI Manual
How to Save an ICM Project File.	HTML GUI Manual
How to Drag and Drop.	HTML GUI Manual
How to: Right Click Options.	HTML GUI Manual
How to Move Windows.	HTML GUI Manual
How to Arrange Windows	HTML GUI Manual

### **2.1.3 How to change Graphics Effects**

<b>How to change Graphics Effects</b>	
How to display the FOG effect.	HTML GUI Manual
How to display side-by-side stereo.	HTML GUI Manual
How to toggle full screen mode.	HTML GUI Manual
How to adjust perspective.	HTML GUI Manual
How to change the lighting.	HTML GUI Manual
How to display sketch accents.	HTML GUI Manual
How to display elegant ribbon and ligand sketch.	HTML GUI Manual

### **2.1.4 How to add Labels and Annotations**

<b>How to add Labels and Annotations</b>	
How to Label Residues.	HTML GUI Manual
How to Label Atoms.	HTML GUI Manual
How to Label Variables.	HTML GUI Manual
How to Display and Undisplay Sites.	HTML GUI Manual
How to Make and Display Annotations.	HTML GUI Manual
How to Make and Display 2D and 3D Labels.	HTML GUI Manual

### **2.1.5 How to Convert Proteins, Display Hydrogens and Ligand Binding Pocket.**

<b>Convert Protein, Display Hydrogens and Ligand Binding Pocket.</b>	
How to Convert a PDB Structure into an ICM Object.	HTML GUI Manual
How to Display Ligand Binding Pocket.	HTML GUI Manual

### **2.1.6 How to Make High Quality Publication Images**

<b>How to Make High Quality Publication Images</b>	
How to Toggle High Quality Display	HTML GUI Manual
How to Toggle Antialiasing.	HTML GUI Manual
How to Copy Image to ClipBoard	HTML GUI Manual
How to Write an Image.	HTML GUI Manual
How to Use the Advanced Write Image Options.	HTML GUI Manual

How to Add an Image to the ICM Photo Album.
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HTML GUI Manual
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### **2.1.7 How to Superimpose Protein Structures.**

<b>How to Superimpose Protein Structures.</b>
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How to Superimpose One or More Protein Structures.
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HTML GUI Manual
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### **2.1.8 How to Measure Distances and Angles.**

<b>How to Measure Distances and Angles.</b>
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How to Measure Distances Between Two Atoms.
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HTML GUI Manual
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How to Measure Distances From One Atom to Many.
---

HTML GUI Manual
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How to Show Corresponding Distances in Two Objects.
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HTML GUI Manual
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How to Display the Ruler Bar.
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HTML GUI Manual
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## **2.2 ActiveICM How To Guide - Create 3D Molecular Documents for the Web and PowerPoint**

This guide is focused on how to make fully interactive 3D documents for Windows PowerPoint and the Web. For more information on the other features in ICM-Browser please see the [ICM-Browser User Guide](#).

### **Creating 3D Documents Is Straightforward**

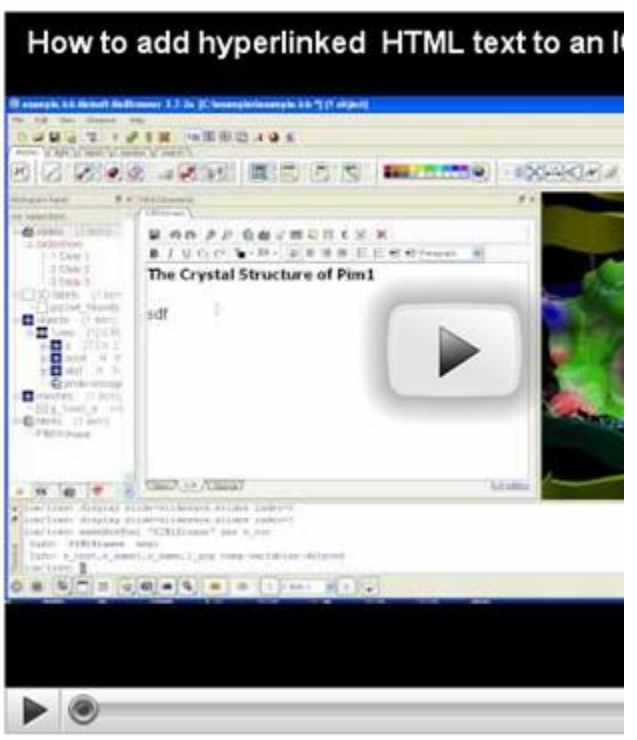
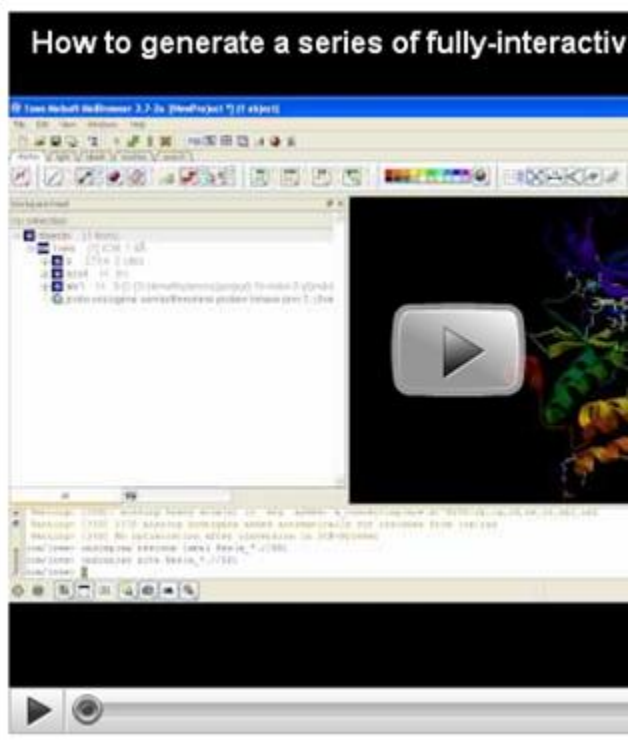
For written documentation please see the [ActiveICM User Guide](#) and the [ICM-Browser User Guide](#). Please see the videos below for a guide to generating fully-interactive 3D molecular files in PowerPoint and on the Web.



How to Download and Install ICM-Browser

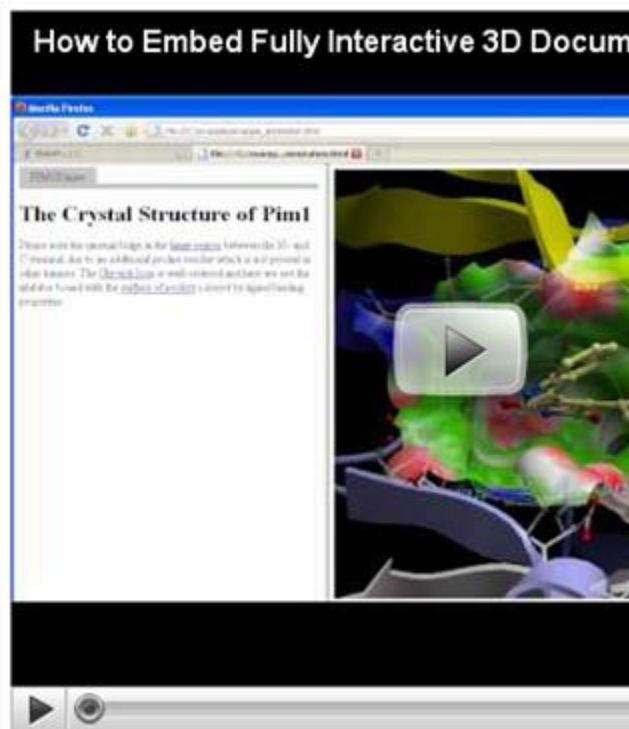
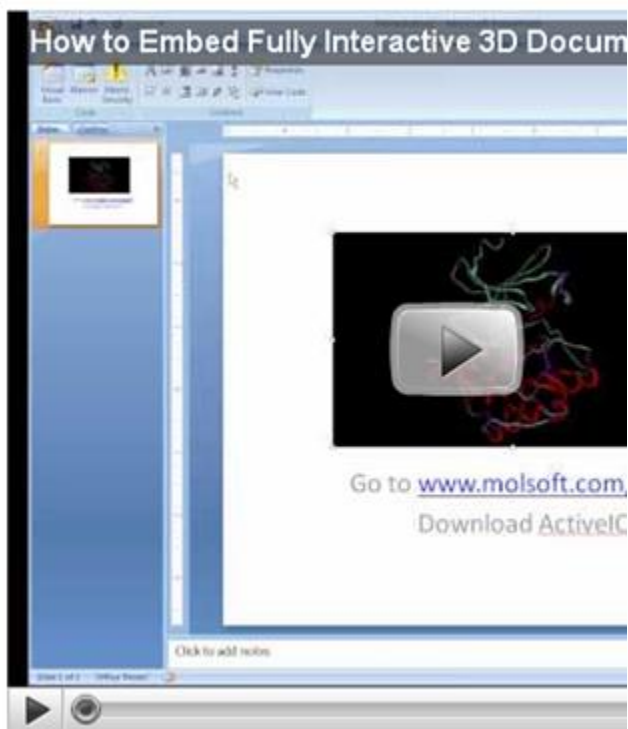


[How to Download and Install ActiveICM](#)



[How to Generate a Series of Fully-Interactive 3D Slides](#)

[How to Add Hyperlinked HTML Text to a 3D Document File](#)



[How to Embed Fully-Interactive 3D Documents into a PowerPoint File](#)

[How to Embed Fully-Interactive 3D Documents into a Web Browser](#)

### 2.2.1 Download and Install ActiveICM.

<b>Getting Started:</b> Download and Install ICM-Browser and ActiveICM.	
Download ICM-Browser Distribution.	<a href="#">Download</a>
Install ICM-Browser Instructions.	Windows Linux Mac
Download ActiveICM Distribution.	<a href="#">Download</a>



Install ActiveICM.	Windows Linux Mac
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### **2.2.2 How to Create a Series of Fully-Interactive 3D Slides.**

<b>Creating Slides</b> How to Create a Series of Fully-Interactive 3D Slides.	
How to Make Fully Interactive 3D Slides	HTML GUI Manual
How to Animate Slides	HTML GUI Manual
How to View and Navigate Slides in the ICM-Browser.	HTML GUI Manual
How to Edit Slides.	HTML GUI Manual
How to Add Smooth Blending and Transition Effects Between Slides.	HTML GUI Manual

### **2.2.3 How to Create Molecular Documents**

<b>How to Create Molecular Documents: Linking Slides to HTML Text.</b>	
How to Create an HTML Document.	HTML GUI Manual
How to Edit an HTML Document.	HTML GUI Manual
How to Make a Hyperlink Between HTML Text and a Slide.	HTML GUI Manual

### **2.2.4 How to Display Molecular Documents in PowerPoint**

<b>How to Display Molecular Documents in PowerPoint</b>	
How to Embed in Microsoft PowerPoint 2003	HTML GUI Manual
How to Embed in Microsoft PowerPoint 2007	HTML GUI Manual

How to Use ActiveICM in PowerPoint	HTML GUI Manual
How to Change ActiveICM Component Properties in PowerPoint	HTML GUI Manual
Advanced use of ActiveICM: Macros to direct visualisation changes.	HTML GUI Manual

### 2.2.5 How to Display Molecular Documents on the Web

<b>How to Display Molecular Documents in Web Browsers</b>	
How to Display Molecular Documents in Web Browsers	HTML GUI Manual

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## 3 Getting Started

**Note:** Click **Next** (top right hand corner) to navigate through this chapter. Headings are listed on the left hand side (web version) or by clicking the **Contents** button on the left-hand-side of the help window in the graphical user interface.

The **Graphical User Interface** (GUI) has many components. When you first use the GUI the default window layout is displayed as shown below.



## 3.1 How to Use the Graphical Display

### 3.1.1 How to load a PDB Structure

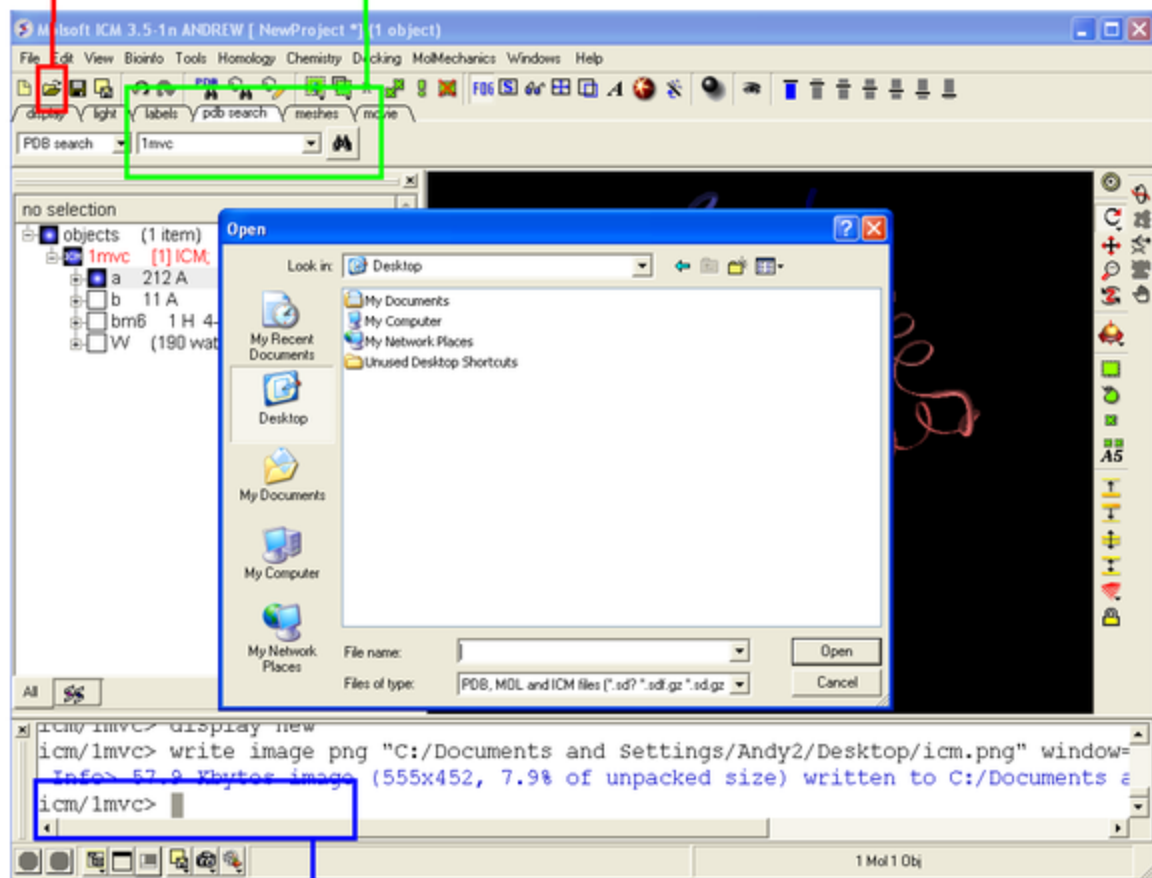
There are three main ways to read in a PDB file.

1. Using the command line.
2. Using File/Open button
3. Using the PDB Search tab

Keyword search "PDB" for more information.

Opens a dialog to locate a PDB file on a local filesystem

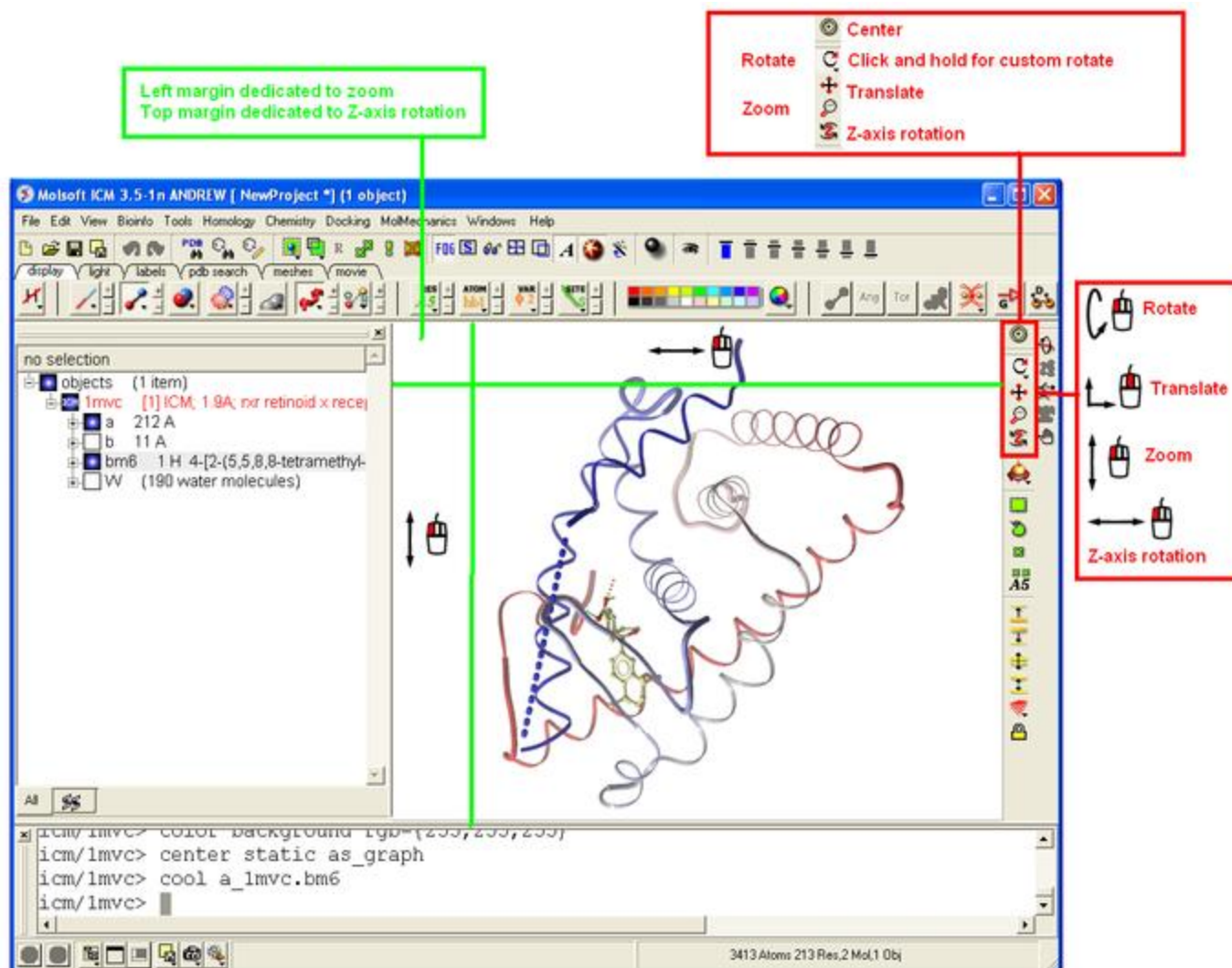
Enter PDB code or a PDB Search String



Simply type the command - read pdb "PDB\_Code" and ICM will fetch the structure from the PDB website

### 3.1.2 How to Move a Structure in the Graphical Display

Ways to move structures using the mouse. Keyword search "mouse" for more information.



### 3.1.3 How to use the Graphics window controls

In the graphics window you can use various `tools` described elsewhere. It is good to know the following:

- **Picking a tool:** the left mouse button will function according to the selected tool
- **Popup menus:** right click on an atom gives a pop-up menu
- **Selecting in the rotation mode:** the right mouse button will select atoms
- **Translating in the rotation mode:** the middle mouse button will translate the scene
- **Zooming and moving clipping planes in the rotation mode:** the left, top and right margins of the graphics window are reserved for other actions, zoom, z-rotation, and clipping plains, respectively. That means that even if you are picking atoms, by pressing control you can still rotate your molecule with the left-mouse-button.

- **Rotating in any non-rotation mode:** if you press **Control** in any mouse mode, e.g. zoom, pick etc., it will temporarily switch to **rotation**
- **Escaping from the connect and continuous movement modes:** pressing **Escape** helps to get out of certain modes, such as Full Screen, Continuous rotation or rocking, the Connect mode.
- **Global rotation in the Connected mode:** pressing **Shift** will temporarily switch to the global rotation/translation mode.

See also: `Graphics controls`.

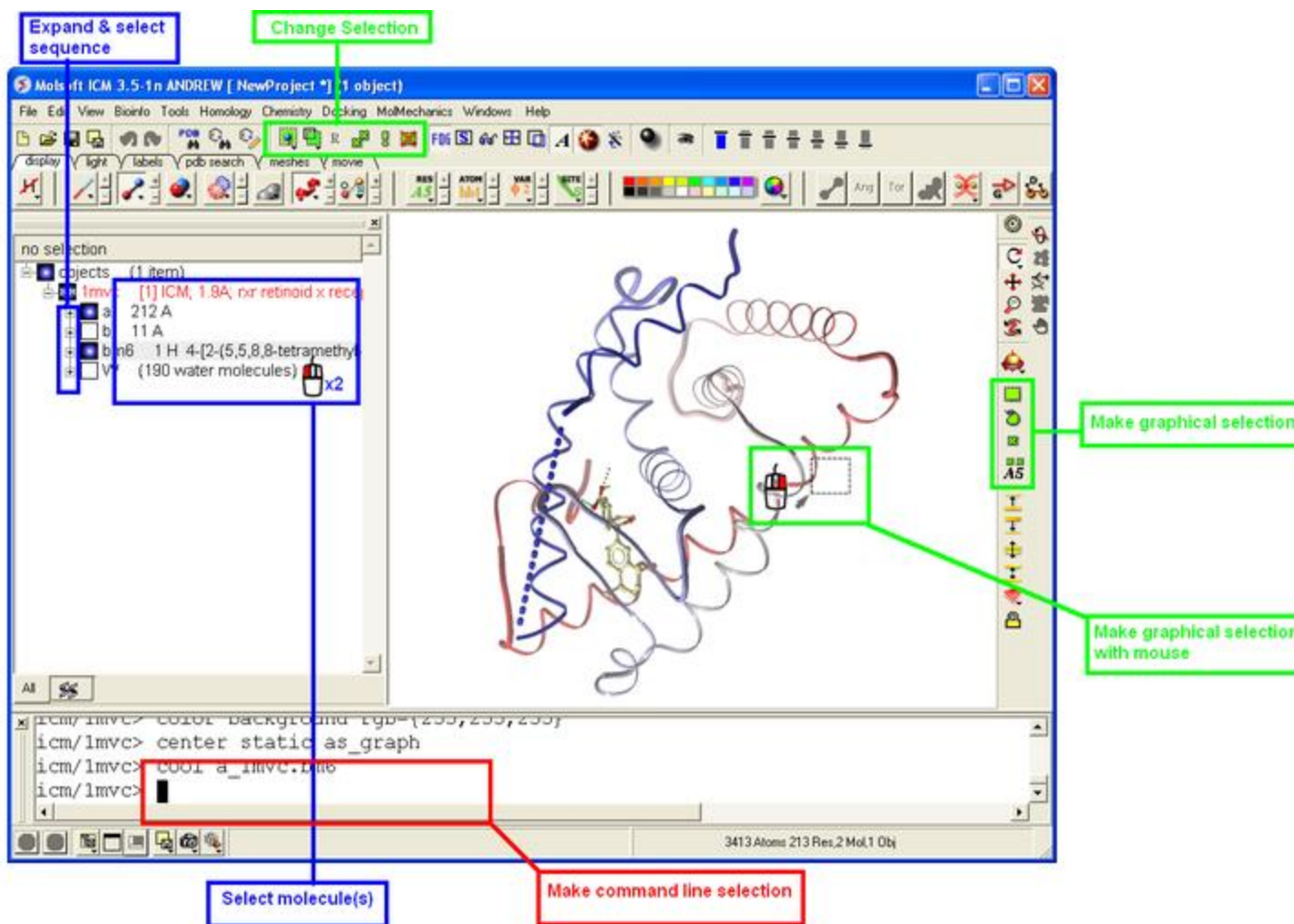
### 3.1.4 How to Make Selections

Making selections in ICM is an important skill to master (e.g. you may want to select a binding pocket for docking or a region of a molecule for coloring). The four levels of selection are:

1. Atoms
2. Residues
3. Molecules
4. Objects (multiple molecules comprising a PDB entry)

There are several ways of making selection in ICM. The simplest is to interact directly with the graphics window - **right-click, hold and drag** around the area of the screen you want to select. Alternatively, in the workspace window, expand the tree of molecules and chains until the relevant protein sequences is displayed. Then left click and drag to mark residues to form a selection.

See the chapter entitled `Making Selections` for more information.



### 3.1.5 How to Change the Selection Level and Mode

It is possible to change the level of selection before or during the building of a selection. The selection level drop-down menu can be used to do this.

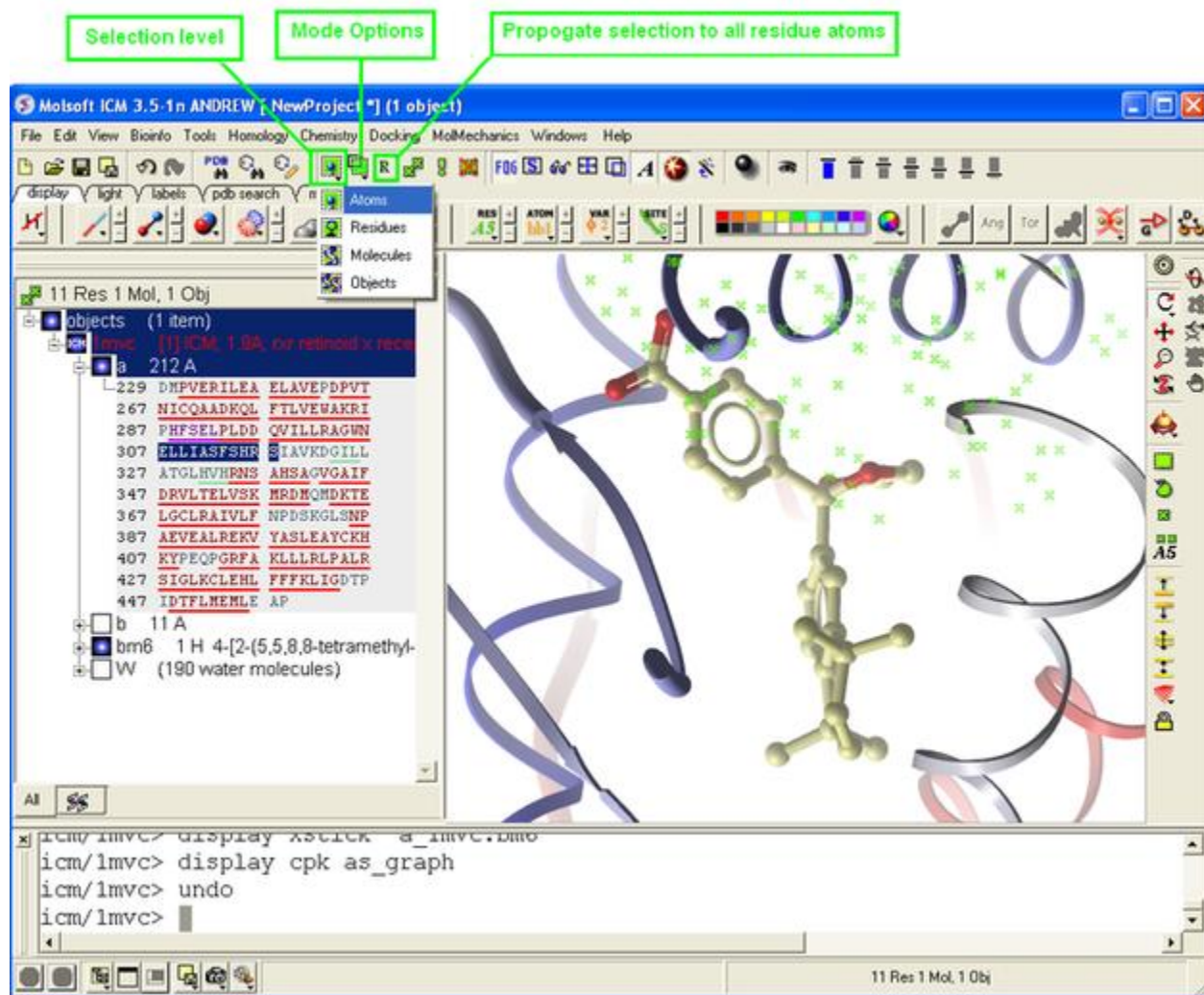
For example, a C-alpha of a residue is selected but one would like to have the whole residue selected (i.e. all atoms). Change the level to **Residues<**. This selection can then be changed into all atoms of the residue by then selecting the **Atoms** level again.

It is also important to observe the selection mode that is being used. There are four modes:

- New: new selection replaces everything selected before
- Add: new selection is added to previous selection(s), if any
- Remove: previously selection (part or whole of it), if included in the new selection will be unselected.

- Toggle: within the new selection, everything that has been selected is unselected and everything that hasn't been selected, will be selected

See the chapter entitled Making Selections for more information.



### 3.1.6 How to Check What is Selected

Once you have made your selection - how can you be sure you have made it and what exactly have you selected. See the chapter entitled Making Selections for more information.



Always check the selection level

Selections are highlighted blue in workspace

Graphical selections are returned to a variable as\_graph

Selections are shown with green crosses in graphical display

A selection tally

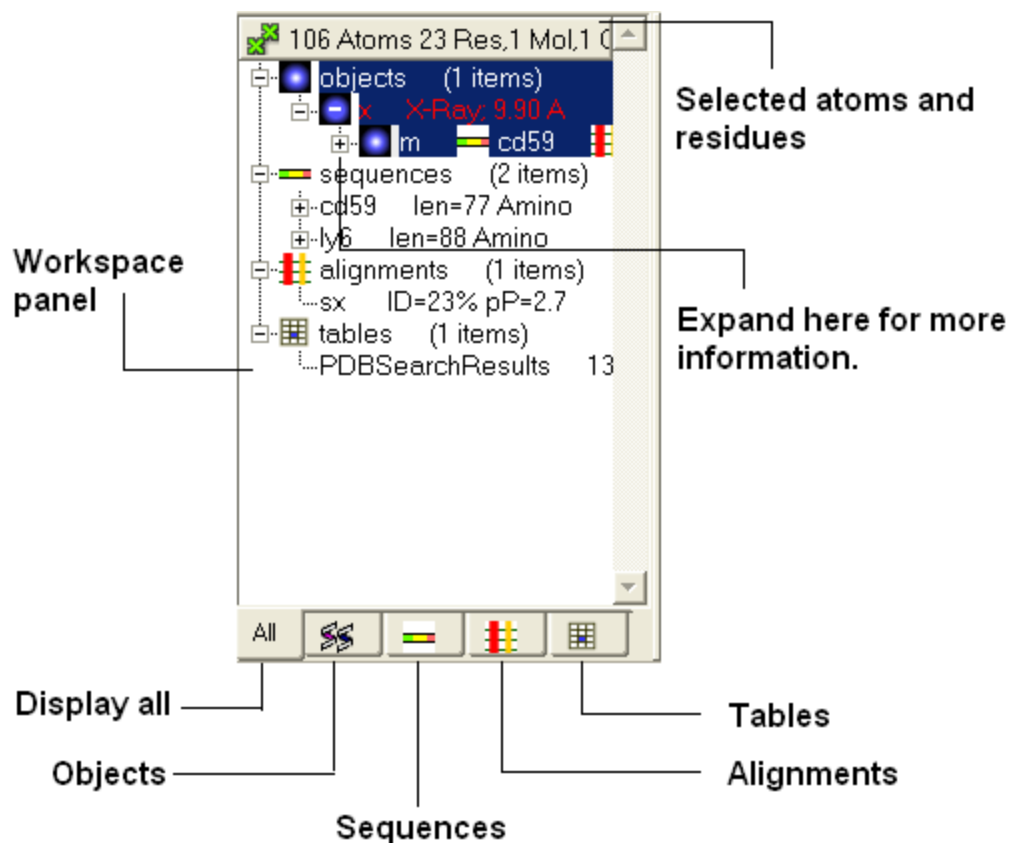
```

icm/lmvc> center static as_graph
icm/lmvc> undisplay store a_lmvc.bm6
icm/lmvc> display xstick a_lmvc.bm6
icm/lmvc> as_graph
  
```

193 Atoms 11 Res: 2 Mol: 1 Obj

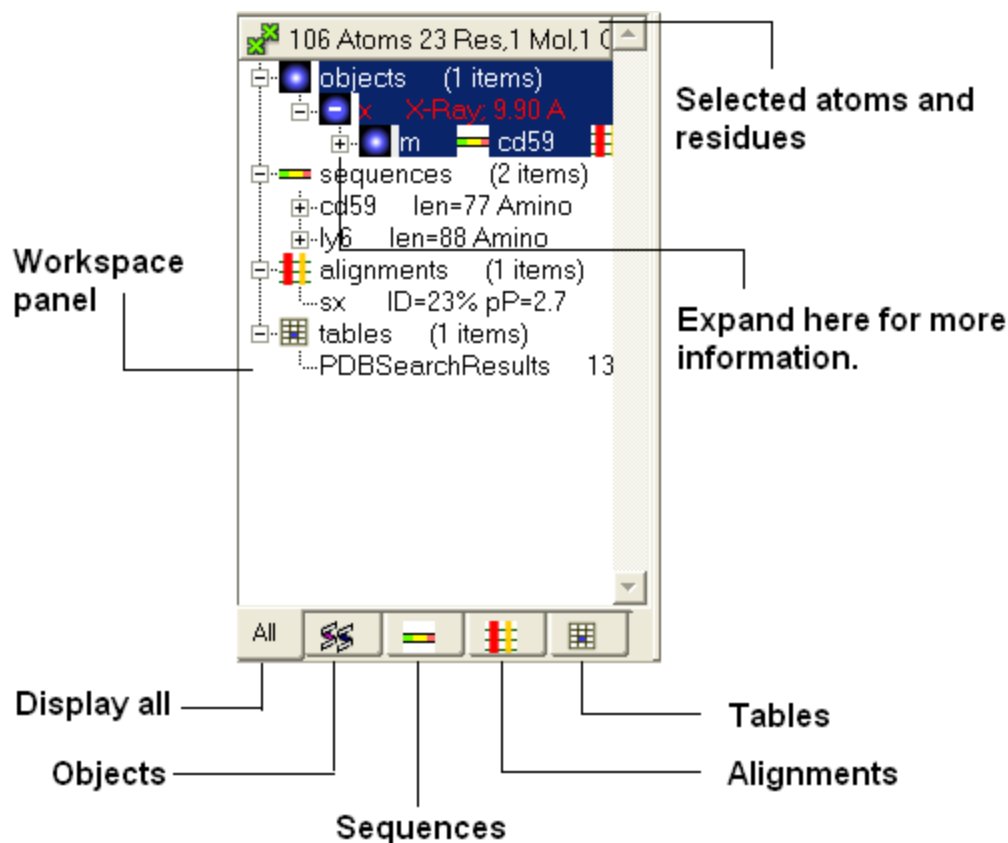
### 3.1.7 How to use the ICM Workspace Panel

The workspace panel (located on the left hand side panel of the gui) is an important place within the graphical user interface because it displays which sequences, structures, objects, tables and alignments are currently loaded into ICM. Also, from this panel you can make graphical selections and drag and drop objects and sequences to other locations within the GUI. More details about how to use the ICM Workspace Panel for displaying structures can be found [here](#).



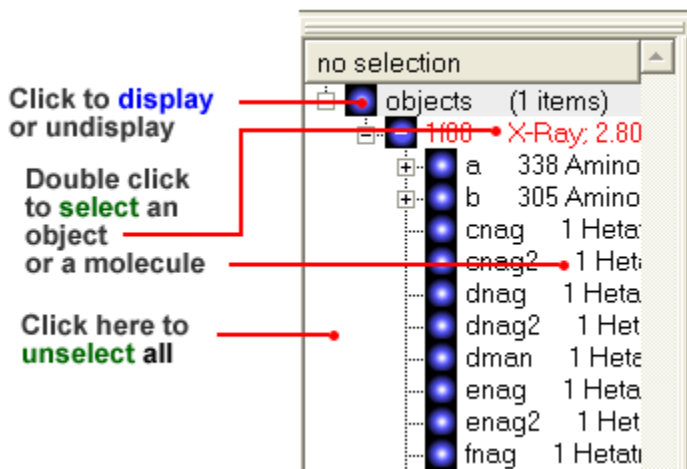
### 3.1.8 How to Display a Molecule

Once a structure has been loaded into ICM the individual components of that structure (i.e. amino acids, metal ions, binding sites etc) are listed in the ICM workspace.



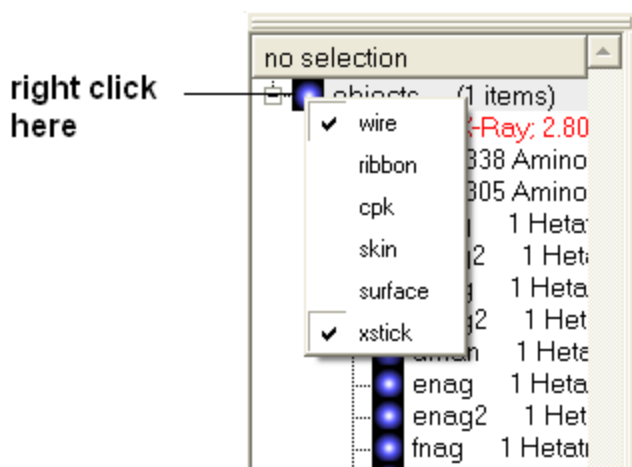
To display every component of the object except for binding sites and water atoms:

- Click on the white box next to the word object at the top of the ICM workspace. This box will be colored blue once the structure is displayed



To display the whole structure in wire, ribbon, cpk, skin, surface and xstick representations:

- Right click on the blue box next to the word object. A menu will be displayed.



- Select which representation you desire for your structure by clicking on the appropriate word. A check mark indicates the representation currently displayed. To un-display a particular representation click on the word again.

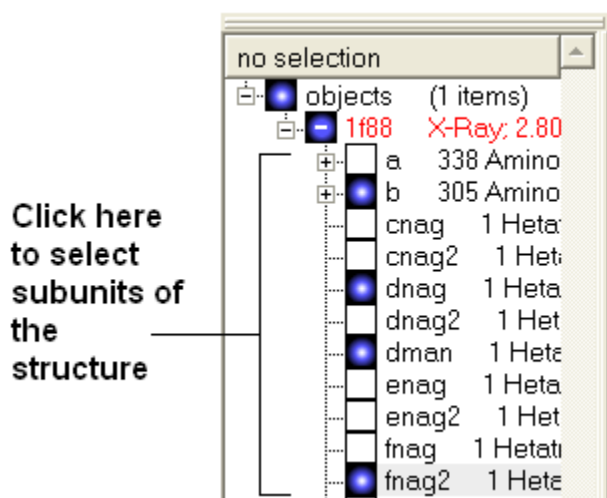
In order to clear your graphical display:

- Select **View/Undisplay All**

If you only wish to display part of the structure then click in the boxes further down the tree in the ICM workspace.

To display the selected regions of the structure in wire, ribbon, cpk, skin, surface and xstick representations:

- Right click on the appropriate box in the **ICM** workspace. A menu will be displayed.
- Select which representation you desire for your structure by clicking on the appropriate word. A check mark indicates the representation currently displayed. To un-display a particular representation click on the word again.

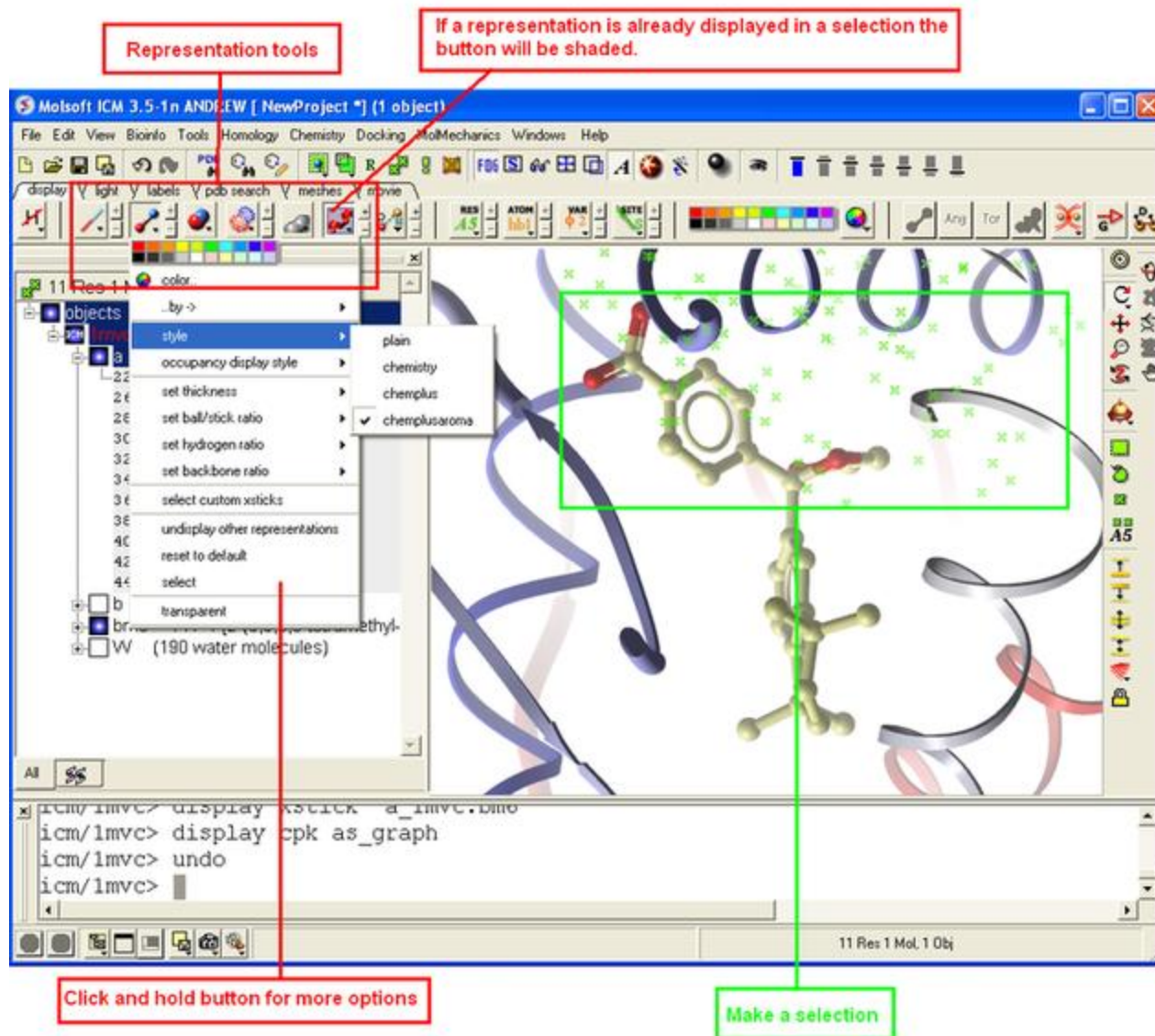


### 3.1.9 How to Change Protein Representation

To change the representation of the protein, make a selection and then use the tools in the display tab.

There are 5 main types of representation:

- **Wire:** Wires connecting covalently bound atoms of a molecule. This representation has no defined thickness as such will not make shadows. Useful for showing the chemical structure of a small molecule.
- **Xstick:** Covalent bonds are represented as cylinders whilst atoms are represented as small spheres..
- **CPK:** Atoms are represented as spheres with their respective van der Waals radius and coloured according to a standard defined by Corey, Pauling and Koltun.
- **Surface:** Solvent accessible surface. This is the center of water sphere as a water probe rolls over the molecule.
- **Skin:** A Connolly molecular surface over the selection. This is a smooth envelope touching the van der Waals surface of atoms as a water probe rolls over the molecule.
- **Ribbons:** Cartoon representation of protein and DNA secondary structure. Protein residues marked as alpha-helices ('H') are shown as a flat, helical ribbon, those marked as beta-sheets ('E') are shown as a flat ribbon with an arrow-head, and the rest are shown as a cylindrical "worm". If secondary elements are not defined everything will be shown as a cylindrical worm. ICM can automatically assign secondary structure: Tools/3D predict /Assign Helices and Strands



### 3.1.10 How to remove chain breaks (dotted lines)

Chain breaks in a protein structure are represented by dotted lines. To remove them use `GRAPHICS.chainBreakStyle=1`

eg

```

read pdb "1xbb"
cool a_
GRAPHICS.chainBreakStyle = 1 # this removes the dotted lines between chain
breaks

```

In version 3.6-1a and above you can use the options in the display tab. Click and hold on the ribbon button. You can then select **Display Chain Breaks/ None**.

### 3.1.11 How to Color

To change the color of the representation you need to use the buttons in the display tab.

Changing the colour of a representation works in much the same way as displaying the representation itself. The selection rationale is the same followed by clicking on a colour in the palette. It is also possible to colour different representations of the same selection independently (e.g. when displaying a loop (selection series of residues), represented as ribbon and xsticks; colour the ribbons of that selection in cyan and the xsticks in red).

To change the color of any representation - click and hold. The color will apply to the selection and the chosen representation only. If nothing is selected then everything displayed in chosen representation will be colored

Left click will change selected foreground color and right click will change the background.

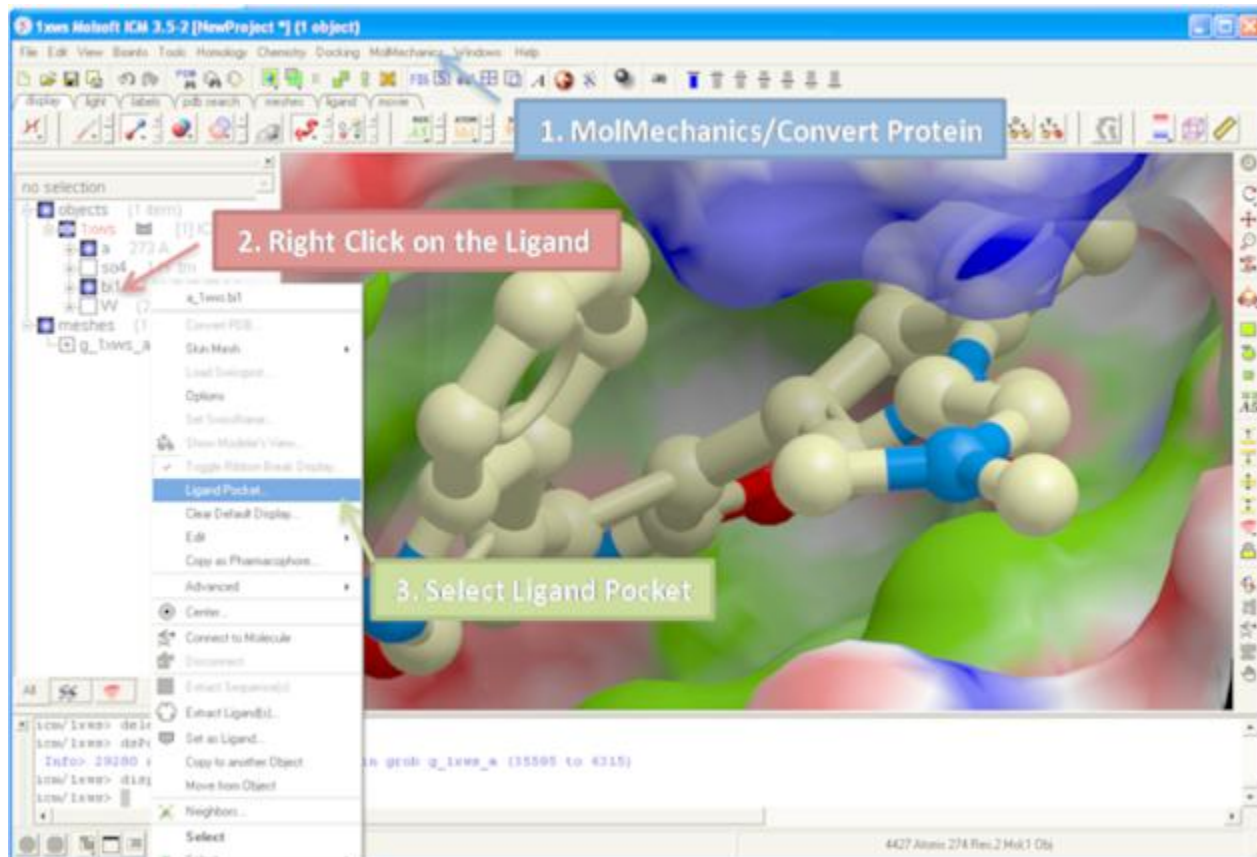
The screenshot shows the Molsoft ICM 3.5.1n software interface. The 'color' menu is open, showing options like 'by->', 'Unlink Color from Alignment', 'Link Color to Alignment', 'assign sec. structure', 'ribbon', 'cylinders', 'protein worm', 'DNA worm', 'undisplay other representations', 'reset to default', 'select', and 'transparent'. The 3D structure is displayed with various representations (stick, ribbon, surface) and colors. The command window at the bottom shows the following commands: `icm/lmvc> display xstick a_lmvc.dmo`, `icm/lmvc> display cpk as_graph`, `icm/lmvc> undo`, and `icm/lmvc>`. The status bar at the bottom right indicates '11 Res 1 Mol, 1 Obj'.

ICM command language can make coloring easier

### 3.1.12 How to Display a Binding Pocket Surface

To display the surface of a small molecule ligand or peptide binding pocket:

- Load the PDB of interest.
- Convert PDB to ICM object. If you do not convert you will not get the properties of the pocket displayed on the surface.
- Right click on the small molecule or peptide in the ICM Workspace and select **Ligand Pocket**.



### 3.1.13 How to Save an ICM Object

Any ICM object such as a structure, sequence, or alignment, can be saved for use at a later time.

To save an object:

- Right click on the object name in the ICM workspace or ICM alignment editor and a menu will be displayed.
- Click on the **Save As...** option.
- Enter the unique name you wish to call your object in the box labeled **File name:**



- Choose which folder or directory you wish to save your object by clicking scrolling down in the box labeled **Save in:**
- Choose which file type you would like to save your object as by scrolling down in the box labeled **Save as type** . ICM structure objects should have the file ending yourfilename.ob and alignments yourfilename.ali
- Once the appropriate information has been entered click on the **Save** button in the bottom right hand section of the window.
- The object is now saved.



To save an ICM object or PDB file right click and select **SaveAs..**

### 3.1.14 How to Save an ICM Project File

All objects contained within an ICM session can be saved in a single file with the extension .icb. The file can then be read into ICM and the exact layout of the file will be preserved. To save a project file go to the **File** menu and select **Save Project**.

### 3.1.15 How to Drag and Drop

**NOTE:** "Drag and Drop" is a useful way of moving objects and sequences around the graphical user interface.

Sequences and objects can be moved around the graphical user interface by dragging and dropping them. All loaded sequences and objects are always displayed in the workspace panel. Select the desired object or sequence from the workspace panel by clicking and holding, move the selection to the desired location and release.

This is a useful application in the graphical user interface. For example, you may have an alignment displayed and you wish to add another sequence to the alignment. This can simply be accomplished by dragging a loaded sequence from the workspace panel into the alignment display panel. Or, you can quickly view an object by dragging and dropping it from the workspace panel into the 3D graphics window.

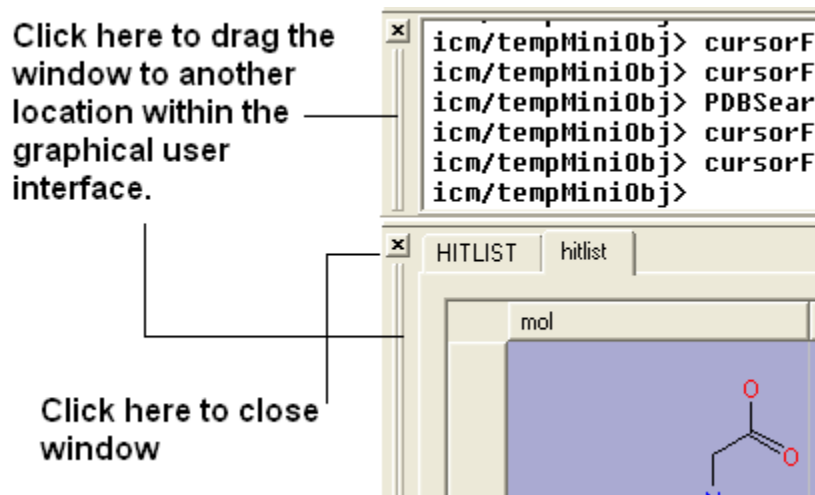
### 3.1.16 How to: Right Click Options

**NOTE:** If you right click on any object you will see a new menu of options related to that object.

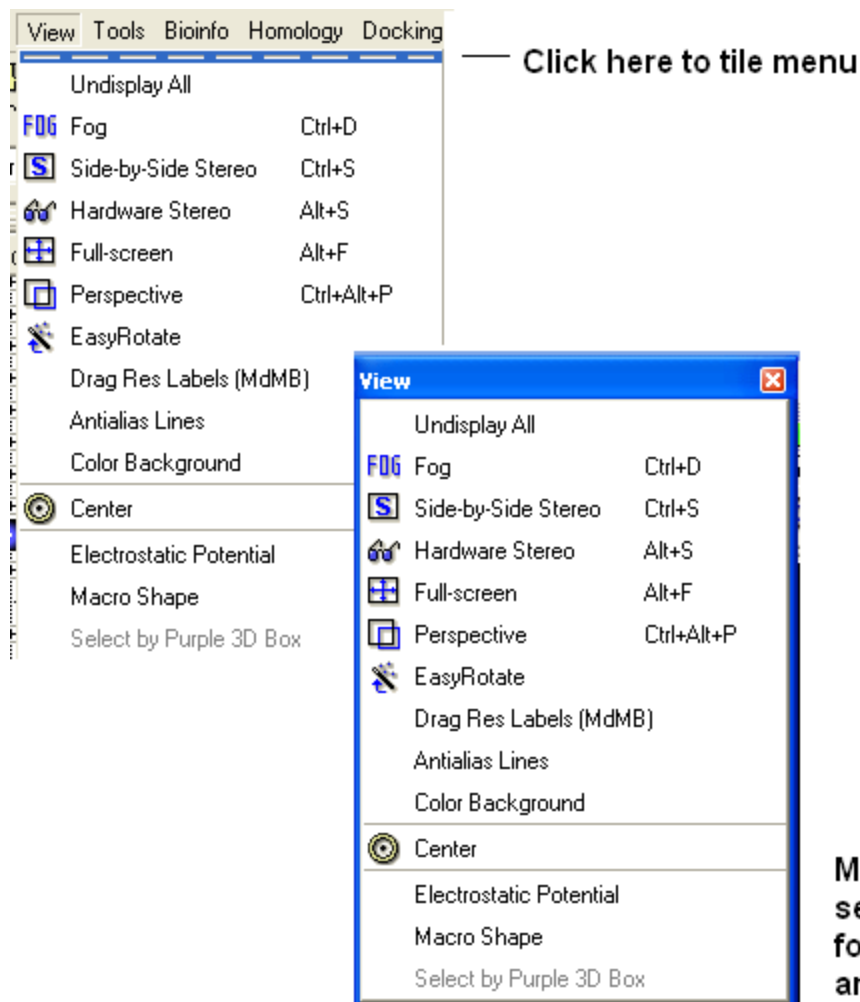
The right click mouse option can be used throughout the graphical user interface. It is a very useful means of opening up a whole new world of menus and options. Most of these options are described in this book. However, when using the graphical user interface it is always a good idea to try right clicking the mouse on an object and seeing which extra options that are available for you to use.

### 3.1.17 How to Move Windows

It is possible to move some windows around the graphical user interface to make viewing easier.



It is also possible to separate menus from the GUI.



**NOTE:** To return to the default display option select the 'Default layout' option in the windows menu.

OR

Click the default layout icon.

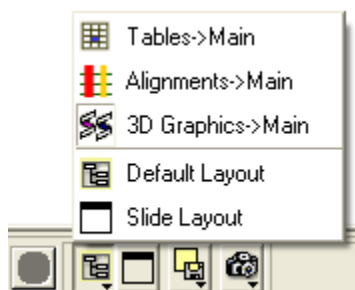


OR

Double click on the window header.

### 3.1.18 How to Arrange Windows

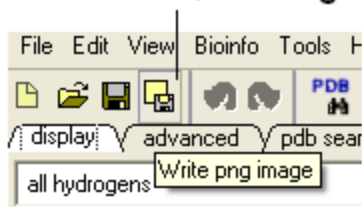
Sometimes when using ICM you may have many items displayed such as structures, alignments and tables. As a default the graphical display is the largest and centered in the middle of the ICM graphical user interface. However if you wish to work on an alignment or table you can place the alignment or table as the main display by clicking on the buttons shown below. The larger display generally makes it easier to manipulate the alignment or table. There are ofcourse other ways to alter the layout such as `tier` the windows but this option is just a simple click and can sometimes come in useful.



### 3.1.19 How to Make a Picture

There are several ways of taking a picture of the contents of the 3D graphical display window see the `write image` section. However the easiest way is to simply click on the camera button in the view tools panel.

**Simply click here for a QUICK high quality image**



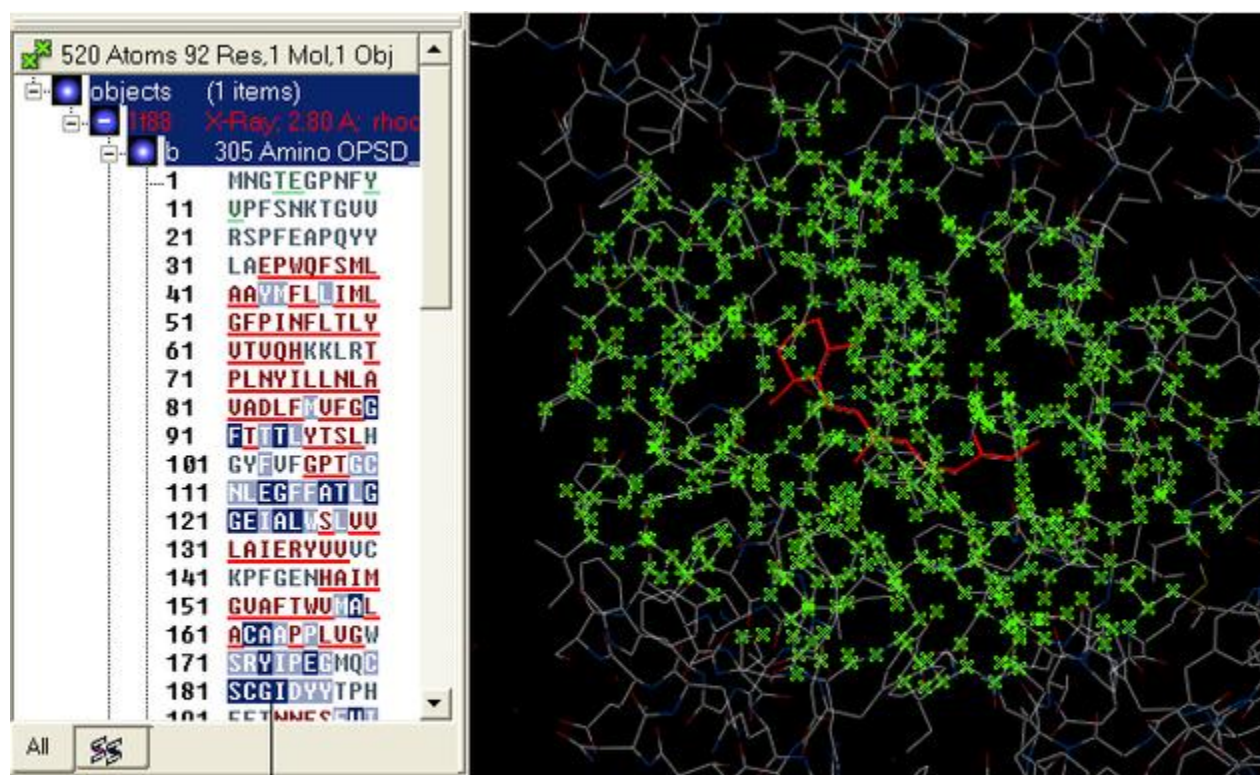
Or select `/File/Quick Image`

The picture will be automatically saved as a PNG file in the directory from which you loaded ICM. The default picture name is `icm[n].png`, where `n` is the number of pictures taken in one ICM session. To save in other picture formats and to change the file name see the `write image` section.

## 3.2 Making Selections

**Note:** Click **Next** (top right hand corner) to navigate through this chapter. Headings are listed on the left hand side (web version) or by clicking the **Contents** button on the left-hand-side of the help window in the graphical user interface.

There will be many occasions when you will have to make selections. For example, if you only wish part of your structure to be displayed or if you want to select residues around a binding pocket. If you have a molecule displayed in the graphics window, then selections will be displayed as green crosses. The selection you have made is also displayed at the top of the ICM Workspace. It is always a good idea to keep an eye on what is selected and what isn't.



Workspace and graphical selections

There are four basic levels of selection

1. Object (eg a PDB structure or ICM object)
2. Molecule

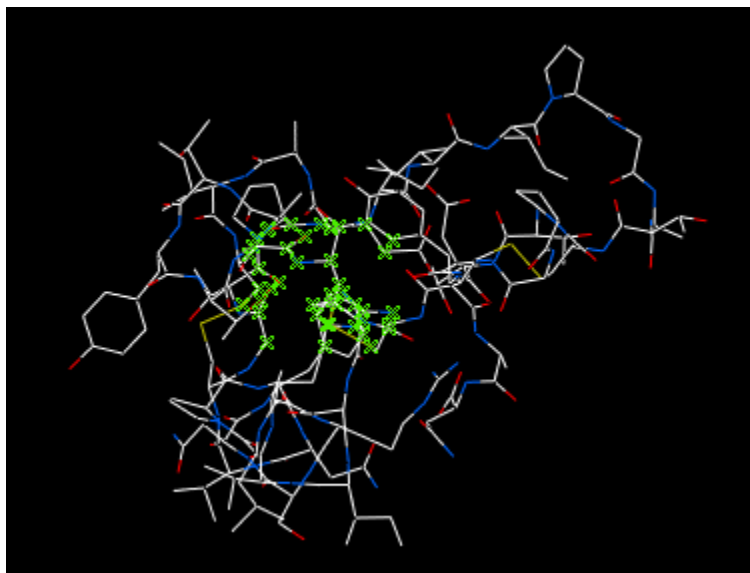
3. Residue
4. Atom

You can make selections in:

- The Graphics Display
- The ICM Workspace (Selections are highlighted in blue)
- Tables
- Alignments

### 3.2.1 Graphical Selections

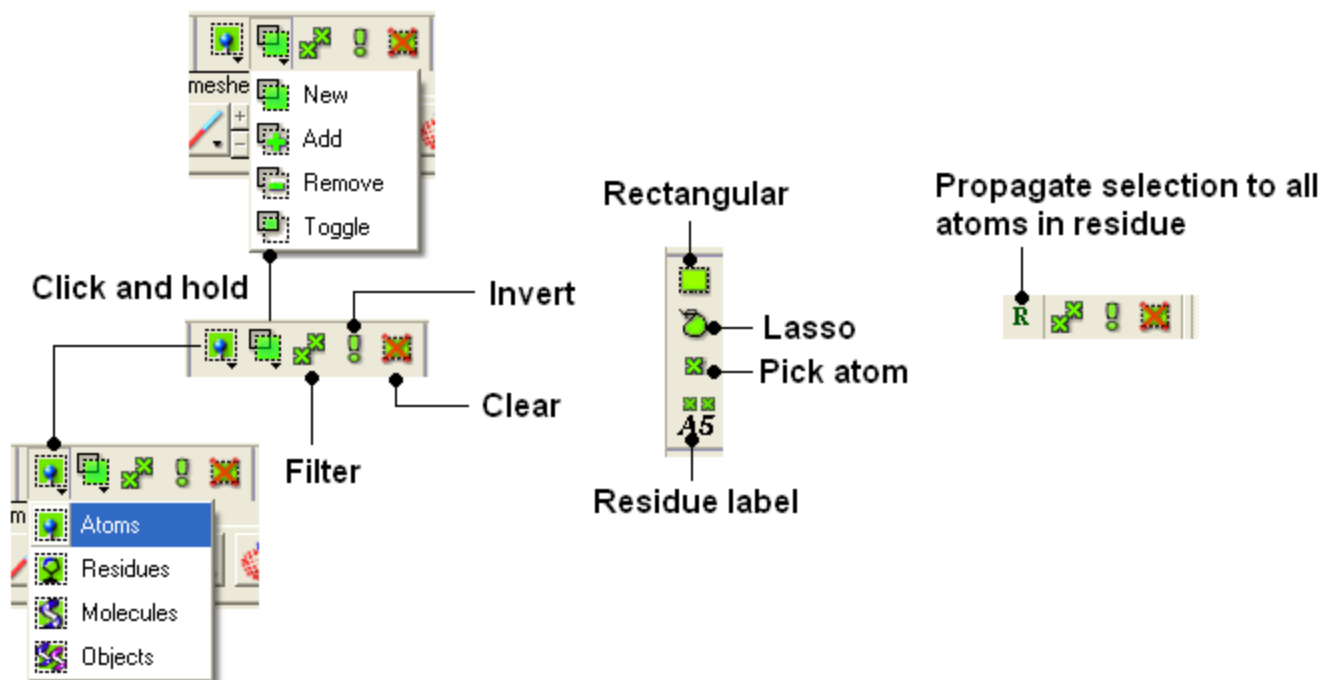
In this section you will learn how to select parts and certain regions of molecules from the 3D graphical display. Graphical and molecule selections are required in many operations within ICM. For example, if you wanted to display graphically part of a molecule or if you wanted to perform a minimization of residues within a sphere of an important atom.



Selection shown  
in green.

### 3.2.2 Selection Tools

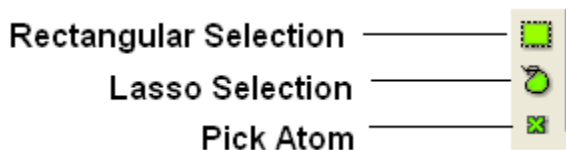
The following buttons can be used to make a selection once a structure is displayed.



**NOTE:** All selection tool buttons are colored green. Graphical selections are represented as green crosses.

### 3.2.3 Basic Selections

To make a basic selection (ie nothing too complicated!) the following buttons can be used.



*To unselect everything you have previously selected:*

- Simply click on the **Unselect** icon on the selection toolbar.

OR

- Right click and drag away from the displayed structure.

*To select parts of your structure:*

- Click on the **Rectangular selection icon** and click and drag around the part of the structure you wish to select.

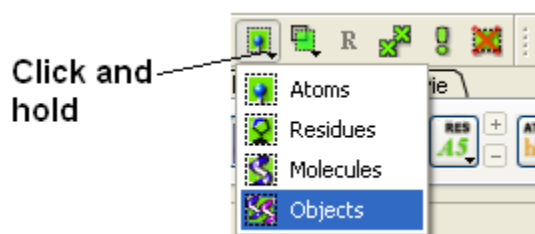
OR

- Click on the **Lasso selection icon** and click and drag your mouse around the area of the structure you wish to select, forming a lasso around it.

*To pick individual atoms:*

- Click on the 'pick atom' button

*You can also change the level of a selection using the button shown below. Click and hold the button to choose the level of selection. For example, if you have selected atoms you can convert the selection to all atoms at the residue level by choosing the Residues option.*

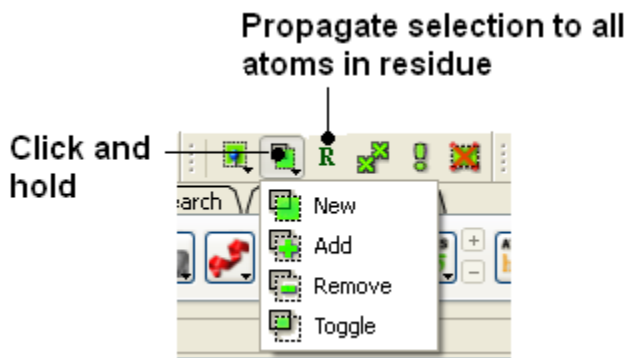


- Click on the **Select objects**, **Select molecules**, **Select residues**, or **Select atoms** icon, depending on which part of the structure you wish to be highlighted.

**NOTE:** The selection you have made is always recorded at the top of the ICM workplace. If you are familiar with using the ICM terminal (See language manual) the atoms, residues, molecules or objects selected interactively in the graphics window are automatically stored in the as\_graph variable.

### 3.2.4 Altering a Selection

Once you have made a selection you may wish to add or remove parts of the selection. The buttons shown below allow you to accomplish this.





*To add or remove from your current selection:*

- Click on the **Selection mode: add** or **Selection mode: remove** icon on the toolbar.
- Click and drag around the part of your structure you wish to add or remove.

*You may also wish to invert your selection in a specific part of the structure.*

The parts that are currently selected will become unselected, and the unselected parts will become selected.

In order to invert a selection:

- Click on the **Invert** icon on the toolbar.

If you wish to select and unselect certain regions of a selection the toggle selection button is very useful.

- Click on the Toggle selection button.
- Right click around the selections you wish to select or unselect.

**NOTE:** The selection you have made is recorded at the top of the ICM workplace. Any selection is stored in the variable as `_graph`.

### 3.2.5 Filter Selection

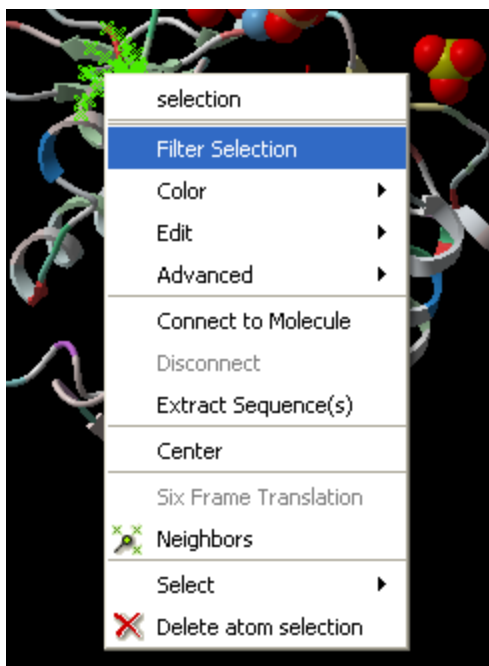
You may want to be very specific about a selection you want to make. For example you may only wish to select protein backbone atoms.

The button shown below enables you to filter your selection:



Or

Right click on a selection and a menu as shown below will be displayed.

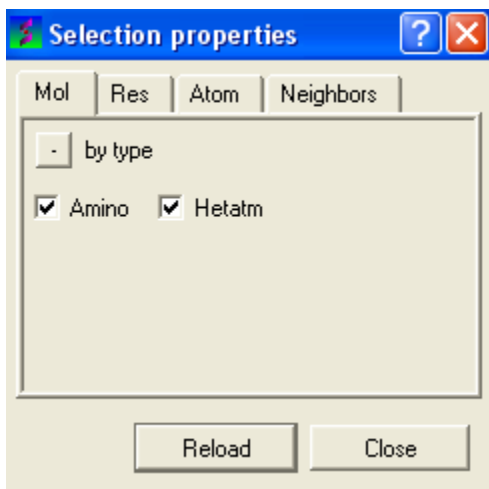


- Select the Filter Selection option.

*If you wish to filter and select by residue or atom type:*



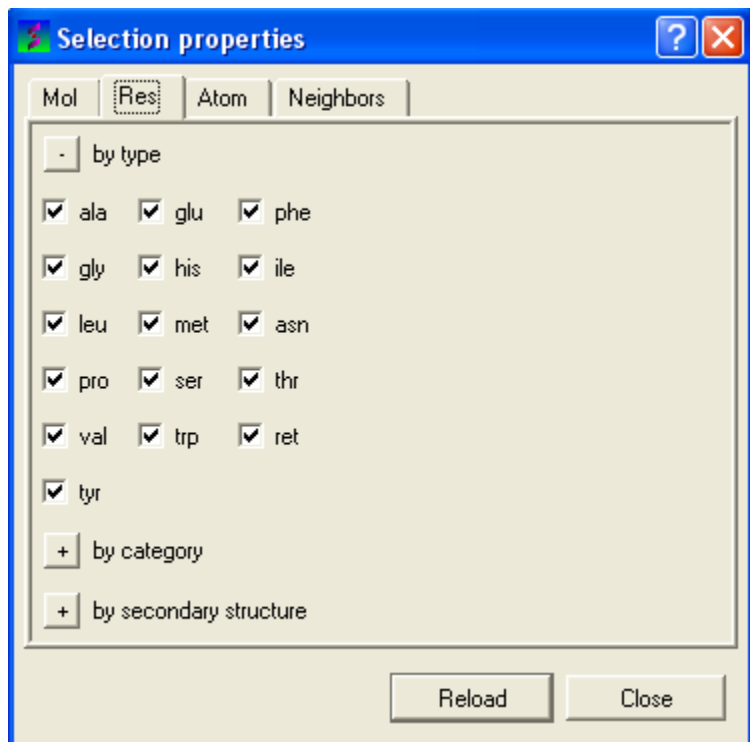
- Click on the Filter graphical selection icon on the toolbar and a data entry box as shown below will be displayed.



*To select just the protein or just the hetatoms as well:*

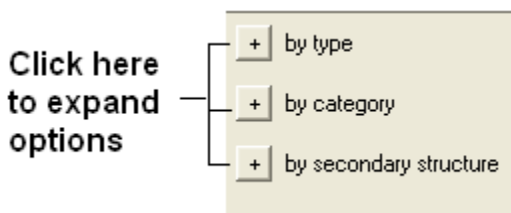
- Click on the Mol tab.
- Check the appropriate boxes depending on your desired selection.

*To filter by residue type or secondary structure:*

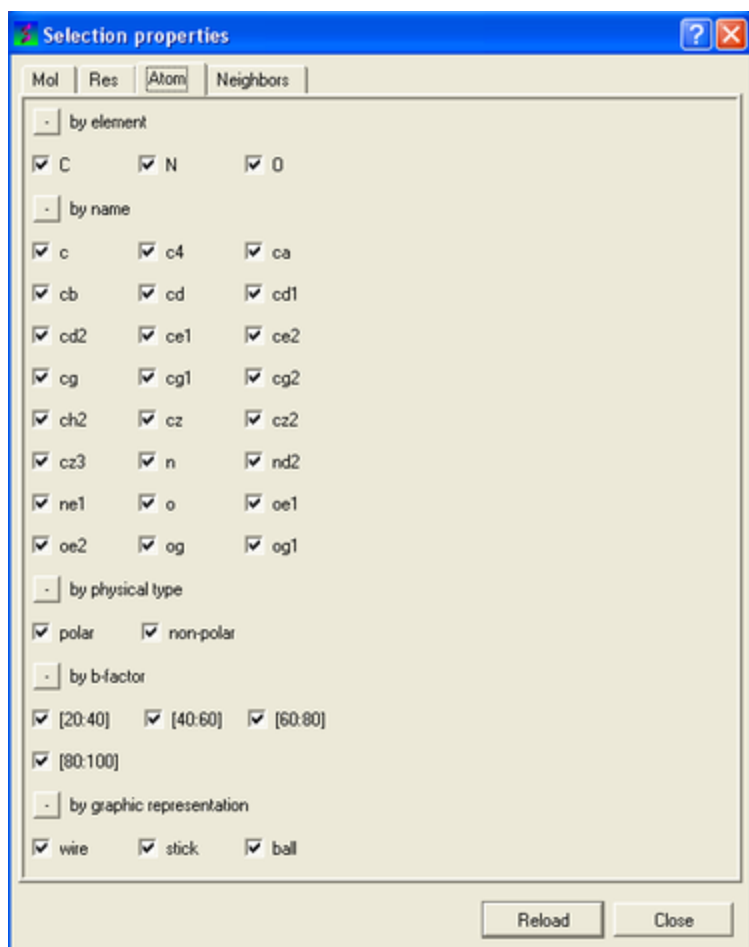


- Click on the Res tab.
- Check the appropriate boxes.

**NOTE:** You may need to click on the button marked with a '+' symbol to expand the options.

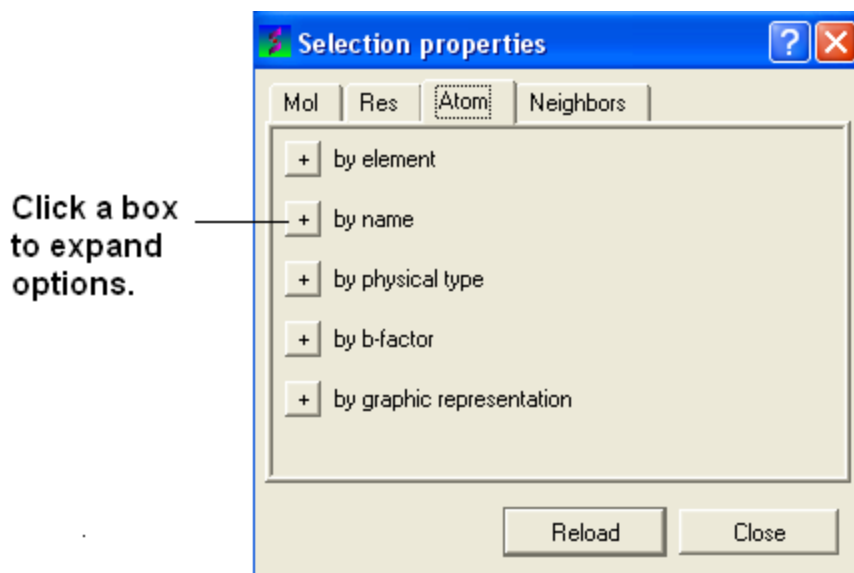


*To filter by atom type.*



- Click on the Atom tab.
- Check the appropriate boxes.

**NOTE:** You may need to click on the button marked with a '+' symbol to expand the options.



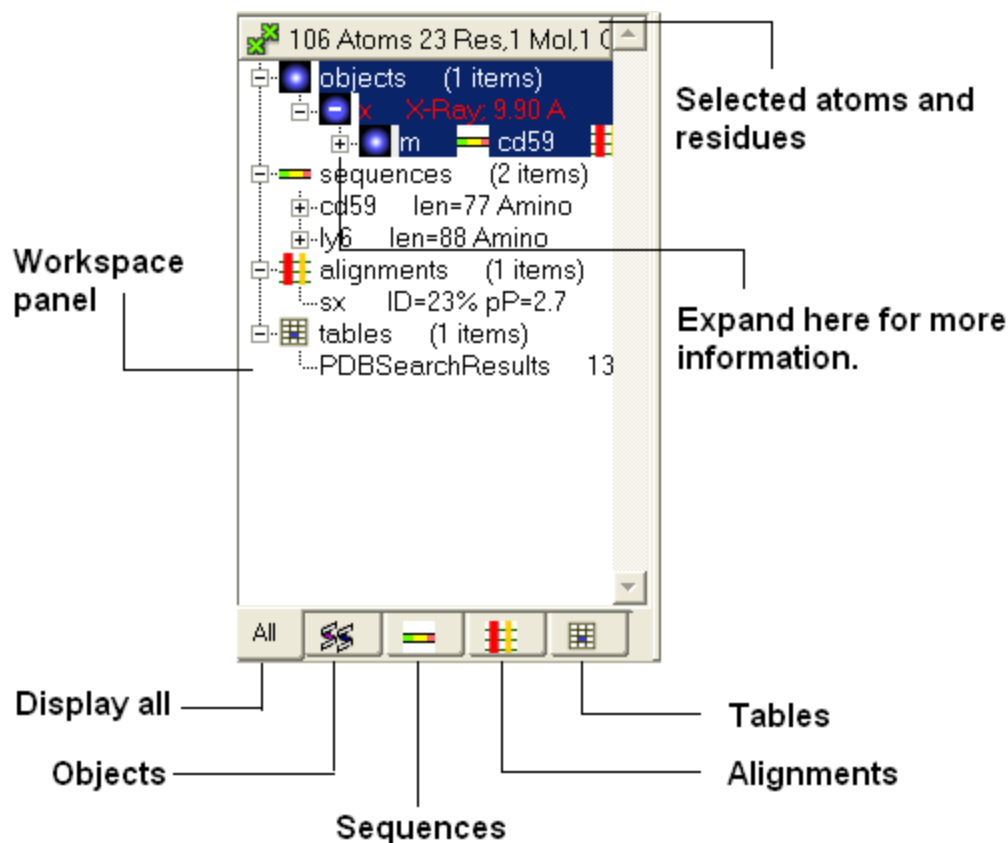
*To select neighbors to a particular selection.*

- See the `select neighbours` section for detailed instructions.

**NOTE:** The selection you have made is always recorded at the top of the ICM workplace. If you are familiar with using the ICM terminal (See language manual) the atoms, residues, molecules or objects selected interactively in the graphics window are automatically s

### 3.2.6 Workspace Selections

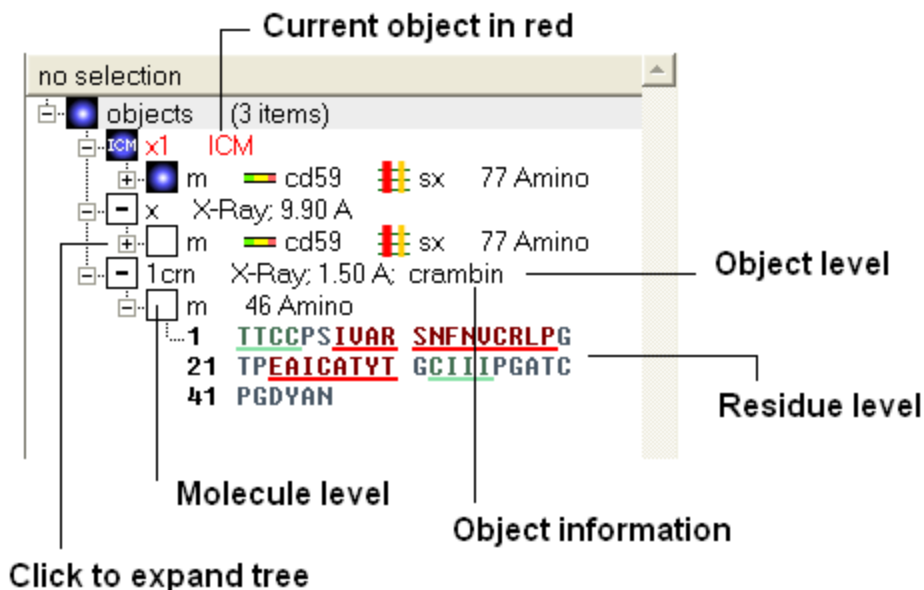
In the default GUI layout the workspace panel is located to the left of the 3D graphics display. It is a great tool for keeping track of all your sequences, pdb structures, objects, tables and alignments. As you will see in this section it also provides a way of making selections.



### 3.2.7 Workspace Navigation

Once you have mastered how to navigate the ICM workspace making a selection will become easier. Each object is divided into 3 levels:

1. Object Level - Shown in red if it is the current object. Holds details about the structure - name, X-ray, NMR, resolution etc. Importantly it will state whether the structure is an ICM object or a structure straight from the PDB. To learn how to convert a PDB into an ICM object go to the section on [converting a PDB](#).
2. Molecular Level - Shows the individual subunits, ligands and hetatoms of a molecule.
3. Residue Level - Shows the sequence.

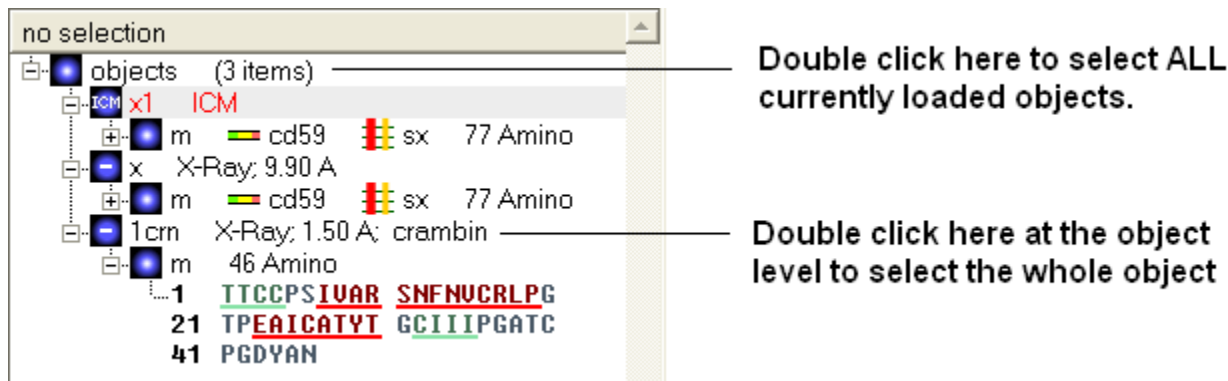


**NOTE:** You can expand each level of the ICM workspace by clicking the "+" button as shown above.

### 3.2.8 Selecting the Whole Object

*To select the whole object:*

- Double click on the object level.



### 3.2.9 Selecting Amino Acids

There are three options to select individual amino acid residues:

### OPTION 1:

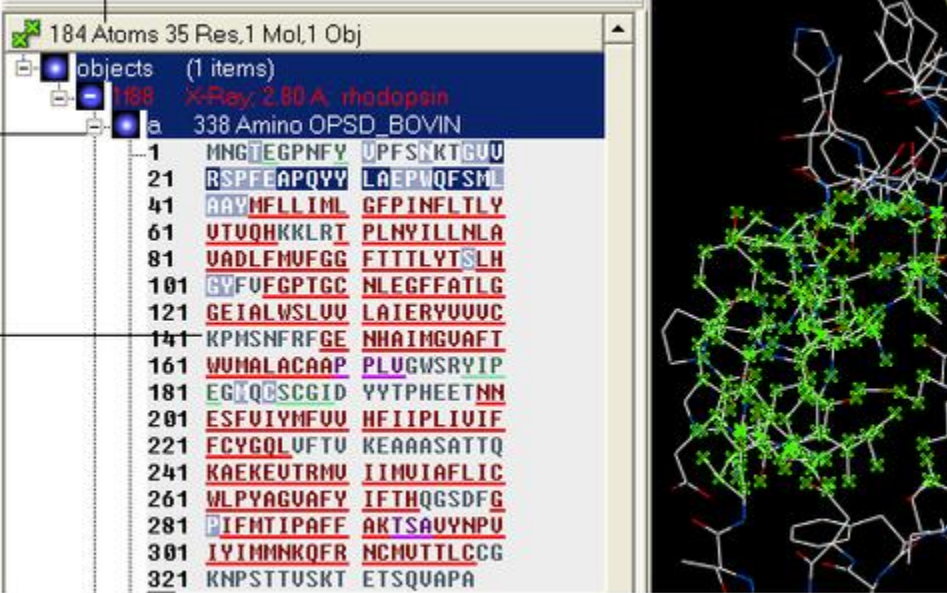
- Click and drag over the residues you wish to select in the ICM workspace. Selected residues will be highlighted in dark blue in the workspace and with green crosses in the graphical display.

Selection information is recorded here

Click here to expand tree to show amino acid residues.

Click and drag over residues you wish to select.

Selected residues will be highlighted in the workspace and graphics window



Residue Number	Residue 1	Residue 2
1	MNGTEGPNFY	UPFSNKTGUU
21	RSPFEAPQVY	LAEPWQFSM
41	AAVHLLIML	GFPINFLTY
61	UTVQHKKLRT	PLNYILLNLA
81	UADLFMVEGG	FTTTLTSLH
101	GVFVFGPTGC	NLEGFFATLG
121	GEIALWLSLV	LAIERYVUUC
141	KPMSNFRFGE	NHAIMGVAFT
161	WMAALACAAP	PLUGWSRYIP
181	EGIQCSGGID	YYTPHEETNM
201	ESFUIYMFUV	HFIIPLIVIF
221	FCYGQLUFTU	KEAASATTQ
241	KAKEEUTRMU	IINUIAFLIC
261	WLPYAGUAFY	IFTHQGSDFG
281	PIFHTIPAFF	ARTSAUYNPU
301	IYIHMNKQER	NCHUTTLCCG
321	KNPSTTUSKT	ETSQUAPA

Any selection is highlighted in the workspace as well as in the 3D graphics window if the structure is displayed.

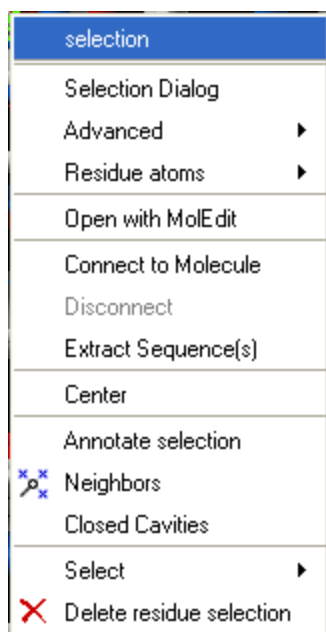
### OPTION 2:

- Click on the **rectangular selection** icon or **lasso selection** icon on the toolbar.
- Click and drag around the residues you wish to select. Selected residues will be displayed by green crosses on the graphical display and blue in the ICM workspace.
- Click on the Pick Atom button.

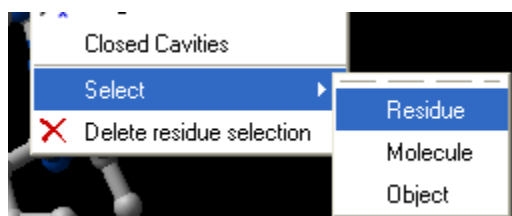
### OPTION 3:

- Right click on the selected residue in the graphical display and a menu as shown here will be displayed.





- Click on **Select** and a further menu will be displayed.
- Click on **Residue, Molecule** or **Object**.



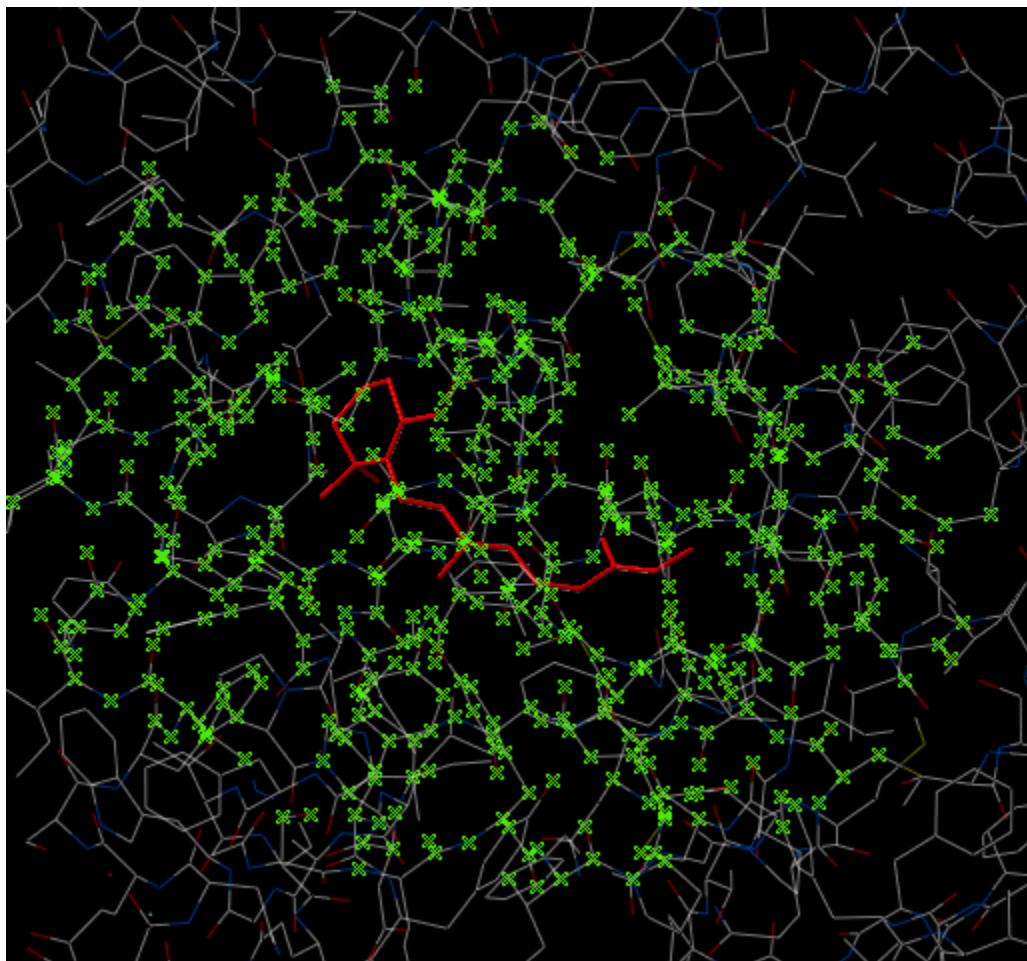
**NOTE:** Ctrl + A will select everything in the ICM workspace, and Ctrl + Shift + A will unselect your objects.

**NOTE:** The selection you have made is always recorded at the top of the ICM workplace. If you are familiar with using the ICM terminal (See language manual) the atoms, residues, molecules or objects selected interactively in the graphics window are automatically s

### 3.2.10 Selecting Neighbors

In some instances you may only want to display or select only a subset of a structure. For example you may only wish to display the residues surrounding a ligand (as shown below (ligand red; graphical selection green crosses). The "Selecting Neighbors" option selects the residues within a sphere of a defined radius.

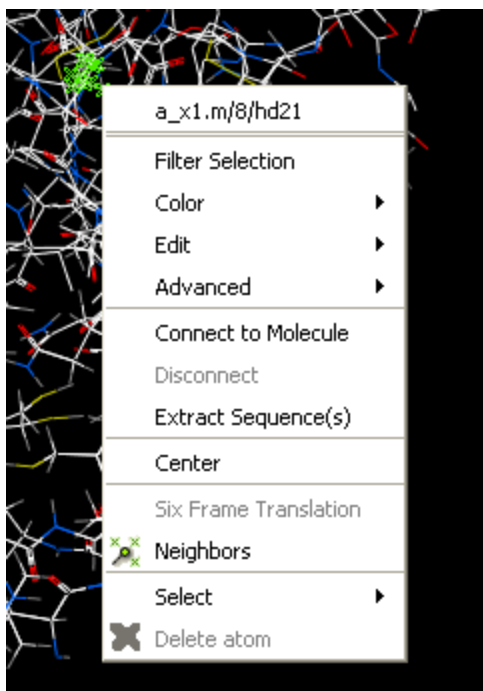
There are two ways of selecting neighbours to a particular atom or residue in ICM. Either by right clicking on the atom or residue in the graphical display or by right clicking in the ICM workspace.



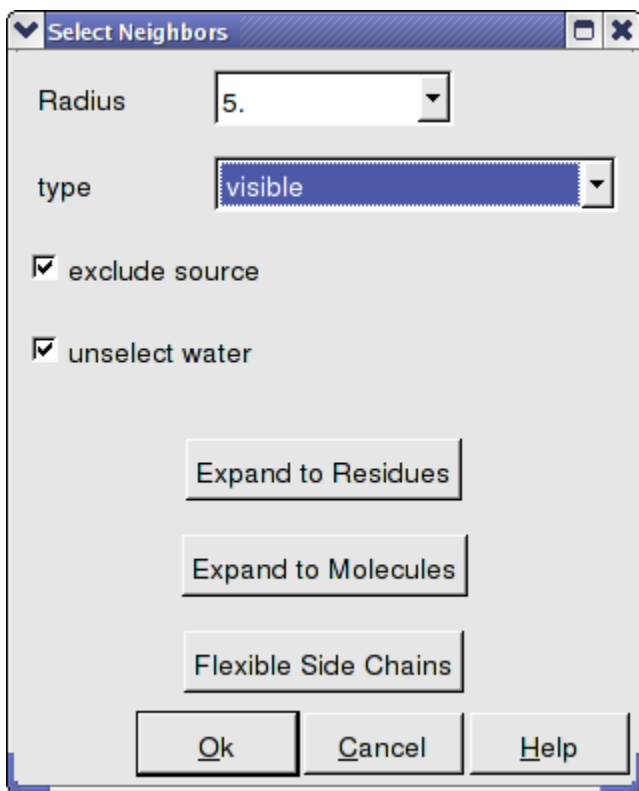
### 3.2.11 Selecting Neighbors: Graphical

*To select neighboring atoms or residues around a sphere of a certain radius:*

- First select the residue(s) or atom(s) around which you wish to select neighbors. (See the Selection Toolbar Section)
- Right click on the selection and a menu as shown below will be displayed or choose Tools/Geometry/Neighbors.

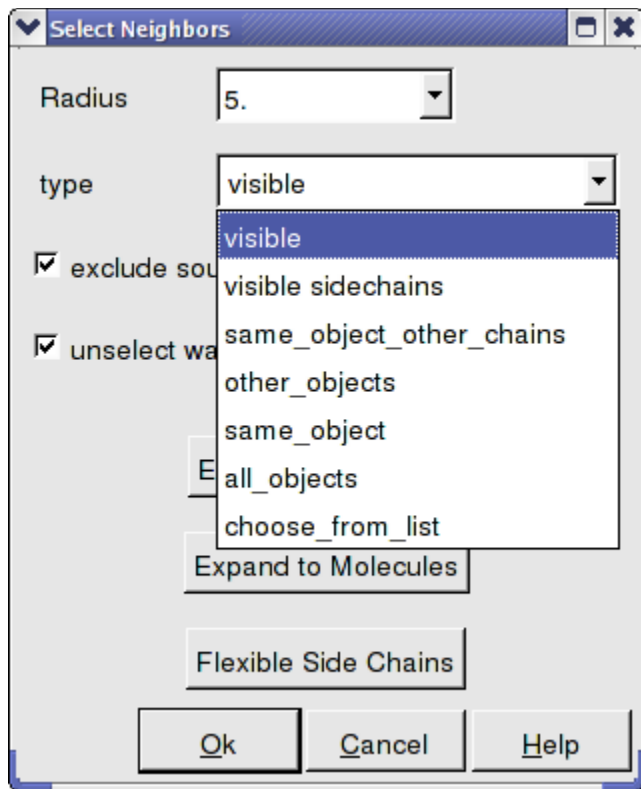


- Select the Neighbors option and a data entry box as shown below will be displayed.



- Enter the selection radius around which you wish to select.

- Select from which object you wish to make the selection from the drop down list in the "type" data entry box.



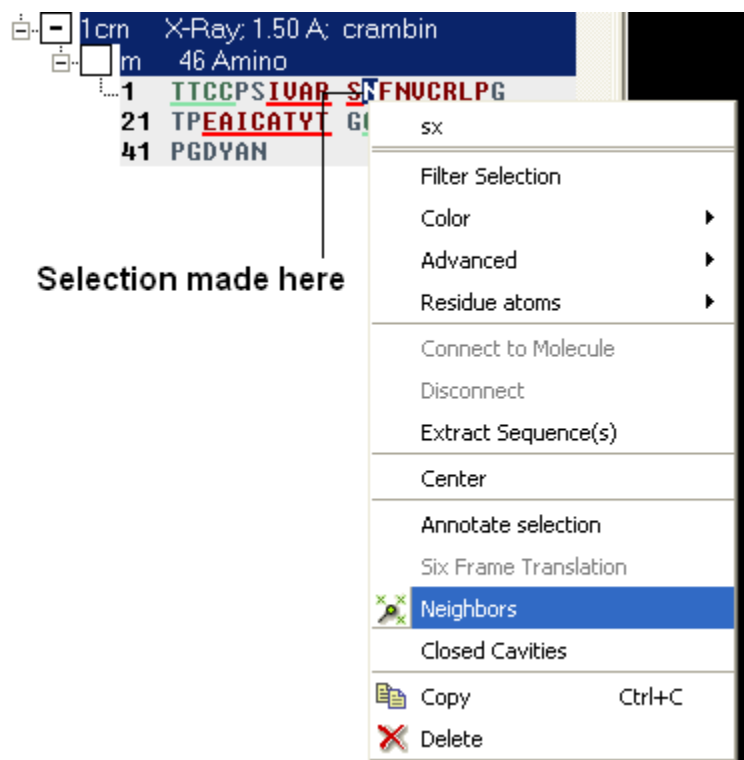
- Select whether you wish your original selection to be selected by checking the "exclude source" box.
- Select whether you wish water molecules to be selected by checking the "unselect water" box.
- There are also options to change the current selection to expand to residues, molecules, or flexible side-chains.
- Click OK and your selection will be displayed as green crosses.

**NOTE:** The selection you have made is always recorded at the top of the ICM workplace. If you are familiar with using the ICM terminal (See language manual) the atoms, residues, molecules or objects selected interactively in the graphics window are automatically saved in the variable `as_graph`. Graphical selections are shown in green (crosses) or highlighted in blue in the ICM Workplace.

### 3.2.12 Selecting Neighbors: Workspace

*To select neighboring atoms or residues around a sphere of a certain radius from a residue in the ICM workspace:*

- First select the residue in the ICM workspace around which you wish to select neighbors. (See the Residue Selection)
- Right click on the selection and a menu as shown below will be displayed.



- Select the Neighbors option and a data entry box as shown below will be displayed.
- Follow the instructions in the previous section.

**NOTE:** The selection you have made is always recorded at the top of the ICM workplace. If you are familiar with using the ICM terminal (See language manual) the atoms, residues, molecules or objects selected interactively in the graphics window are automatically s

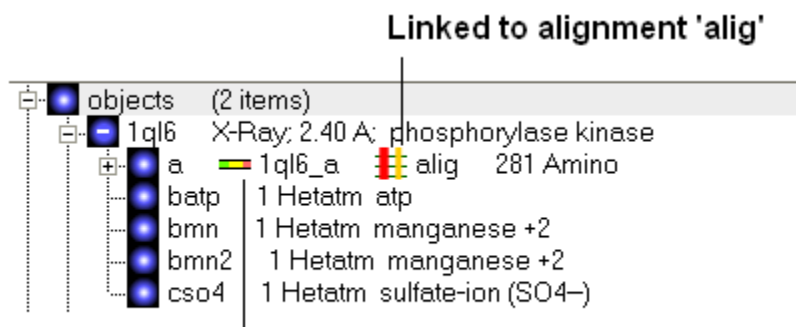
### 3.2.13 Alignment and Table Selections

Descriptions on how to make selections in Alignments and Tables are in the sections entitled Making Selections in Alignments and Making Table Selections.

### 3.2.14 Making Links

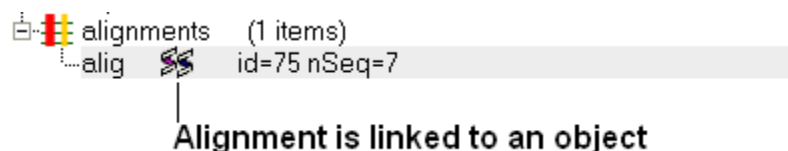
It is sometimes necessary to make links between sequences objects and alignments. A link enables you to make selections in one environment such as an alignment and then these selections are transferred to the object such as the PDB structure displayed.

If a link is made then a symbol will be displayed next to the object in the ICM workspace. In the example shown below subunit\_a of the X-ray structure 1ql6 is linked to the sequence 1ql6\_a and the alignment called 'alig'.



**Linked to sequence 1ql6\_a**

If an object is linked to an alignment a symbol as shown below will be displayed.



To link a sequence from an object - extract the sequence from the object.

- Right click on the object in the ICM workspace.
- Select extract sequence.

To link a sequence and object to an alignment.

Use the extracted sequence as described above to build your alignment.

In addition a link can be made between a structure and alignment by:

- Bioinfo/Link to Structure.
- Enter alignment name.
- OK

### 3.3 Menu Option Guide

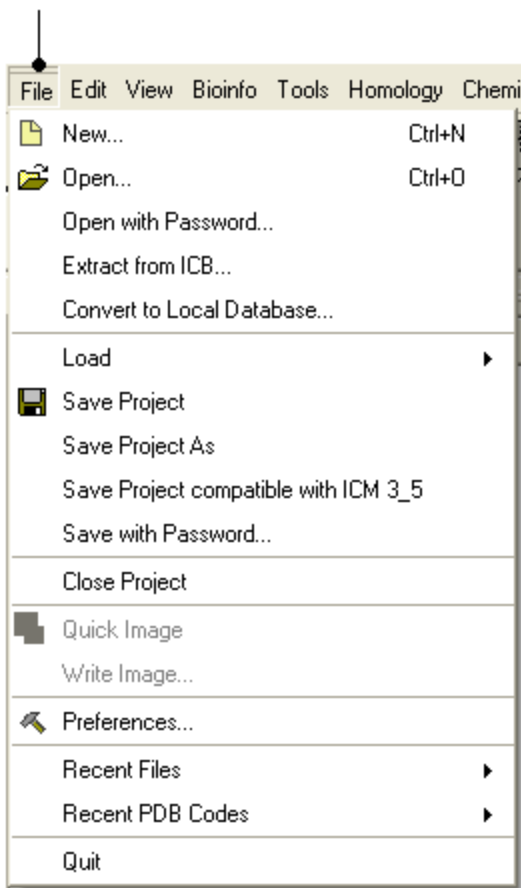
**Note:** Click **Next** (top right hand corner) to navigate through this chapter. Headings are listed on the left hand side (web version) or by clicking the **Contents** button on the left-hand-side of the help window in the graphical user interface.

Here we describe all the options in the drop down graphical user interface menus.



### 3.3.1 File Menu

## File Menu

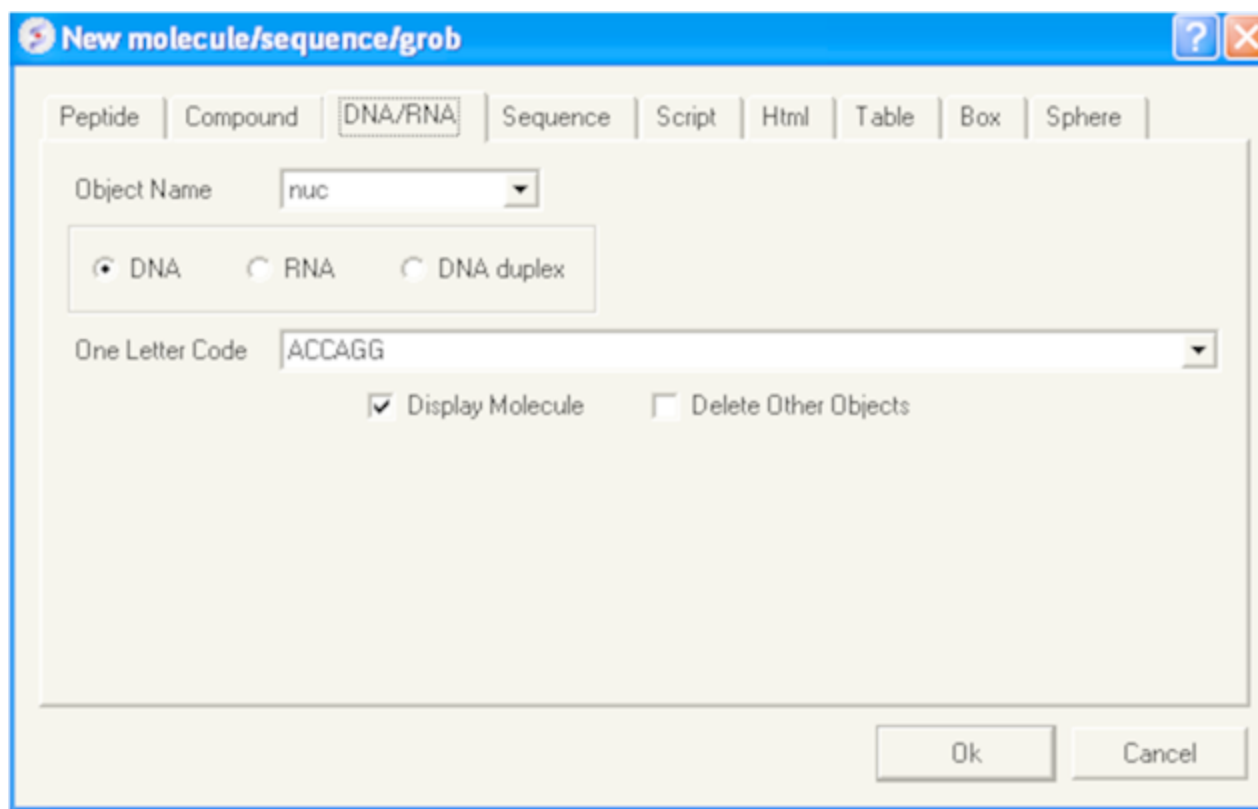


### 3.3.1.1 New

ICM can read as well as create several different entities. This dialog box helps you to create new entities from scratch:

All the processes in this section can be found under **File/New**, in the **New molecule/sequence/grob window**





#### 3.3.1.1.1 HTML

- File/New HTML tab provides a window to enter HTML code. This window is a good starting point for generating new molecular documents.

#### 3.3.1.1.2 New Table

##### *To generate a new empty table:*

- File/New and select the **Table** tab and a window as shown below will be displayed.
- Enter the number of rows and columns you wish to include in your table and whether you wish to add a column with chemical data.

#### 3.3.1.1.3 arrow

Creates a 3D arrow as a new graphical object ('grob' or 'mesh'). This arrow can be generated both as a solid object or as a simpler line representation. The name of the object can be defined in the 'Arrow Name' field.

The start (StartXYZ) and end (End XYZ) points of the arrow are defined in cartesian coordinates (X, Y, Z). The quality of the arrow can be adjusted (the higher the value, the smoother the arrow will be). Color can be assigned by simply clicking on the desired one or using rgb scale (eg. for red: `rgb={1. 0. 0.}`).

The Arrow Radius is defined in Angstroms. The size of the head, shown as a solid cone is defined as a fraction of the whole length of the arrow. Thus 0.1 means that the height of the head will take 10% of the total size of the arrow, while 1.0 means that the head will take the whole arrow (resulting in a shaftless arrow). The width of the head refers to the diameter of the head cone and it is defined as a multiplier of the Arrow Radius.

Tip: the arrow can be moved independently using 'connect'

#### **3.3.1.1.4 Box**

Creates a 3D box as a new graphical object ('grob' or 'mesh'). This box can be generated both as a solid object or as a simpler wire representation. The name of the box can be defined in the 'BoxName' field.

Dimensions of the box (X, Y, Z) are given in Angstroms and the angles connecting the sides are given in degrees. Color can be assigned by simply clicking on the desired one or using rgb scale (eg. for red: `rgb={1. 0. 0.}`).

Tip: the box can be moved independently using 'connect'

#### **3.3.1.1.5 sphere**

Creates a 3D sphere as a new graphical object ('grob' or 'mesh'). This sphere can be generated both as a solid object or as a simpler wire representation. The name of the sphere can be defined in the 'BoxName' field.

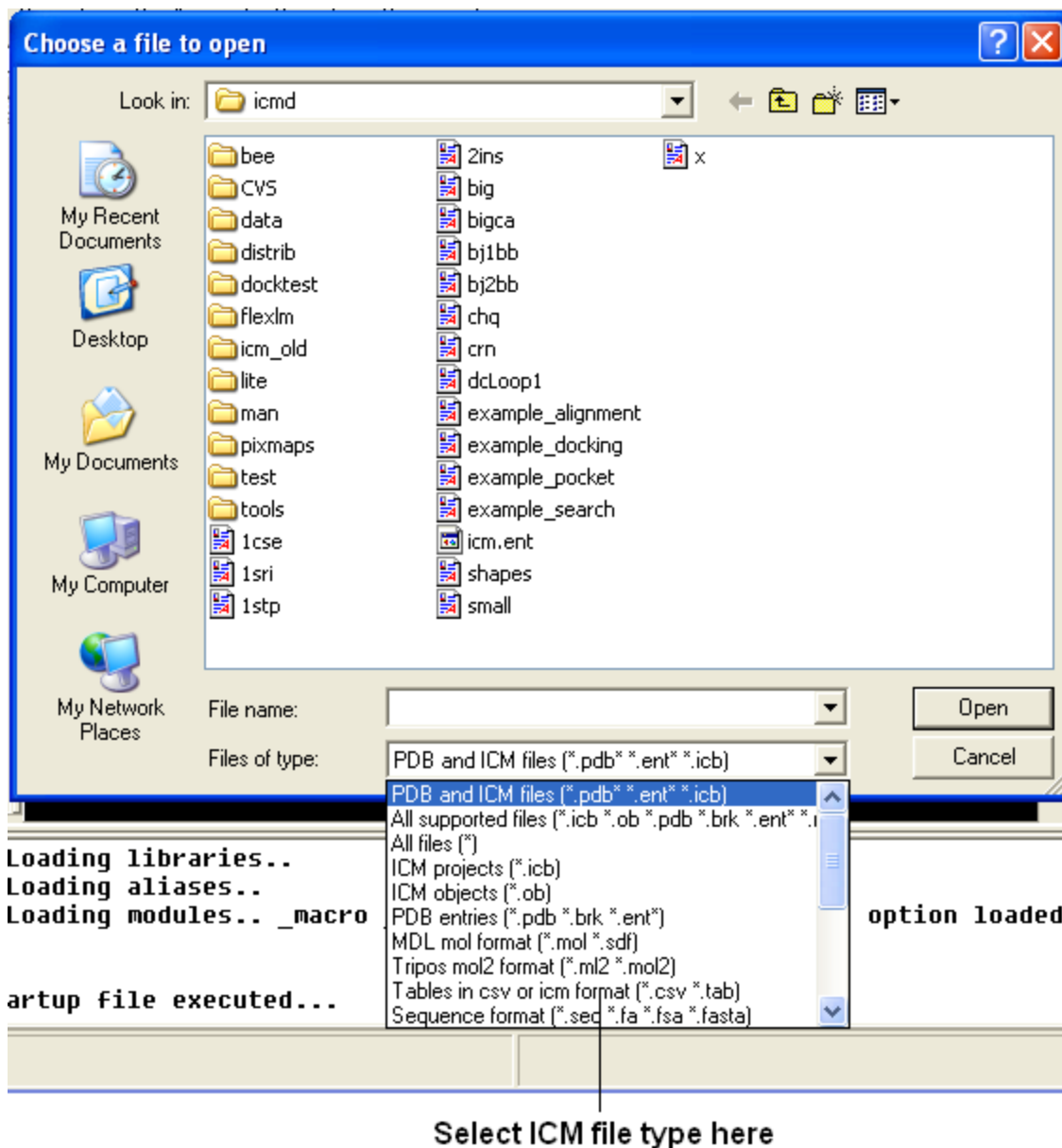
Dimensions of the sphere (X, Y, Z) are given in Angstroms and the angles connecting the sides are given in degrees. Color can be assigned by simply clicking on the desired one or using rgb scale (eg. for red: `rgb={1. 0. 0.}`).

Tip: the arrow can be moved independently using 'connect'

#### **3.3.1.2 Open**

Any file that ICM can understand can be opened by:

- Selecting File/Open.



### 3.3.1.3 Open with Password

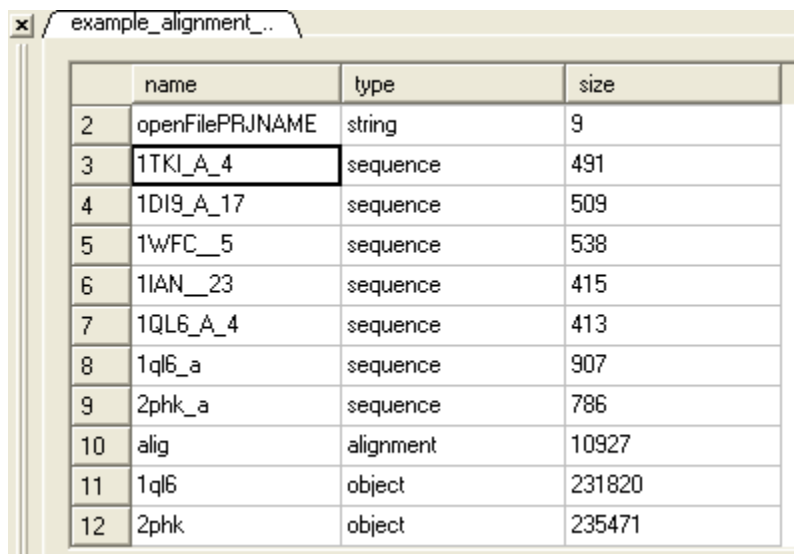
To open a file that is password protected:

- File/Open with Password

### 3.3.1.4 Extract from ICB

An **icb** file is an `icm project file` and this option allows you to view a tabulated list of what the icb file contains.

- File/ Extract from ICB
- Locate the saved icb file.
- A table as shown below will be displayed
- Double-click on any of the entry to extract that item from ICB



	name	type	size
2	openFilePRJNAME	string	9
3	1TKI_A_4	sequence	491
4	1DI9_A_17	sequence	509
5	1wFC__5	sequence	538
6	1IAN__23	sequence	415
7	1QL6_A_4	sequence	413
8	1ql6_a	sequence	907
9	2phk_a	sequence	786
10	alig	alignment	10927
11	1ql6	object	231820
12	2phk	object	235471

### 3.3.1.5 Load

*Options* contained within the menu File/Load

**PDB** - read PDB from FTP, http, and local PDB

**From Multiple Object File** - A multiple object file will have a file extension \*.ob and you can select which member of the multiple object is displayed.

**PFam Alignment** - PFam is a collection of multiple sequence alignments - enter FASTA ID

**SwissProt** - Download SwissProt sequence.

**All Images from Dir** - Read into ICM multiple image files png or jpg.

**Electron Density Map** - Download electron density map from Uppsala electron density server  
<http://eds.bmc.uu.se/eds/>

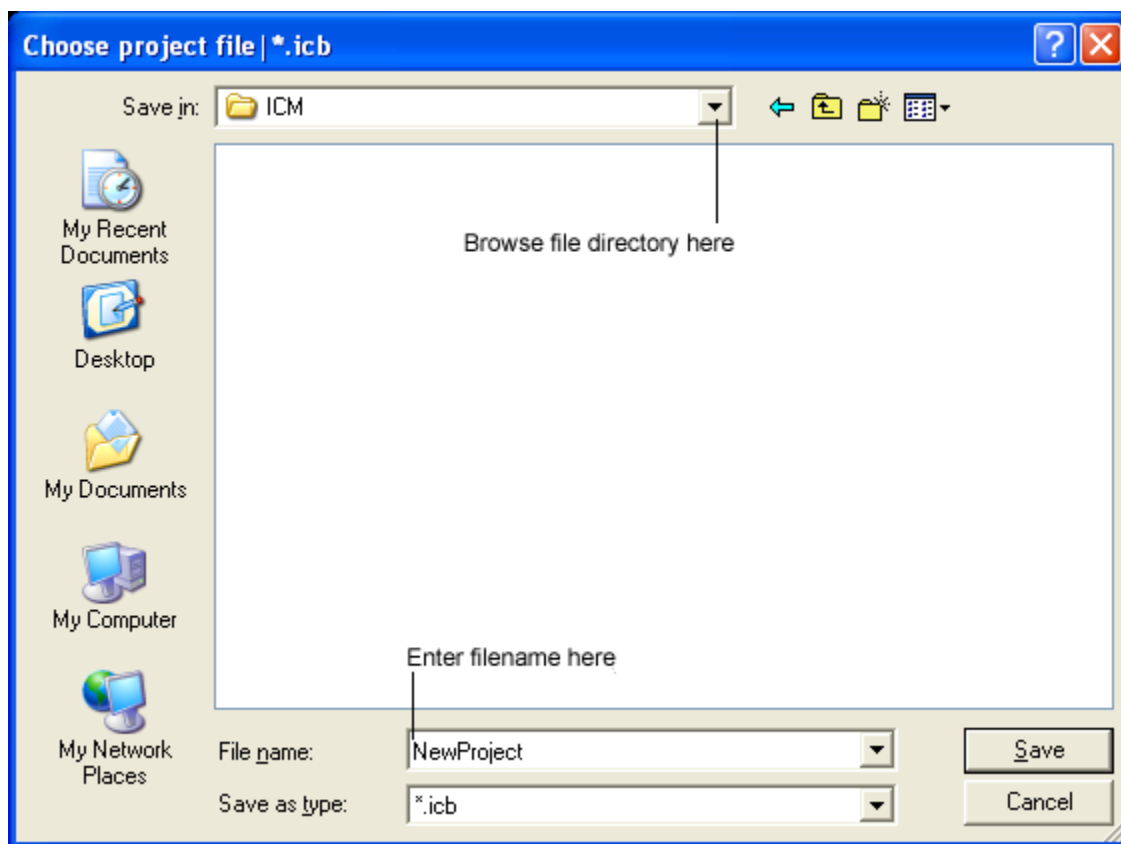
**3D Mesh in KMZ or COLLADA Format from Google** - see  
<http://sketchup.google.com/3dwarehouse/> to download KMZ or COLLADA.

### 3.3.1.6 Save Project

Saving a project will allow you to quit from ICM and then return to the exact set-up and display at which you left off at a later date. The projects are saved in files with the extension \*.icb

*To save a project:*

- Select **File/Save Project** and a data entry window will be displayed. This window will only appear if this is the first time you have saved a project.
- Enter the unique name you wish to call your project in the box labeled **File name:**



- Choose which folder or directory you wish to save your project in by scrolling down in the box labeled **Save in:**
- Once the appropriate information has been entered click on the **Save** button in the bottom right hand section of the window.
- The project is now saved as yourfilename.icb.

**NOTE:** An alternative way to save a project is to click on the save icon on the toolbar.



### 3.3.1.7 Save Project As

If you wish to re-name the project or save different versions of the same project use the **Save Project As** option.

To rename a project:

- Click on the **File/Save Project** option and a data entry window will be displayed. This window will only appear if this is the first time you have saved a project.
- Enter the unique name you wish to call your project in the box labeled **File name:**
- Choose which folder or directory you wish to save your project by scrolling down in the box labeled **Save in:**
- Once the appropriate information has been entered click on the **Save** button in the bottom right hand section of the window.
- The project is now saved as yourfilename.icb.

#### 3.3.1.7.1 Reloading a Saved ICM Object when ICM is Running

Once an ICM object has been saved you can re-read it by:

- Click on **File/Open** and a data entry window will be displayed (below).
- Locate your saved ICM Object by clicking on the **Browse** button in the bottom right hand section of the window.

**NOTE:** To make your search easier you can limit the number of files you search through by scrolling down in the Open as section and selecting the appropriate file ending.

- Click on the **OK** button when the file has been located and your saved ICM Object will load.

**NOTE:** If the file you wish to load has been viewed recently then it will be in the drop down menu in the Open box.

#### 3.3.1.7.2 Reloading a Saved ICM Object in Windows when ICM is not Running

To reload a saved project in Windows simply find the file in the "My Computer" file store and double-click on the icon.

### 3.3.1.8 Save Project Compatible with ICM 3\_5

#### File/Save Project Compatible with ICM 3\_5

Use this option to save a version of your ICM project compatible with an older version of ICM. Version 3.5 or older. If you have an ICM license you can update your version of ICM by visiting our support site at [www.molsft.com/support](http://www.molsft.com/support)

### 3.3.1.9 Save with Password

To save a project which is protected by a password:

- File/Save with Password
- Enter a file name or browse for a previously saved project.
- Enter a password
- Determine whether you want the file to be **Fully Protected, read only** or **Read Only and Allow Comments** .

### 3.3.1.10 Export as ActiveICM Html

To embed in a web browser.

1. Download ActiveICM from here  
<http://www.molsoft.com/getbrowser.cgi?product=activeicm&act=list> (it is free!).
2. Create an HTML page in ICM (File/New/Html).
3. Add a series of slides.
4. File/Export As ActiveICM Html..

### 3.3.1.11 Close Project

To close a project:

## File/Close Project

### 3.3.1.12 Quick Image

A quick image can be saved using this option. The image will be saved as icm1.png in the current directory in which you are working. Each subsequent image produced will be incrementally numbered.

This option is also available via a button as shown below:

#### Quick image button



### 3.3.1.13 Write Image

Before saving an image it is best to improve the quality of the image using the "High Quality Image" and antialias buttons shown below.

#### antialias

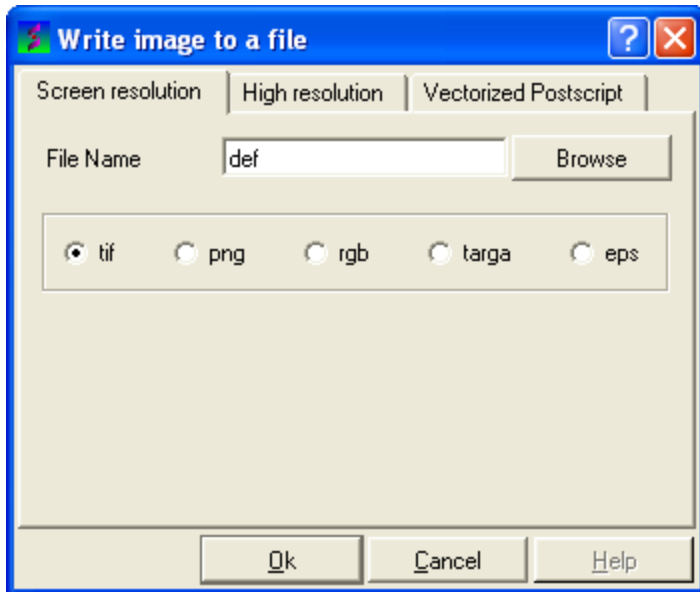


#### high quality image

To save and write an image:

- Select **File/Write Image** and the following window will be displayed:





- Enter the name for the picture in the **File name** data entry box.
- Select which file format you would like to save the picture in by clicking in the circular selection button next to the file types. The options are .tif; .png; .rgb; .targa .eps.
- To specify which resolution you wish the picture to be saved click on the **High resolution** button at the top of the panel.
- Click the drop down arrow in the **Resolution Increase** data entry box and select which resolution you require the picture to be. Alternatively you can type the resolution you require into this box.

**NOTE:** A quick way to save an image is to use the Quick Capture Graphics button on the toolbar which is described in the `Picture Tips` section of this manual.

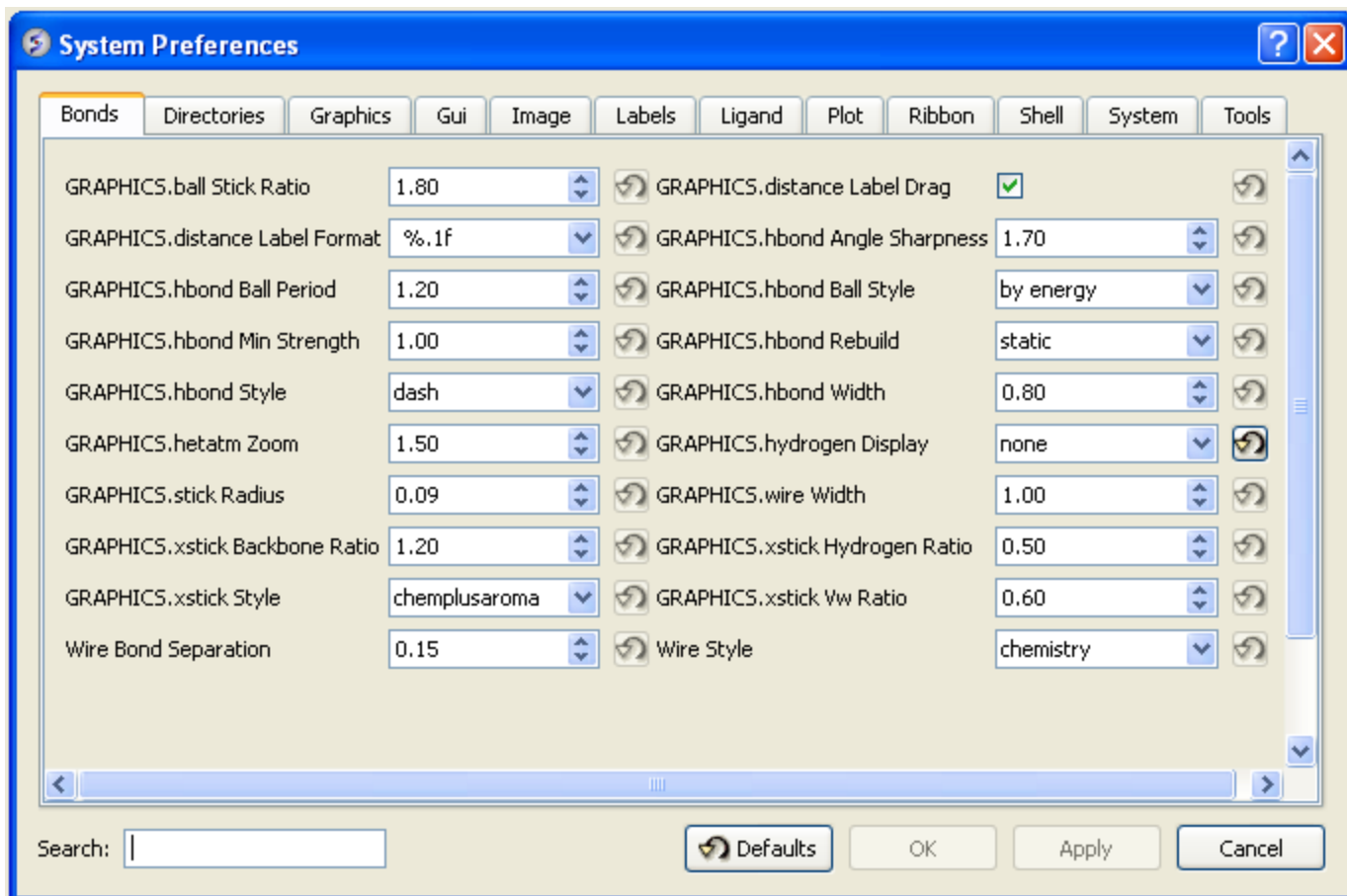
### 3.3.1.14 Preferences

*Your ICM preferences can be changed by:*

- Select File/Preferences.

**NOTE:** There is a "Reset to Default" button in case you make any changes you are not happy with.

#### 3.3.1.14.1 Bonds Preferences



***GRAPHICS.ballStickRatio*** - A default ratio of ball and stick radii. This ratio is applied when the styles are switched from the GUI xstick toolbar. Default (1.4)

***GRAPHICS.hbond Ball Period*** - Default (3)

***GRAPHICS.hbondMinStrength*** - parameter determines the hbond strength threshold for hbond display. The strength value is between 0. and 2. By changing 1. to 0.2 you will see more weak hydrogen bonds. Default: (1).

***GRAPHICS.hbondStyle*** - determines the style in which hydrogen bonds are displayed. Here hbond-Donor, Hydrogen, and hbond-Acceptor atoms will be referred to as D, H and A, respectively,

***GRAPHICS.hetatmZoom*** - The default ball and stick radii of a ligand can be different by the GRAPHICS.hetatmZoom factor. This makes a better ligand view since the ligand stands out from the surrounding protein atoms.

***GRAPHICS.stickRadius*** - radius (in Angstroms) of a cylinder displayed as a part of stick or xstick graphical representation of a molecule. Individual (residue-wide) control of stick radii.

***GRAPHICS.xstick Backbone Ratio*** - Default (1.2)

**GRAPHICS.xstick Style** - xstick style

**wireBondSeparation** the distance between two parallel lines representing a chemical double bond if wireStyle = "chemistry". Default (0.2 Angstroms).

**GRAPHICS.distance Label Drag** - enable distance label dragging

**GRAPHICS.hbondAngleSharpness** determines how the strength depends on the D-H...A(lone pair) angle. The preference can be found the general Preferences menu Default (1.7)

**GRAPHICS.hbond Ball Style** even, by atom size, by energy or telescopic

**GRAPHICS.hbond Rebuild**

**GRAPHICS.hbondWidth** relative width of a displayed hbond .

**GRAPHICS.hydrogenDisplay** determines the default hydrogen display mode for the display command.

```
GRAPHICS.hydrogenDisplay = "polar"
    1 = "all"      # all hydrogens are shown
    2 = "polar"   <-- current choice # polar displayed, the non-polar
hidden
    3 = "none"   # no hydrogens are displayed
```

**GRAPHICS.wire Width** - relative width of wire Default (1)

**GRAPHICS.xstick Hydrogen Ratio** - Default (0.5)

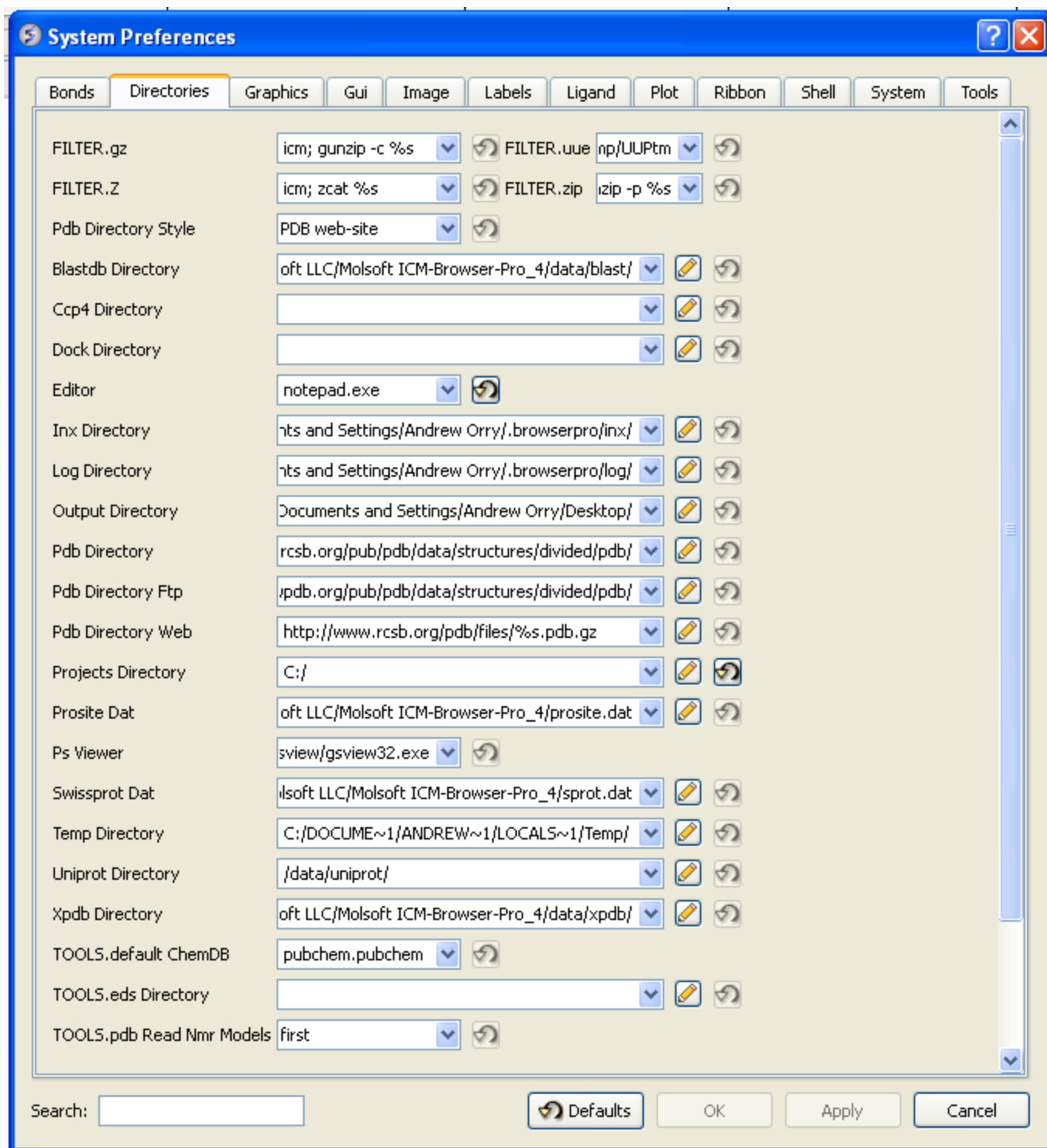
**GRAPHICS.xstick Vw Ratio** - Default (0.6)

**Wire Style** - change the default wire style

```
GRAPHICS.hbondStyle = "dash"
    1 = "wire"      # Just a line
    2 = "chemistry" # shows different types of chemical bonds.
    3 = "tree"     # shows a directed graph of the ICM-molecular tree
    4 = "aromatic" #
```

### 3.3.1.14.2 Directories Preferences

**DIRECTORIES TAB:**



Within this tab you can select the default directories for:

***FILTER.gz***, ***FILTER.uue***, ***FILTER.Z***, ***Filter.zip*** allows you to read compressed files .gz, .uue, .Z, and, .zip files automatically leaving the compressed file intact.

**PDB Directory Style** - The style of your Protein Data Bank directory/directories. ICM will understand all of the listed styles, including distributions with compressed \*.gz , \*.bz2 and \*.Z files

**BlastDB Directory** - return directory with Blast-formatted sequence files for ICM sequence searches. You can download Blast formatted databases from here  
`ftp://ftp.ncbi.nih.gov/blast/db/`

**Dock Directory** - Default directory for storing docking files.

**CCP4 Directory**

**Editor** - Select a default text editor

**Inx Directory** - location of stored index (\*.inx) files.

**Log Directory** - when you quit an icm-session, a \_seslog.icm file is automatically stored. If the s\_logDir variable is empty, it is stored to the s\_userDir + "/log/" directory. However one can redirect it to the current working directory ( "." ) or any other directory.

**Output Directory** -

**PDB Directory** - directory containing the PDB database of 3D structures. These files can also be easily downloaded directly from the PDB site if the variables are set as in the example below. PDB distributions can exist in several styles (all files in the same directory, or divided etc.).

**PDB Directory FTP**

**PDB Directory Web**

**Projects Directory** - Select the default location for storing ICM projects. Save your data in an ICM project. It is a convenient way of keeping all your structures, alignments, tables, docking results etc... in one place. A description on how to save an ICM project is described in the GUI Basics section of this manual.

**Prosite Dat** - location of the prosite.dat file a dictionary of protein sites and patterns, (Copyright by Amos Bairoch, Medical Biochemistry Department, University of Geneva, Switzerland).

**Ps Viewer** - Select a postscript viewer

**Swissprot Dat** - location of swissprot.dat file

**Temp Directory** - scratch directory for temporary files ( some montecarlo files will be saved there ).

**Uniprot Dat** - location of uniprot.dat file

***XPDB Directory*** - Path to the ICM XPDB database of compact binary ICM objects which are annotated with the site information. The advantage of the XPDB database is the speed of reading and smaller size than PDB. XPDB entries are read about 80 times faster!

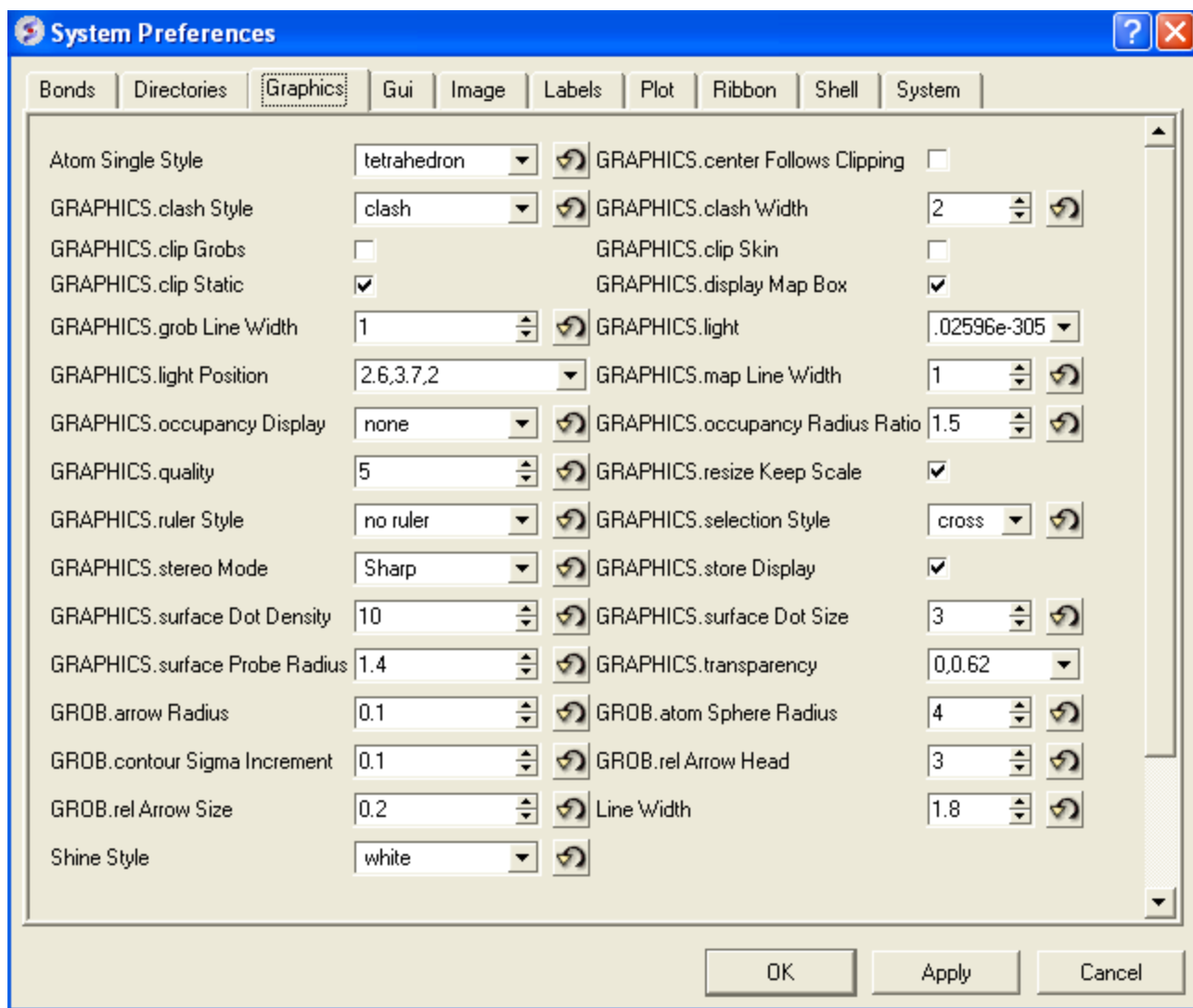
***TOOLS.default ChemDB***

***TOOLS.eds Directory***

***TOOLS.pdb Read Nmr Models***

1. = "first" : reads only one model from a multi-model (e.g. NMR) pdb file
2. = "all" : reads all models from a multi-model (e.g. NMR) pdb file and creates a separate object for each of them
3. = "all stack" : creates one object and loads all other models as a stored cartesian stack

**3.3.1.14.3 Graphics Preferences**



**Atom Single Style** - display style of isolated atoms in the wire mode.

1. "tetrahedron"
2. "cross"
3. "dot"

**GRAPHICS.clash Style** - choose clash length, strain or length.

**GRAPHICS.clip Grobs** - enable grob clipping.

**GRAPHICS.clip Static** -

**GRAPHICS.grobLineWidth** - relative width of displayed lines of 3D meshes ( grobs ). Also affects the interatomic distance display.

**GRAPHICS.lightPosition** - X, Y and Z position of the light source in the graphics window. The X and Y coordinates are usually slightly beyond the [-1, 1] range where [-1, 1] is the size of the window, and the Z position is perpendicular to the screen and is set to 2. (do not make it negative).

**GRAPHICS.occupancyDisplay** preference controlling if and how the partial or zero atom occupancies are displayed. The abnormal occupancies are shown as circles around atoms. These following values are allowed.

```
1. = "none" # nothing is displayed
2. = "circle" # a circle is displayed
3. = "label" # a circle and a label with the value (zero values are not shown)
```

**GRAPHICS.quality** - integer parameter controlling quality (density of graphical elements) of such representations as cpk, ball, stick, ribbon. Do not make it larger than about 20 or smaller than 1.

**GRAPHICS.ruler Style** - change ruler from center to side

**GRAPHICS.stereoMode** - 1. "up-and-down", 2. "line interleaved" 3. "in-a-window"

\*a simple hardware stereo mode for workstations with a horizontal frame splitter. \*In the "up-and-down" mode a longer frame with two stereo images on top of each other is generated and the two halves are then superimposed with the splitter. This mode does not require anything from a graphics card, but does require a frame splitter. A frame splitter box was connected between a monitor and a graphics card output. This mode has an unpleasant side effect, the rest of the screen (beyond the OpenGL window) becomes stretched and the lower part of the screen is superimposed on the top half. \*The "line interleaved" mode can be used with a new type of frame splitter at the line level. In this case the odd lines from one stereo-image are interleaved with the even lines of another. The side-effect of this mode is that the intensity is reduced in half since at each moment one sees only one half of the lines. The splitter device for this mode can be purchased from Virex ([www.virex.com](http://www.virex.com)). This mode produces a dark stereo image but is easily available (requires stereo goggles, e.g. from Virex). \*The "in-a-window" mode is used in SGI workstations and in a Linux workstation with an advanced graphics card supporting a quad graphics buffer. In this mode the hardware stereo regime applies only to an OpenGL window. This is the best mode but it requires an expensive graphics card (plus the stereo goggles).

**GRAPHICS.surfaceDotDensity** - Determines the number of dots per square Angstrom on the graphical solvent accessible surface.

**GRAPHICS.surfaceProbeRadius** - An increment to the van der Waals radii of atoms at which the dotted atomic surface is calculated. It is used by the display surface command to display dotted



van der Waals surface. If the GRAPHICS.surfaceProbeRadius is set to 1.4 the surface becomes equivalent to the solvent accessible surface with a probe of 1.4Å

**GROB.arrowRadius** - a real arrow radius in Angstroms used by the Grob( "ARROW", R\_ ) function. Default: 0.5.

**GROB.contourSigmaIncrement** - a real increment in the sigma level used to re-contour an electron density map using the make grob m\_ed add r\_increment command. This parameter is used in the GUI when plus and minus are pressed.

**GROB.relArrow Size** - a real ratio of the arrow head radius to the arrow radius. This parameter is used by the Grob( "ARROW", R\_ ) function. Default: 3.0.

**shineStyle** - defines how solid surfaces of cpk , skin and grobs reflect light. Possibilities:

1. "white" <- default
2. "color"

The first option gives a more shiny and greasy look.

**GRAPHICS.center Follows Clipping** - determine the function of center button.

**GRAPHICS.clashWidth** - relative width of a displayed clash .

**GRAPHICS.clip Skin** - enable skin clipping.

**GRAPHICS.displayMapBox** - controls if the bounding box of a map is displayed

**GRAPHICS.light** - a rarray of 13 elements between 0. and 1. which controls the main properties of lighting model in GL.

**GRAPHICS.mapLineWidth** - relative width of lines and dots of a displayed map.

**GRAPHICS.occupancy Radius Ratio** - preference controlling the radius of the partial or zero atom occupancies

**GRAPHICS.resize Keep Scale**

**GRAPHICS.selectionStyle** - preference for the style in which the graphical selection is shown. The preference may have the following values.

**GRAPHIC.store Display** - maintains representation and coloring for an object.

**GRAPHICS.surfaceDotSize** - Determines the size of the dot on the solvent accessible graphical surface.

**GRAPHICS.transparency** - Two parameters regulating the transparency of grobs.

**GROB.atomSphereRadius** - default radius (in Angstroms) which is used to select a patch on the surface of a grob.

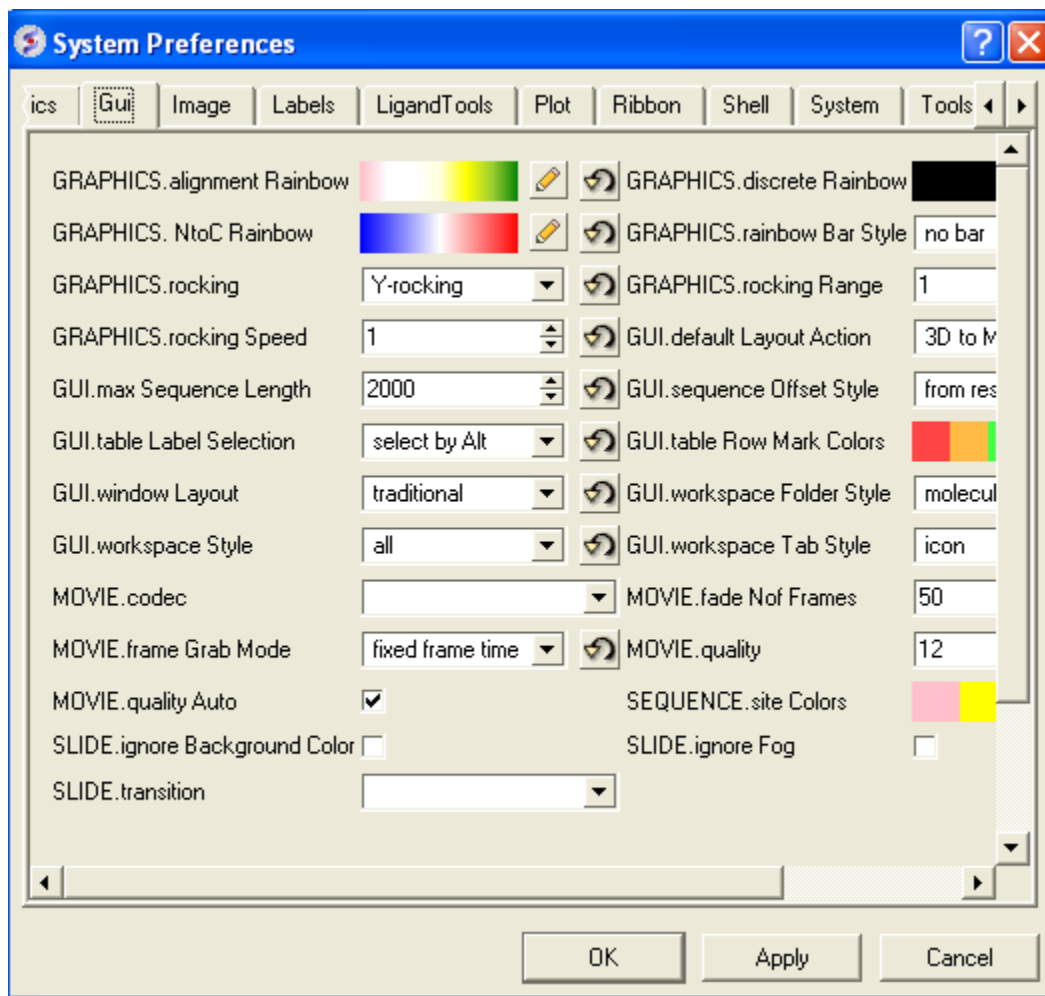
**GROB.relArrowHead** - a real ratio of the arrow head radius to the arrow radius.

**lineWidth** - the real width of lines used to display the wire representation of chemical bonds.

#### 3.3.1.14.4 GUI Preferences

##### **GUI TAB:**

The options contained within the Preferences/Gui tab are described below.



**GRAPHICS.alignment Rainbow** - This option controls how alignments are colored by default.

**GRAPHICS.NtoC Rainbow** - Controls the coloring of structural representation from the N-terminal to the C-terminal

**GRAPHICS.rocking** - Controls default `rocking motion`.

**GRAPHICS.rocking Speed** - Controls rocking or rotation `speed`.

**GUI.auto Save Interval** - Controls auto save period (minutes)

**GUI.table Row Mark Colors** - Controls colors used for marking tables.

**GUI.workspaceTabStyle** - Controls the style of ICM-object tabs created in the `workspace panel` of ICM GUI.

**Movie.fade Nof Frames** - Controls number of frames for the fade out option in screenshot movie making.

**Movie.quality** - Controls the resolution of the movie

**SEQUENCE.site Colors** - Controls coloring of sequence sites.

**SLIDE.ignore Fog** - Fog representations can be ignored in `slide` preparation if desired.

**GRAPHICS.discrete Rainbow** -

**GRAPHICS.rainbow Bar Style** - determines if and where the color bar will appear after a molecule is colored by an array.

**GRAPHICS.rocking Range** - real value of rocking range.

**GUI.auto Save** - auto save on or off

**GUI.max Sequence Length** - maximum sequence length displayed in ICM

**GUI.workspace Folder Style** - `workspace` folder style.

**MOVIE.frame Grab Mode** - with screenshot movie making you can choose either fixed frame time or real time.

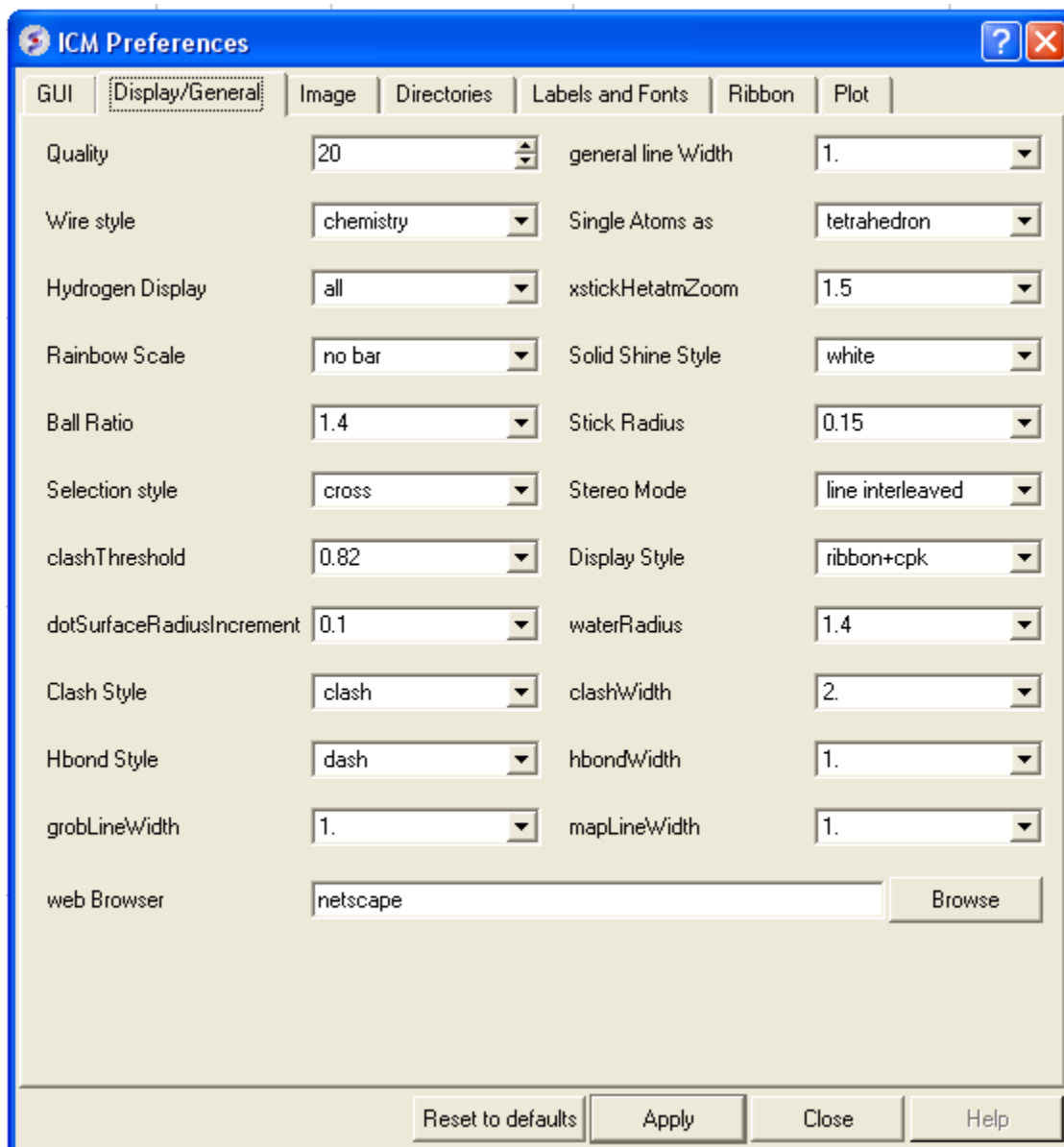
**Movie.quality Auto** - with screenshot movie making you can allow ICM to control the movie resolution.

**SLIDE.ignore Background Color** - Ignore background color when you are making a `slide`.

#### 3.3.1.14.5 General Preferences

## DISPLAY/GENERAL TAB:

Here is a summary of the important options in the DISPLAY/GENERAL Preferences Tab.



**Quality** - controls the quality (density of graphical elements) of such representations as cpk, ball, stick, ribbon. Do not make it larger than about 20 or smaller than 1. We recommend to make this parameter at least 15 if you want to make a high quality image. You can also increase the number of image resolution by making the image window 2,3,4 times larger (in the example below it is 2 times larger) than the displayed window.

**Wire Style** - Four different wire styles are available.

**Hydrogen Display** - Select whether you always want all hydrogens displayed or just-polar hydrogens or no hydrogens at all.

**Rainbow Scale** - determines if and where the color bar will appear after a molecule is colored by an array. Coloring by an array is one of the options of the display and color commands.

```
1. = "left" <- default choice
2. = "right"
3. = "no text"
4. = "no bar"
```

**Ball Ratio** - The ratio of ball and stick radii. This ratio is applied when the styles are switched to xstick from the GUI xstick toolbar.

**Selection Style** - Change the graphical display of your selections. Default is a green cross.

**Clash Threshold** - a clash is defined as an interatomic distance less than a sum of van der Waals radii of two atoms of interest multiplied by the clashThreshold parameter. For hydrogen bonded atoms, the distance threshold is additionally reduced by 20% . Default = 0.82

**DotSurfaceRadiusIncrement** - radius of a probe sphere used to display a dotted surface of a molecule. All van der Waals radii are expanded by this value. vwExpand=0 corresponds to the CPK surface, vwExpand=1.4 corresponds to the water-accessible surface. Be aware of the difference between the waterRadius and vwExpand parameters: waterRadius is used in

- show energy "sf"
- show [area|volume] skin
- display skin while vwExpand is used in
- show [area|volume] surface
- display surface

Default (1.4).

**H Bond Style** - How do you wish your H-Bonds to be displayed by default? Dashes, Bond Length, Bond Length and Angle.

**grobLineWidth** - relative width of displayed lines of 3D meshes ( grobs ). Also affects the interatomic distance display.

**general line with** - the real width of lines used to display the wire representation of chemical bonds. See also IMAGE.lineWidth parameter which controls line thickness in molecular images generated by the write postscript command, and the PLOT.lineWidth which controls the width for the plot command. Default (1.0)

**single atom as** - display style of isolated atoms in the wire mode.

1. "tetrahedron"
2. "cross"
3. "dot"

The size of the first two representation is controlled by the GRAPHICS.ballRadius parameter and the line width (especially important for the "dot" style) is controlled by the lineWidth parameter.

***xstickhetatomzZoom*** - The default ball and stick radii of a ligand can be different. This makes a better ligand view since the ligand stands out from the surrounding protein atoms.

***solid shine style*** - choose either white or color

***Stick Radius*** - radius (in Angstroms) of a cylinder displayed as a part of stick or xstick graphical representation of a molecule. Individual (residue-wide) control of stick radii.

***Stereo Mode*** - Select a default stereo mode

***Display Style*** - A default display style can be chosen using a combination of styles.

***Water Radius*** - radius of water sphere which is used to calculate an analytical molecular surface (referred to as skin) as well as the solvent-accessible surface (centers of water spheres).

***clashWidth*** - relative width of a displayed clash.

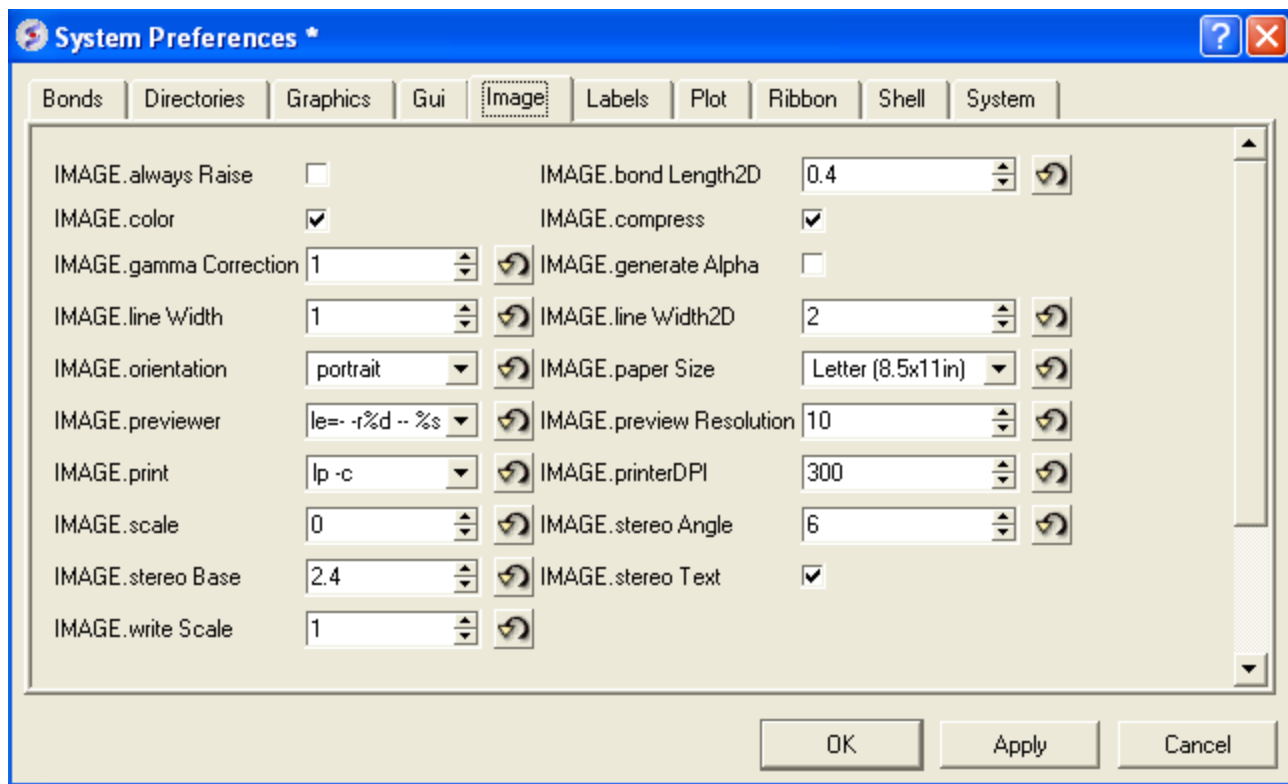
***hbondWidth*** - relative width of hydrogen bond display

***mapLineWidth*** - relative width of lines and dots of a displayed map.

#### 3.3.1.14.6 Image Preferences

##### ***IMAGE TAB:***

Here is a summary of the important options in the IMAGE Preferences Tab.



***IMAGE.color*** - logical to save color or black\_and\_white ('bw') images.

***IMAGE.gammaCorrection*** - real variable to to lighten or darken the image by changing the gamma parameter. A gamma value that is greater than 1.0 will lighten the printed picture, while a gamma value that is less that 1.0 will darken it.

***IMAGE.lineWidth*** - this real parameter specifies the default line width for the postscript lines.

***IMAGE.orientation*** - image orientation.

***IMAGE.previewer*** - a string parameter to specify the external filter which creates a rough binary (pixmap) postscript preview and adds it to the header of the ICM-generated high resolution bitmap or vectorized postscript files saved by the write image postscript, and write postscript , respectively .

***IMAGE.print*** - unix command for printer.

***IMAGE.scale*** - real variable. If non zero, controls the image scale with respect to the screen image size.

***IMAGE.stereoBase*** - real variable to define the stereo base (separation between two stereo panels) in the write image postscript and write postscript command.

***IMAGE.writeScale*** - an integer parameter used to increase the image resolution in the `Quick Image Write` tool.

***IMAGE.bondLength2D*** - real length of a chemical bond (in inches) in chemical 2D drawings upon the `Copy Image` command.

***IMAGE.compress*** - logical to toggle simple lossless compression, standard for .tif files. This compression is required to be implemented in all TIFF-reading programs.

***IMAGE.generateAlpha*** - logical to toggle generation of the alpha (opacity) channel for the SGI rgb, tif and png image files to make the pixels of the background color transparent.

***IMAGE.lineWidth2D*** - integer thickness of bonds in chemical 2D drawing upon the `Copy Image` command. This is useful for cutting and pasting from ICM to external documents.

***IMAGE.paper Size*** - specify paper size.

***IMAGE.previewResolution*** - integer resolution of the rough bitmap preview added to the vectorized postscript file in lines per inch.

***IMAGE.printerDPI*** - this integer parameter the printer resolution in Dot Per Inch (DPI). Important for the `write image postscript` command.

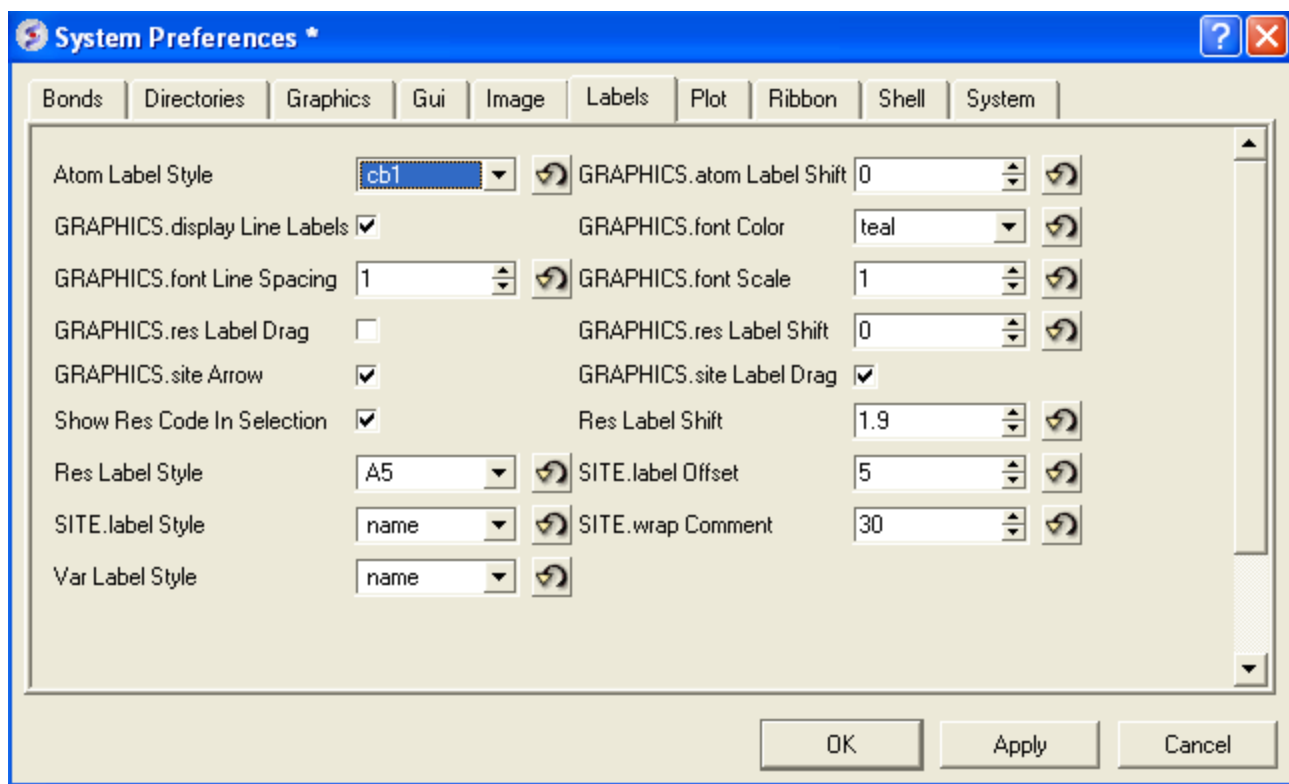
***IMAGE.stereoAngle*** - real variable to define stereo angle (relative rotation of two stereo images) in the `write image postscript` and `write postscript` command.

***IMAGE.stereoText*** - logical to make text labels for only one panel or both panels of the stereo diagram.

#### 3.3.1.14.7 Font Preferences

***LABEL FONT TAB:***





**atomLabelStyle** style of atom labels invoked by clicking on an the atom label button.

**GRAPHICS.displayLineLabels** - enables/disables the display of edge lengths (inter-point distances) of a grob generated with the Grob( "distance" .. ) function.

**GRAPHICS.font Line Spacing** - Change the spacing between lines in labels.

**GRAPHICS.resLabelDrag** - if yes, enables dragging of the displayed residue labels with the middle mouse button.

**GRAPHICS. site Arrow** - Highlight sites with an arrow yes or no.

**Show Res Code In Selection** - When you make a selection the icm selection language will be displayed when you right click on the selection.

**Res Label Style** - Default residue label style.

**SITE.label Style** - Default label sites style.

**Var Label Style** - Default label variable style.

**GRAPHICS.atomLabelShift** - a non-negative integer number of spaces preceding an atom label. This parameter is useful for displaying labels next to a solid representation,

**GRAPHICS.fontColor** - set font color

**GRAPHICS.font Scale** - set font size

**GRAPHICS.site Label Shift** - GRAPHICS.resLabelShift a non-negative integer number of spaces preceding a site label.

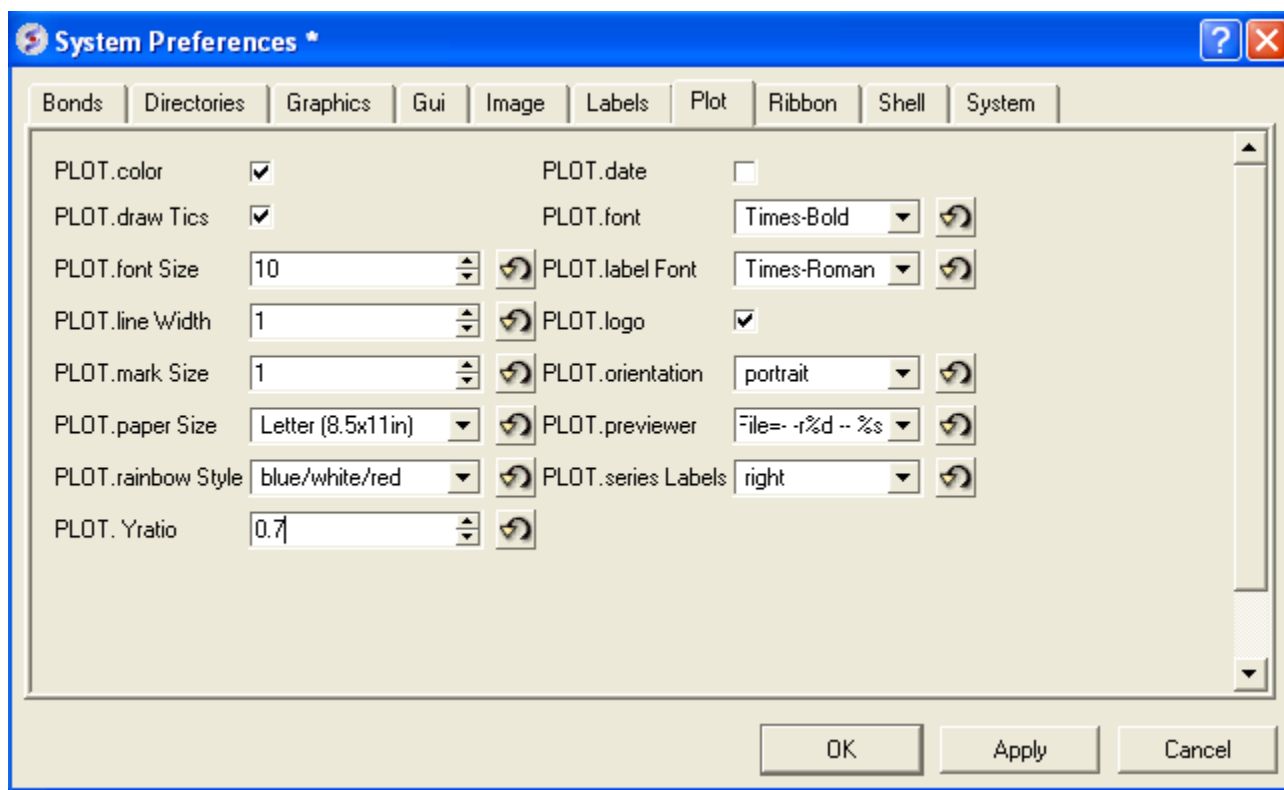
**GRAPHICS. site Label Drag** - if yes, enables dragging of the displayed site labels with the middle mouse button.

**Res Label Shift** - a non-negative integer number of spaces preceding a residue label. This parameter is useful for displaying residue labels next to a solid

**SITE.labelOffset** - (default 5. A) the real offset of the site label with respect to the residue label atom.

**SITE.wrap Comment** - Number of characters per comment line.

### 3.3.1.14.8 Plot Preferences



**PLOT.color** - logical to generate a color plot. Usually it does not make sense to switch it off because your b/w printer will interpret the color postscript just fine anyway.

***PLOT.draw Tics*** logical yes or no

***PLOT.fontSize*** real font size. Any reasonable number from 3. (1 mm, use a magnifying glass then) to 96.

***PLOT.lineWidth*** - real line width for graphs (not the frame and tics)

***PLOT.markSize*** - real mark size in points. Allowed mark types: line, cross, square, triangle, diamond, circle, star, dstar, bar, dot, SQUARE, TRIANGLE, DIAMOND, CIRCLE, STAR, DSTAR, BAR. Uppercase words indicate filled marks.

***PLOT.paper Size*** - preference to specify plot paper size

***PLOT.rainbowStyle*** - preference defining the color spectrum used by the plot area command.

***PLOT.Yratio*** - real aspect ratio of the ICM plot frame. Using link option of the plot command is equivalent to setting this variable to 1.0. If ***PLOT.Yratio*** is set to 0. , the ratio will be set automatically to fill out the available box optimally.

***[PLOT.date]*** - display date on plot

***PLOT.font*** - preference for the title/legend font.

***PLOT.labelFont*** - preference for the data point label font.

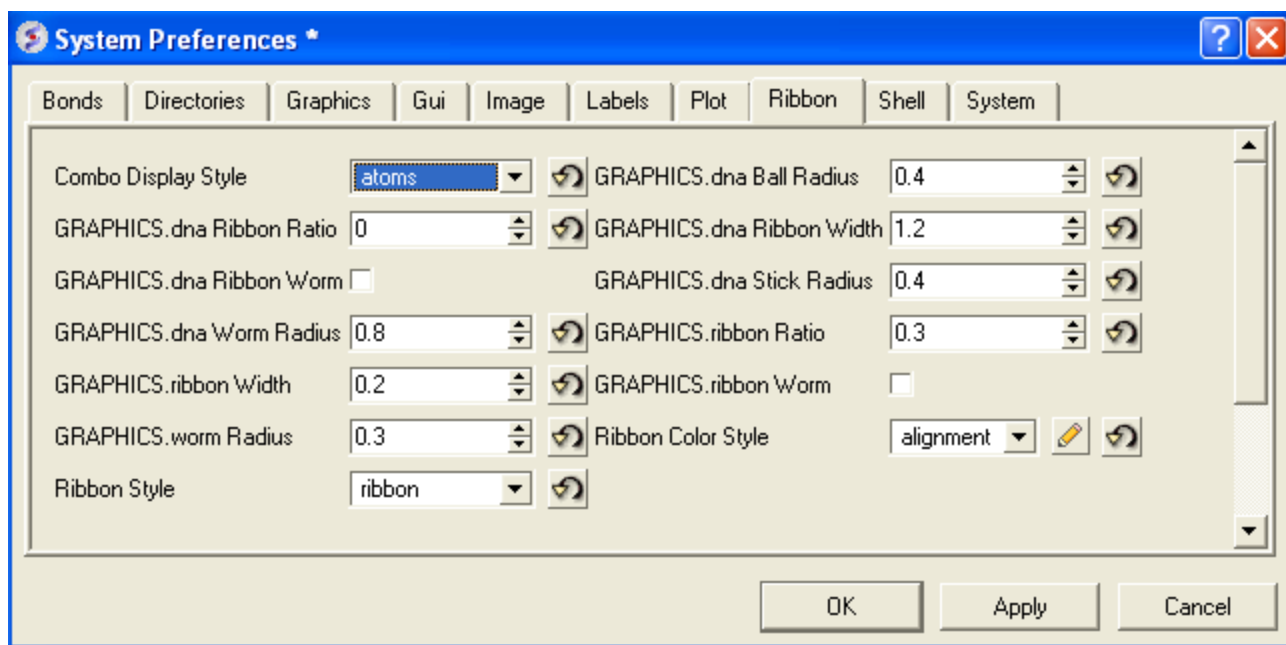
***PLOT.logo*** - logical switch for the ICM-logo on the plot.

***PLOT.orientation*** - preference for the plot orientation.

***PLOT.previewer*** - command to local ps viewer

***PLOT.seriesLabels*** - preference to indicate position of a series/color legend inside the plot frame.

#### **3.3.1.14.9 Ribbon Preferences**



**Combo Display Style** - select ribbon-cpk, atoms, ribbon-ligand, chemical

**GRAPHICS.dnaRibbonRatio** - real ratio of depth to width for the DNA ribbon .

**GRAPHICS.dnaRibbonWorm** - logical which, if yes, makes the DNA backbone ribbon round, rather than rectangular. Default: no

**GRAPHICS.dnaWormRadius** - real radius of the worm representing bases in DNA ribbon .

**GRAPHICS.ribbonWidth** - real width of the protein ribbon .

**GRAPHICS.wormRadius** - radius of coiled segments (i.e. those where the secondary structure is marked as "\_") of a polypeptide chain in ribbon representation. Default (0.3).

**Ribbon Style** - specifies default style when ribbon is displayed.

**GRAPHICS.dnaBallRadius** - DNA bases in ribbon representation are shown as balls controlled by this real parameter.

**GRAPHICS.dnaRibbonWidth** - real width (in Angstroms) of the DNA ribbon .

**GRAPHICS.dnaStickRadius** - real radius of the sticks representing bases in DNA ribbon .

**GRAPHICS.ribbonRatio** - real ratio of depth to width for the protein ribbon .

**GRAPHICS.ribbonWorm** - logical parameter, if yes, makes the ribbon round, rather than rectangular.

## *ribbonColorStyle* -

- sets the ribbon coloring scheme.

1 = "type" default. colors by secondary structure type or explicit color

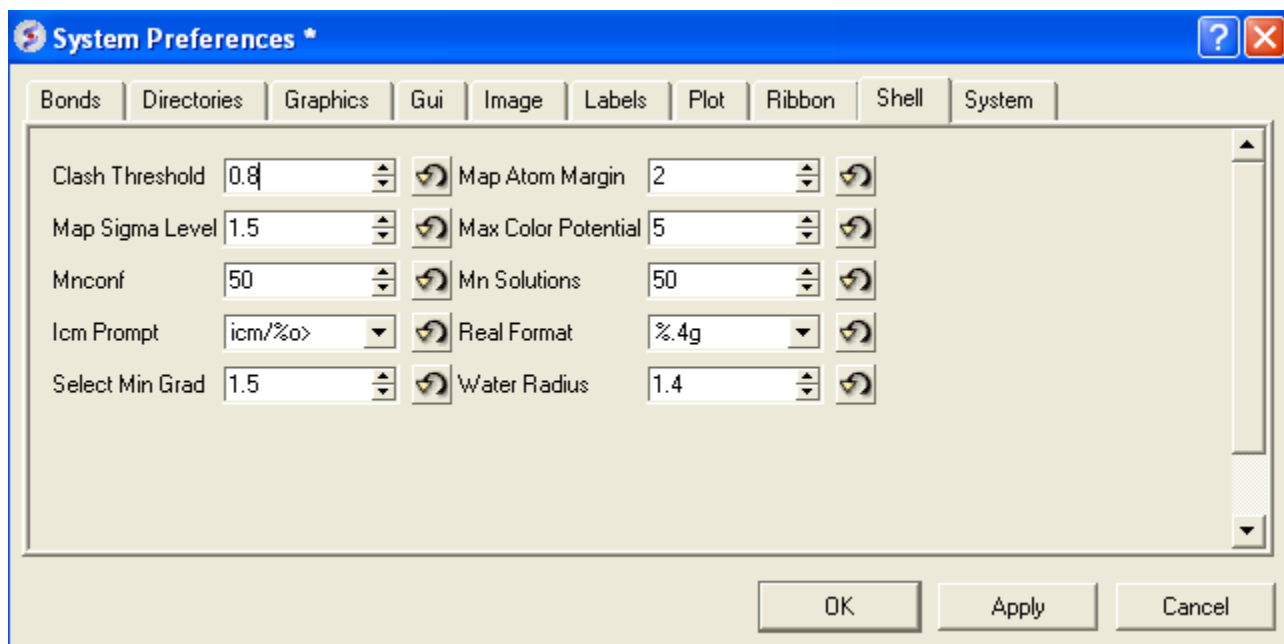
2 = "NtoC" colors each chain gradually blue-to-red from N- to C- (or from 5' to 3' for DNA)

3 = "alignment" if there is an alignment linked to a protein, color gapped backbone regions gray

4 = "reliability" 3D gaussian averaging with selectSphereRadius of alignment strength in space

If ribbonColorStyle equals to 4, the conserved areas will be colored blue, while the most divergent will be red, and the intermediate conservation areas will be colored white. Example:

### 3.3.1.14.10 Shell Preferences



**Clash Threshold** - a clash is defined as an interatomic distance less than a sum of van der Waals radii of two atoms of interest multiplied by the clashThreshold parameter.

**Map Sigma Level** - (in Rmsd values over the mean value). Margin value used for making graphical objects contouring the 3D density map .

**Mnconf** - maximal number of conformations in the conformational stack . The stack stops growing after this number is achieved and starts replacing representative conformations with higher energy values by new conformations with superior energies, if the latter are found.

**Icm Prompt** - defines the ICM-prompt string.

**Select Min Grad** - default minimal gradient vector length for gradient atom selection (  $a_{//G}$ ). This parameter is also used by the montecarlo fast command, which requires a value of 2. to 10. for optimal performance.

**Map Atom Margin** - Margin in Angstroms around selected atoms. The margin is added to the positional boundaries to define a submap index box in the Map ( map\_source , as\_ ) function.

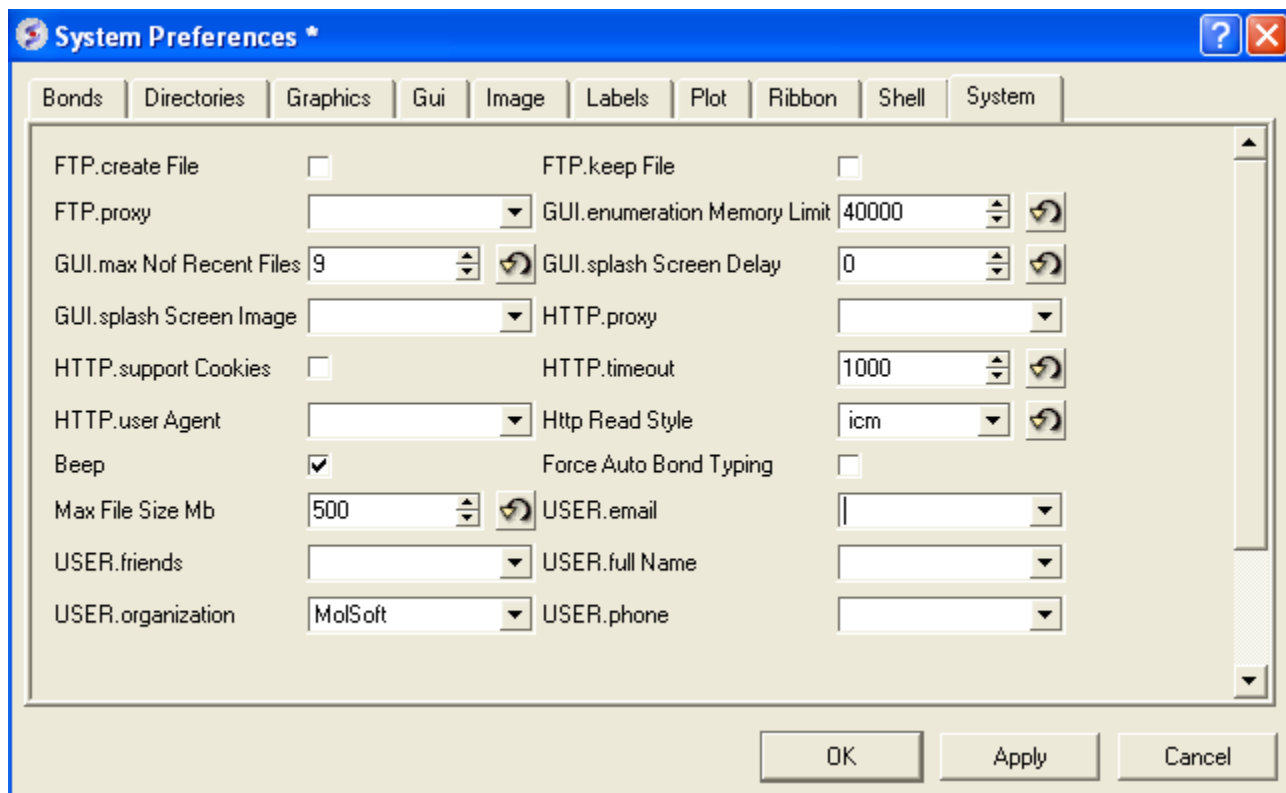
**maxColorPotential** - local electrostatic potential in kcal/e.u.charge units at which the surface element is colored by extreme red or extreme blue. All higher values will have the same color. This absolute scaling is convenient to develop a feeling of electrostatic properties of molecular surfaces.

**mnSolutions** - this parameter limits the number of hits retained by the program after a search.

**Real Format** - format of real numbers

**Water Radius** - radius of water sphere which is used to calculate an analytical molecular surface

```
system-preferences{FTP.createFile, FTP.proxy, GUI.max Nof Recent Files, GUI.splash Screen Image, HTTP.support Cookies, HTTP.user Agent, Beep, Max File Size Mb, USER.friends, USER.organization, FTP.keep File, GUI.enumeration Memory Limit, GUI.splash Screen Delay, HTTP.proxy, Http Read Style, Force Auto Bond Typing, USER.email, USER.full Name, USER.phone} h4-- System Preferences {System Preferences}
```



***FTP.createFile*** -

***FTP.proxy*** - string path to the proxy server for connections through firewall. Default: "" (empty string).

***GUI.max Nof Recent Files*** - maximum number of `recent files` stored.

***GUI.splash Screen Image*** - path to splash image displayed on startup

***HTTP.support Cookies*** - http support cookies yes or no

***HTTP.user Agent*** - client application used within a particular network protocol for www

***Beep*** - warning beep yes or no

***Max File Size Mb*** - Maximum file size in MegaBytes that can be loaded into ICM.

***USER.friends***

***USER.organization***

***FTP.keep File*** - (default no ). If yes, the temporary file is kept in the `s_tempDir` directory. Otherwise the file is deleted.

***GUI.enumeration Memory Limit*** - memory limit for enumeration operations.

***GUI.splash Screen Delay***

***HTTP.proxy*** - string for HTTP server for connection through firewall

***HTTP.timeout*** - timeout in seconds

***Http Read Style*** icm or lynx

***Force Auto Bond Typing*** - yes/no

***USER.email, USER.full Name, USER.phone***

### **3.3.1.15 Recent Files**

Recently viewed projects and files can be easily downloaded from the "Recent Files" option. To access this:

- Select File/Recent Files.

- Select the desired project by clicking on it once.

### 3.3.1.16 Recent PDB Codes

Quickly retrieve and display PDB structures that have recently been viewed.

- Select File/Recent PDB Codes
- Select desired PDB code by clicking on it once and it will be loaded into the graphical display.

### 3.3.1.17 Quit

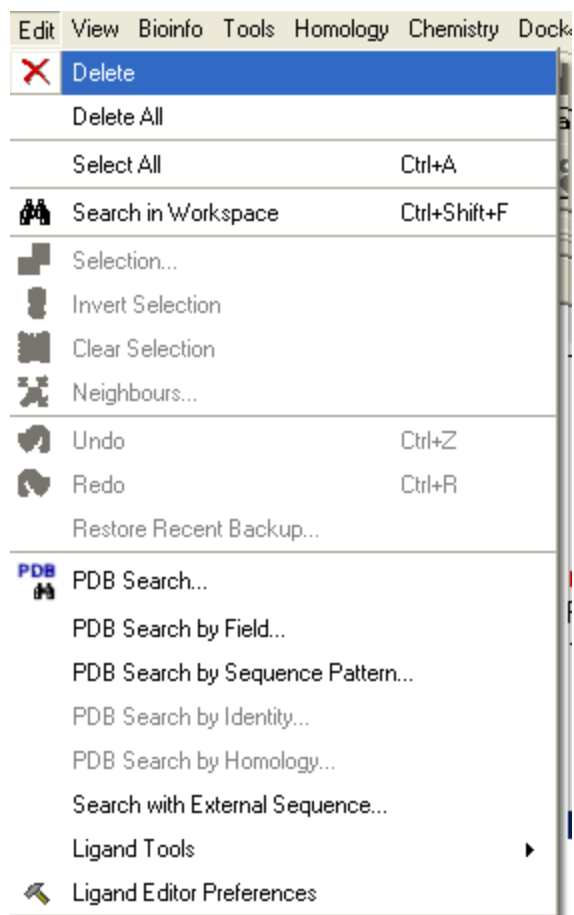
Need to close down ICM - no problem. You do one of the following:

1. Select **File/Quit**. ICM will quit without saving files.
2. Save and Click **X** at the upper right corner of the ICM window.
3. Type `quit` in the terminal window.

**NOTE:** You may want to save the icm session as an `ICM Project file` before quitting.

### 3.3.2 Edit Menu





### 3.3.2.1 Delete

This option will delete anything that is selected.

### 3.3.2.2 Delete All

This option will delete everything e.g. sequences, structures, tables ... Use with care!

### 3.3.2.3 Select All

This option will select everything e.g. sequences, structures, tables...

### 3.3.2.4 Search in Workspace

This option allow you to search for a particular text in the workspace

### 3.3.2.5 Selection

This option allows you to make a precise selection either by neighbors or specifying a particular atom or neighbor. Click on the tabs to jump between selection levels.

### 3.3.2.6 Invert Selection

This option will select everything that is not currently selected.

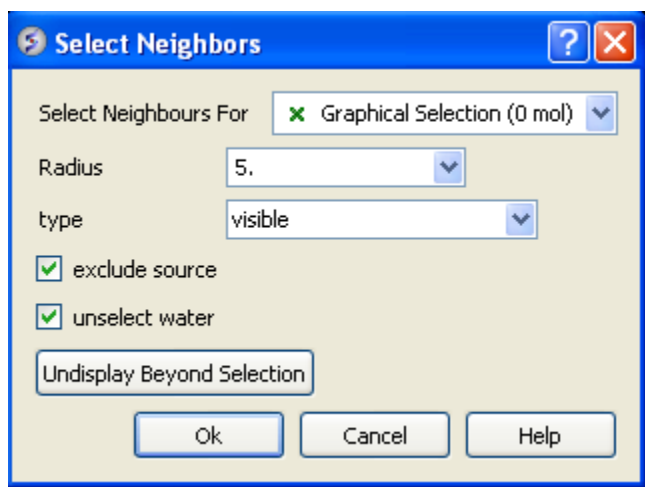
### 3.3.2.7 Clear Selection

This option will remove all selections. For more information on selections see the [Making Selections Chapter](#).

### 3.3.2.8 Neighbor Selection

This option will allow you to make a spherical selection.

The window will open as displayed as below:



- Select the molecule you wish to select neighbors around. For example you can select a ligand in the ICM Workspace and then choose the **Graphical Selection** option in the

"Select Neighbors For" dialog entry box. Or alternatively you can select the object by clicking on the drop down button next to the "Select Neighbors For" dialog entry box.

- Enter the radius in Angstroms for the neighbor selection. e.g. 5.
- **Type** - this option is **important**. This option relates to what is going to be selected. For example if you leave this option as **visible** and you only have ribbon representation displayed for your receptor (e.g. when selecting neighbors for a ligand) then only backbone atoms will be selected.

Selection **Type** option includes:

- **visible** - will select all atoms displayed within the radius selected.
- **visible sidechains** will select all visible side-chains - not backbone atoms.
- **same\_object\_other\_chains** will select all atoms in other chains in the same object as the original selection.
- **other objects** will select atoms in objects other than the original selection.
- **same object** will select atoms in the same object as the original selection.
- **all\_objects** will select atoms in all objects
- **choose\_from\_list** will allow you to select the object you wish to include in the neighbors selection.
  
- **exclude source** if checked will not include your original selection in the spherical selection.
- **unselect water** if checked will not select water molecules
- **Undisplay Beyond Selection** will only display the atoms selected.

### 3.3.2.9 Undo

Due to the complexities of working in an internal coordinates environment not everything can be undone or redone. Certain things like coloring and representations can be undone or redone.

### 3.3.2.10 Redo

Due to the complexities of working in an internal coordinates environment not everything can be undone or redone. Certain things like coloring and representations can be undone or redone.

### 3.3.2.11 Restore Recent Backup

ICM periodically makes a backup of your ICM project. If for whatever reason you lose an ICM session and you want to load the backup for the file use:

## **Edit/Restore Recent Backup**

### **3.3.2.12 PDB Search**

See PDB Search Tab

### **3.3.2.13 PDB Search by Field**

See PDB Search Tab

### **3.3.2.14 PDB Search by Identity**

See PDB Search Tab

### **3.3.2.15 PDB Search by Homology**

See PDB Search Tab

### **3.3.2.16 PDB Search with External Sequence**

See PDB Search Tab

### **3.3.2.17 Ligand Tools**

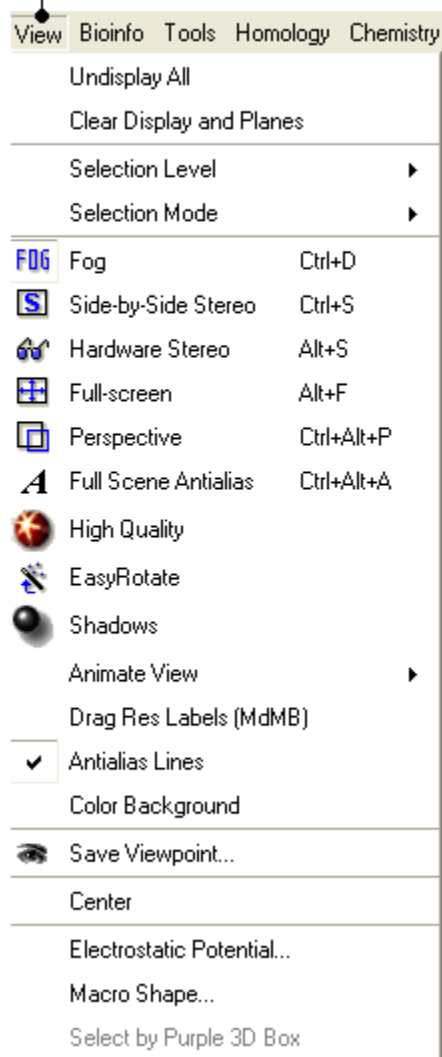
See the ligand editor section of the manual.

### **3.3.2.18 Ligand Editor Preferences**

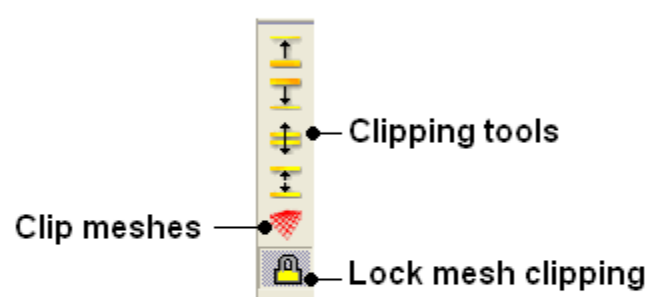
See the ligand editor section of the manual.

## **3.3.3 View Menu**

### View Menu



### View Buttons



### 3.3.3.1 Undisplay All

*To undisplay everything currently displayed in the graphical display*

- View/Undisplay All

**Note** For more details on displaying structures please see the GUI Overview chapter.

### 3.3.3.2 Clear Display & Planes

### *To clear the display and planes*

- View/Clear Display and Planes

**NOTE:** For more details on planes please see the sections on `clipping tools` and `mesh clipping`.

### **3.3.3.3 Selection Level**

There are four levels of selection - atom, residue, molecule and object. For more details on selections please see the `Making Selections` section.

### **3.3.3.4 Selection Mode**

There are four different ways to make selections - new, add, remove and toggle. For more details on selections please see the `Making Selections` section.

### **3.3.3.5 Fog**

**Fog Toggle**(Ctrl + D) : this feature creates a fog-like environment for your object, so that the part of your structure that is closer appears clear and the distant parts are faded as if they are in fog. The `clipping planes` control the point at which the fog begins.

- View/Fog

### **3.3.3.6 Side-by-Side Stereo**

**Side-by-side stereo toggle**(Ctrl + S) : this feature allows you to view your structure in 3D form without any 3D goggles.

- View/Side-by-Side Stereo

### **3.3.3.7 Hardware Stereo**

**Hardware stereo toggle**(Alt + S) - if you have 3D goggles and you wish to view your structure in 3D form, this feature will allow you to do so.

- View/Hardware Stereo

### 3.3.3.8 Full Screen

**Full screen toggle**Alt\_F - this makes your graphical display fill the entire screen. If you wish to exit this mode, press escape.

- View/Full Screen

### 3.3.3.9 Perspective

**Toggle perspective** Ctrl\_P this will add perspective to your structure, enhancing depth in the graphical display.

- View/Perspective

### 3.3.3.10 Full Scene Antialias

Anti-aliasing is the technique of minimizing the distortion artifacts known as aliasing when representing a high-resolution signal at a lower resolution. Always use this option before making high resolution images.

- View/Full Scene Antialias

### 3.3.3.11 High Quality

**Toggle High Quality:** this option will give your ICM object better resolution and higher quality. The change in quality is most visible at a high magnification. However, if your object is very large, this feature could slow down your program.

Always use this option before making high resolution images.

- View/High Quality

### 3.3.3.12 Easy Rotate

**Toggle easy rotation:** this feature is necessary if your structure is very large or perhaps your computer cannot quickly `rotate` it. It will prevent your structure from fully loading each time you rotate it, therefore speeding up the process.

- View/Easy Rotate

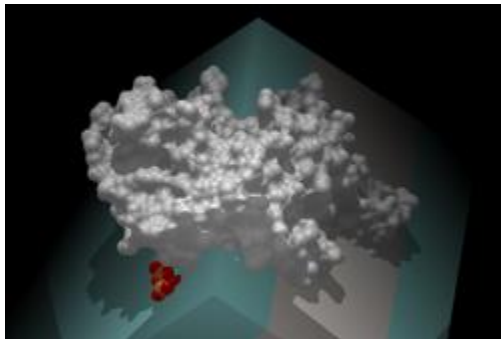
### 3.3.3.13 Shadows

- View/Shadows

OR

select the shadow button shown below.

Toggle shadow

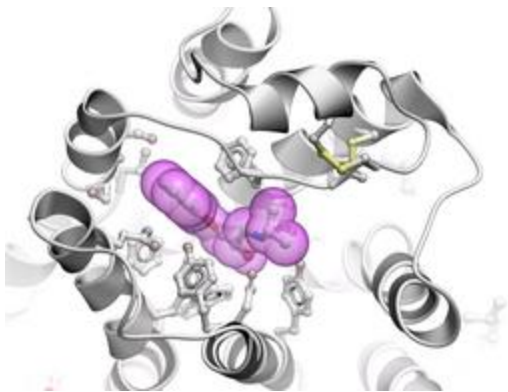


### 3.3.3.14 Sketch Accents

*To make images as shown below use:*

- View/Sketch Accents





### 3.3.3.15 Animate View

This tool is described in more detail in the [Molecular Animations and Transitions](#) section.

### 3.3.3.16 Drag Res Labels

*To change the location of your residue label:*

- Select View/Drag res labels.
- If your mouse has a middle mouse button, then click on handle (as shown) of the label you wish to move, and drag it to your desired area.

Click on  
this area  
to drag  
your  
label.



- If your mouse has no middle mouse button, then click on the Translation icon on the toolbar, and click on the handle (as shown) of the label you wish to move, and drag it to your desired area.

The +/- buttons on the side of the Residue and Atom buttons will shift the label. There are also other **residue label move** options available when you click and hold the residue label button. These options include **Shift to Sidechain Tips**, **Shift to Calphas**, and **Restore Positions**

### 3.3.3.17 Antialias Lines

Use this option to activate antialias lines. It is recommended to leave this option selected.

- View/Antialias Lines

### 3.3.3.18 Color Background

*To change the background color*

- View/Color Background
- Select a color from the panel and press OK.

This option is also in the more convenient `display` tab.

### 3.3.3.19 Save Viewpoint

It is possible to store a current view using the button shown below.



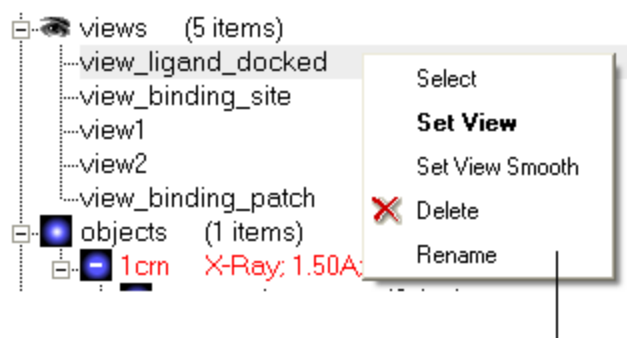
**Store Current View**

Click on the button and the current view will be stored so that you can view it later. A data entry box will be displayed asking you to name the view. All stored views can be found in the ICM workspace as shown below.



- Double click on the view in the ICM Workspace to display it.

A number of view display options are available by right clicking on the view in the ICM workspace as shown below.



Store current view right click menu

The option in the right click menu called "set view smooth" returns to the view slowly showing the trajectory between the original view and the current one.

### 3.3.3.20 Center

*To center on an object displayed in the graphical display*

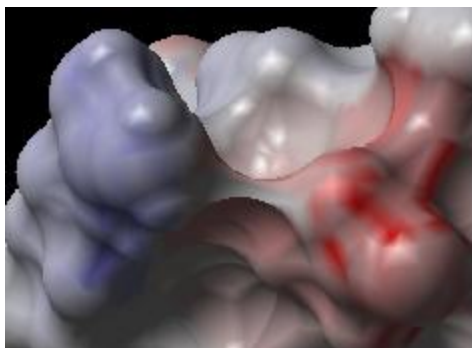
- Make a selection on the region on which you wish to center on.
- Tools/Center (or use the `center` button on the right hand-side of the graphical display).

### 3.3.3.21 Electrostatic potential

This option generates the skin representation of the molecular surface colored according to the electrostatic potential calculated by the REBEL method (hydrogen atoms are ignored). REBEL is a method to solve the Poisson equation for a molecule. REBEL is a powerful implementation of the boundary element method with analytical molecular surface as dielectric boundary. This method is fast (takes seconds for a protein) and accurate. REBEL stands for Rapid Exact-Boundary ELectrostatics. The energy calculated by this method consists of the Coulomb energy and the solvation energy

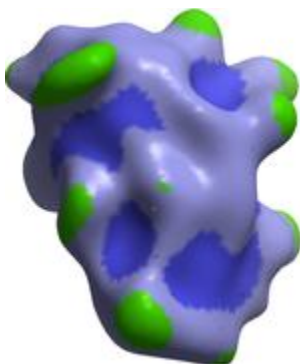
*In order to color the skin of your molecule by electrostatic potential:*

- Select **View/Electrostatic** potential.
- Enter the potential scale value. This is the local electrostatic potential in kcal/e.u.charge units at which the surface element is colored by extreme red or extreme blue. All higher values will have the same color. This absolute scaling is convenient to develop a feeling of electrostatic properties of molecular surfaces.
- Areas colored blue represent positive areas and red represents negative areas.



### 3.3.3.22 Macro Shape

A macroshape allows easy viewing and manipulation of a structure. A macroshape representation is ideal for large structures which allows the user to easily identify important regions of the structure and facilitate the return to the 'standard' view of a particular molecule. The level of detail displayed in the macroshape can be controlled by changing the number of harmonics, gridStep, and, contour level.



- View/Macro Shape

### 3.3.3.23 Select by Purple 3D Box

An alternative way to make a make-selection{selection} is to use the purple 3D box. To do this:

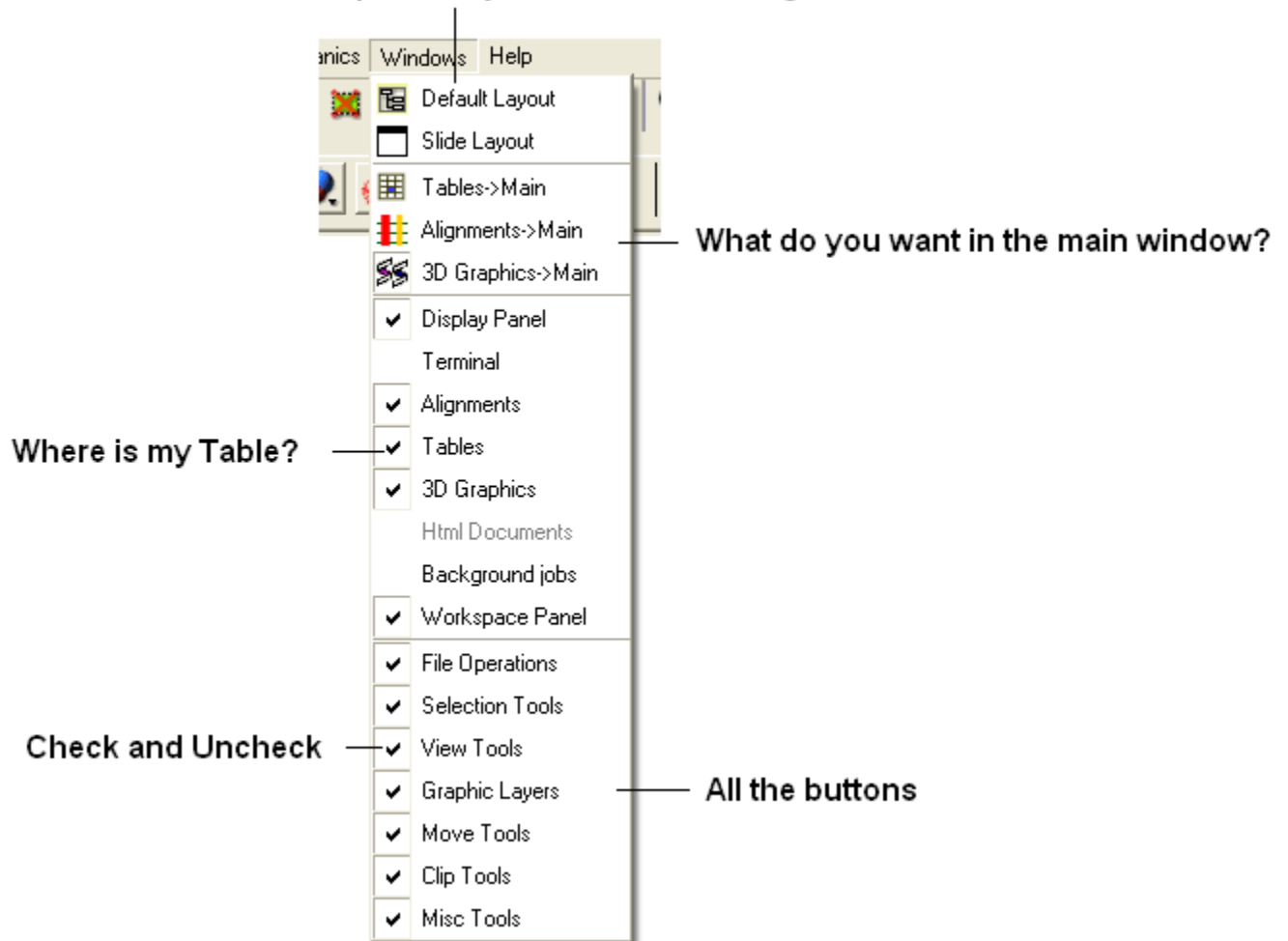
- Select the **display** tab and the purple box button
- View/ Select by Purple 3D Box
- The atoms contained within the purple box will be selected.

### 3.3.4 Windows Menu

This menu allows you to choose the windows you wish to display. The windows which open automatically when you first open GUI are shown in the Default GUI section. Other windows can be displayed by selecting the windows menu. For example, if you have loaded a table but cannot see it in the GUI it may be because the Tables option in the window menu hasn't been selected.

To add or remove windows from the GUI display select the 'window menu'. Other windows not included in the default display such as tables and alignments can be added.

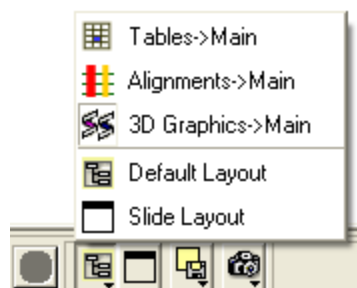
**I have windows open everywhere - Please bring some order.**



To return to the default display option select the 'Default layout' option in the windows menu.

OR

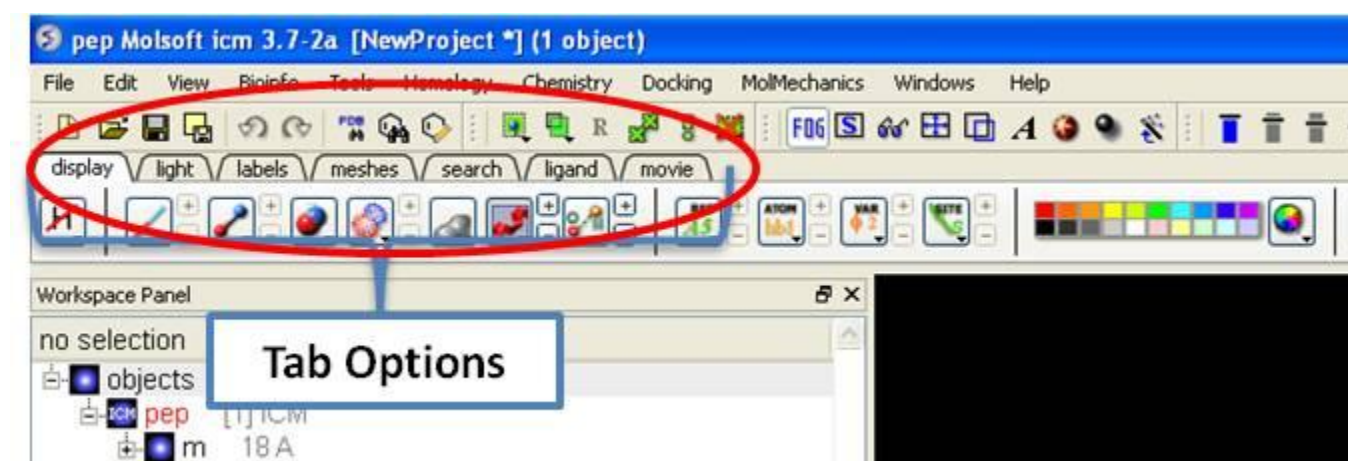
Click the default layout icon.



Some options can be accessed at the bottom of the GUI.

## 3.4 Tab Guide

In this section we describe the contents of the tabs in the graphical user interface.

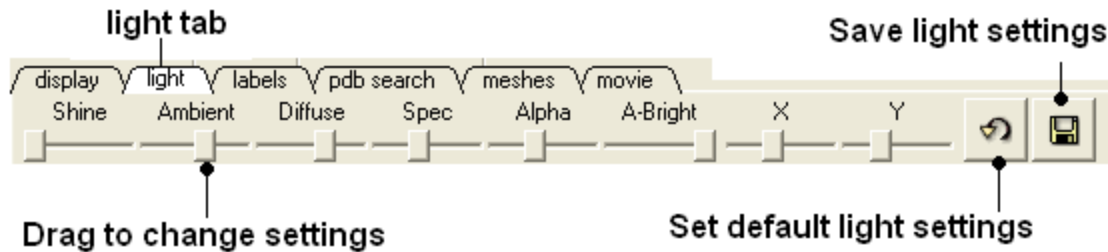


### 3.4.1 Display Tab

The display tab contains tools for a variety of functions including - structural representations, coloring, labeling and superposition. This tab is shown below.

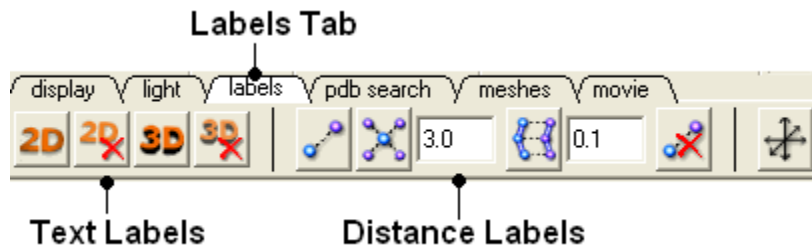


### 3.4.2 Light Tab



The options in this tab are described in the [Lighting](#) Section.

### 3.4.3 Labels Tab



The options in this tab are described in the [labels](#) section of this manual.

### 3.4.4 PDB Search Tab

Instructions on how to use this tab can be found in the [Search PDB](#) section.

### 3.4.5 Meshes Tab

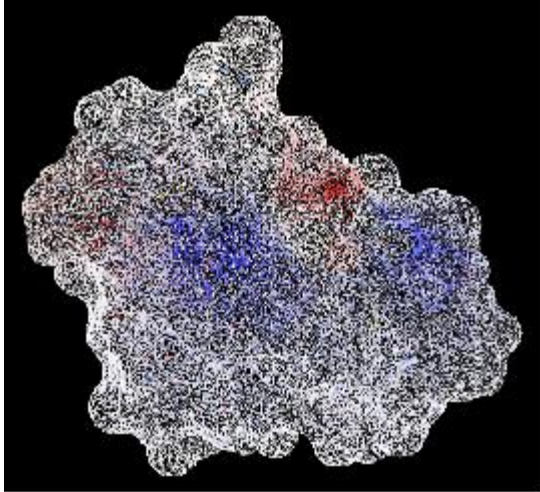
**Note:** Click **Next** (top right hand corner) to navigate through this chapter. Headings are listed on the left hand side (web version) or by clicking the **Contents** button on the left-hand-side of the help window in the graphical user interface.

Click on the tab button entitled '**meshes**' and three different graphical display tools are available for you to use. The three displays are surface, meshes and macroshape and are collectively referred to as meshes.



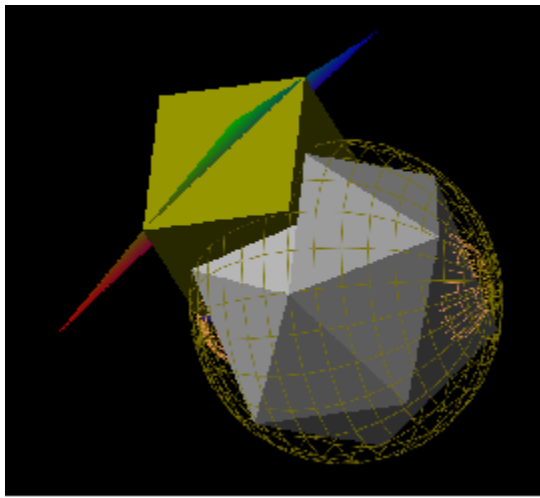
The benefits and applications of each display are described in this section.



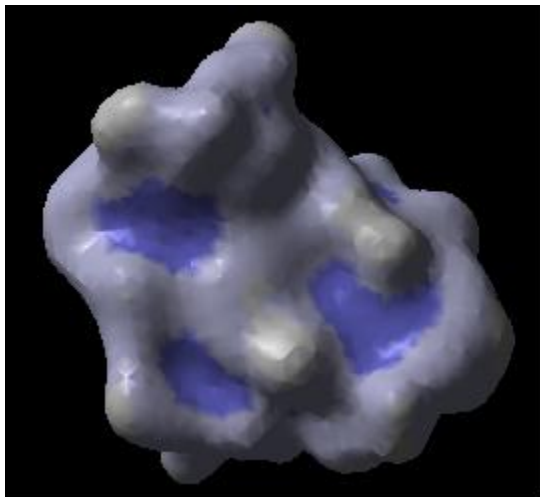


Surface:

Meshes:



Macroshape:

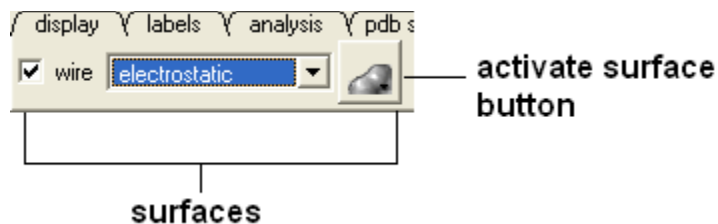


### 3.4.5.1 Surfaces

The surface of your structure can be displayed and colored by **electrostatics** or **binding** properties. To do this:

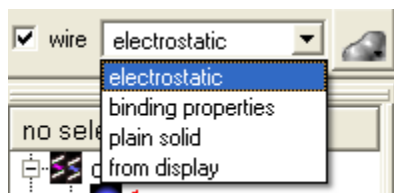
- Load a structure into ICM `File/Open` or `tab-pdb{PDB Search}`
- Convert the structure into an ICM object.
- Select the 'meshes' tab button.

The buttons and options you need to use are shown below:



First you need to decide by what parameter you wish to color the surface:

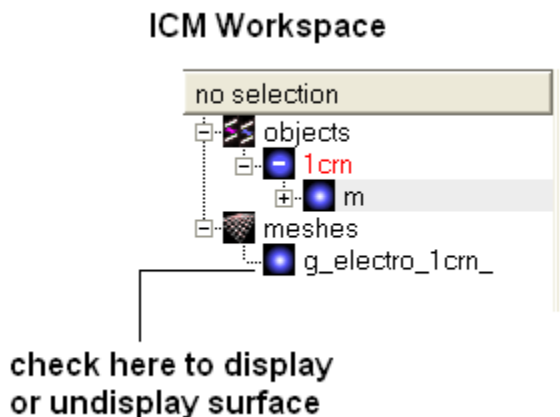
- Click on the drop down arrow menu shown below and select which parameter you wish to color the surface by.



- Click the button next to the menu to color the surface of your molecule.

If you wish to have your surface displayed in wire check the 'wire' box next to the menu.

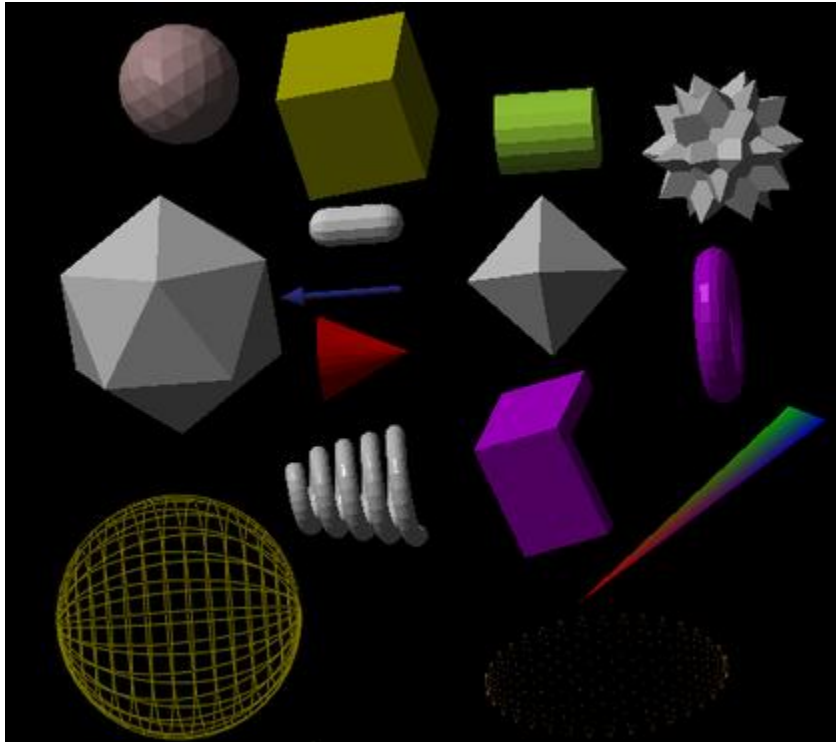
To display or undisplay the surface click in the box in the ICM workspace as shown below:



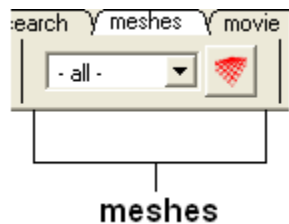
**NOTE:** All surfaces, meshes and macroshapes come under the one heading of **meshes** in the workspace panel.

### 3.4.5.2 Meshes and Macroshape

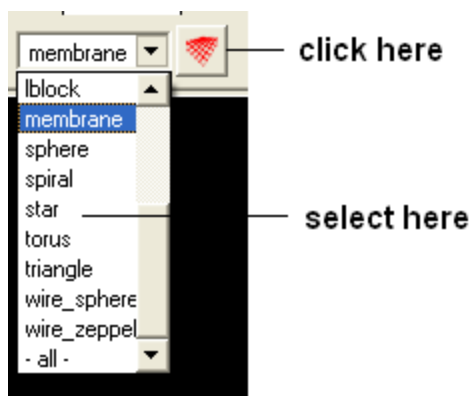
A variety of shapes can be constructed using ICM. These shapes are referred to as meshes. The types of shapes you can build are shown below:



All the buttons for creating these shapes are shown here:

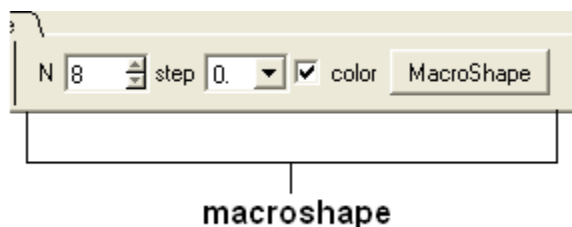


To make a shape select it from the menu by clicking on the down arrow and then click the button next to the menu. The shape will then be displayed in the 3D graphics window.



### 3.4.5.3 Macroshape

A macroshape can be constructed and allows easy viewing and manipulation of the structural representation. A macroshape representation is ideal for large structures which allows the user to easily identify important regions of the structure and facilitate the return to the 'standard' view of a particular molecule. All the buttons needed to display a macroshape structure are shown below in the 'meshes' tab.



*To construct a macroshape:*

- Load a molecule into ICM *File/Open* or *tab-pdb{PDB Search}*
- Select the amount of detail required in the shape by increasing the values in 'N' or 'step' data entry box (note the default values are usually sufficient).
- Check the 'color' if you wish your molecule to be colored.
- Click the button labeled 'MacroShape'.

Macroshape can also be used from the View menu: *View/Macro Shape*

### 3.4.5.4 Google 3D Objects (Sketchup)

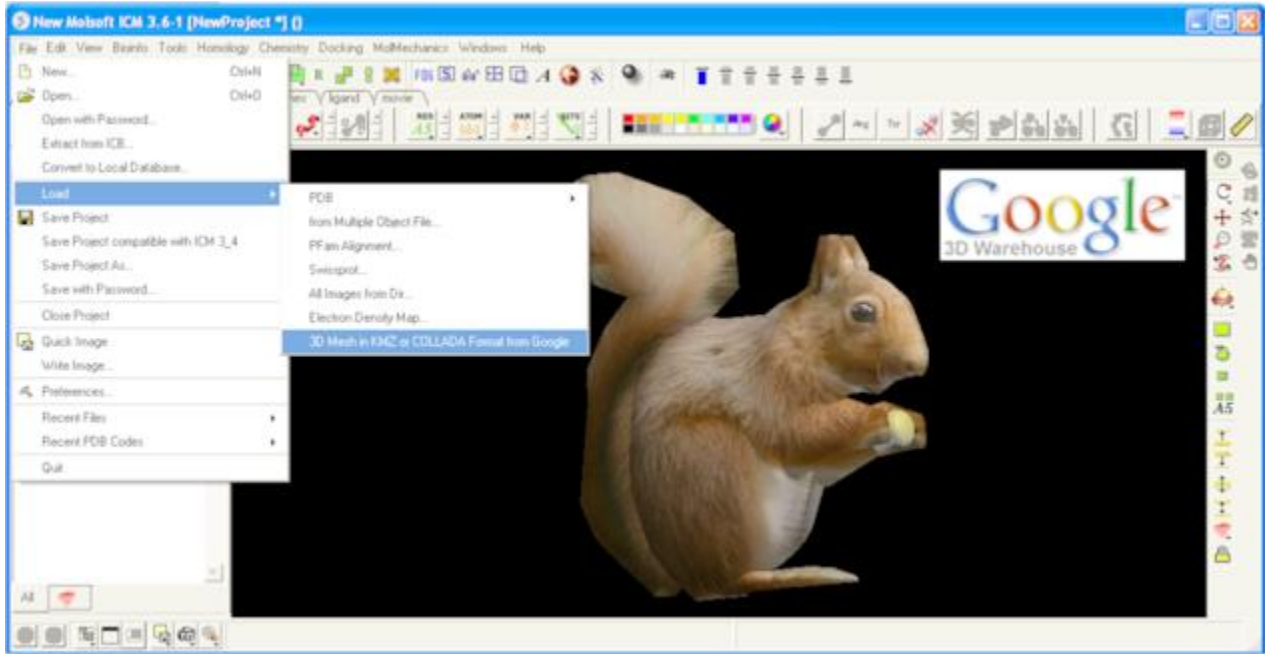
*To read in a 3D Mesh from Google in KMZ or COLLADA format:*

- *File/Load/ 3D Mesh in KMZ or COLLADA Format from Google*

- Search for the object you would like to view and download it.
- To read the file go to File/Open

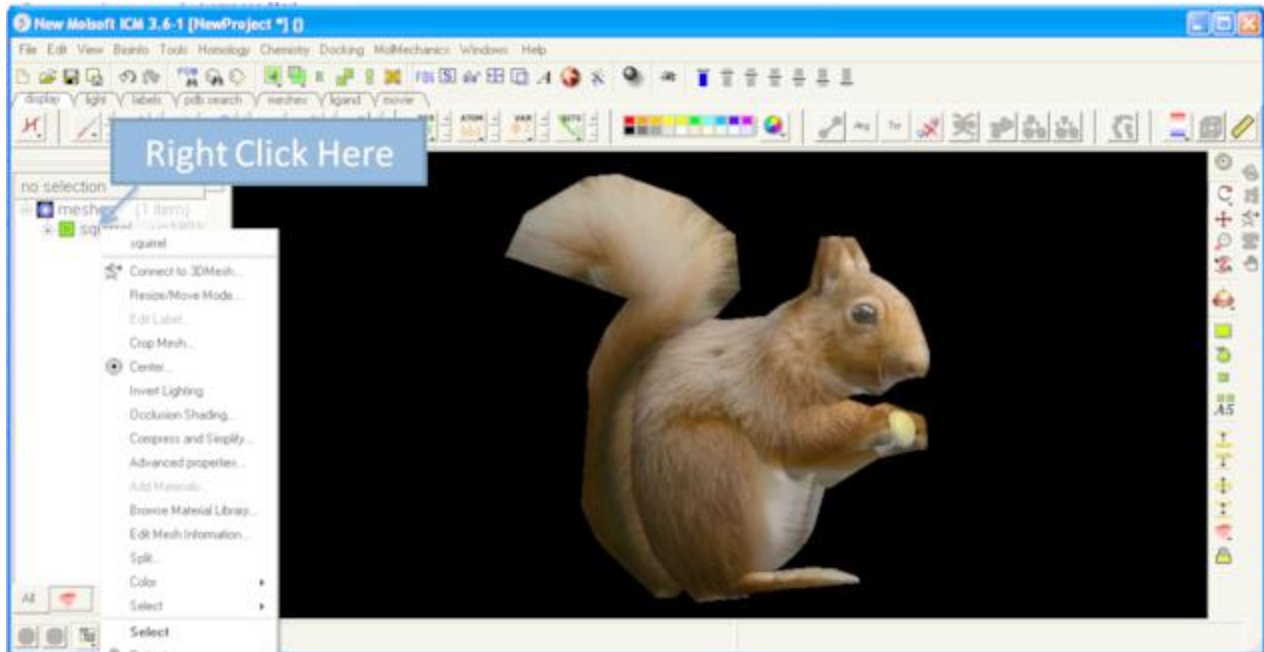
An example of a KMZ file can be found in the distribution (a squirrel model by **ilikipie**, provided with author's permission).

- File/Open, and choose the squirrel.kmz file



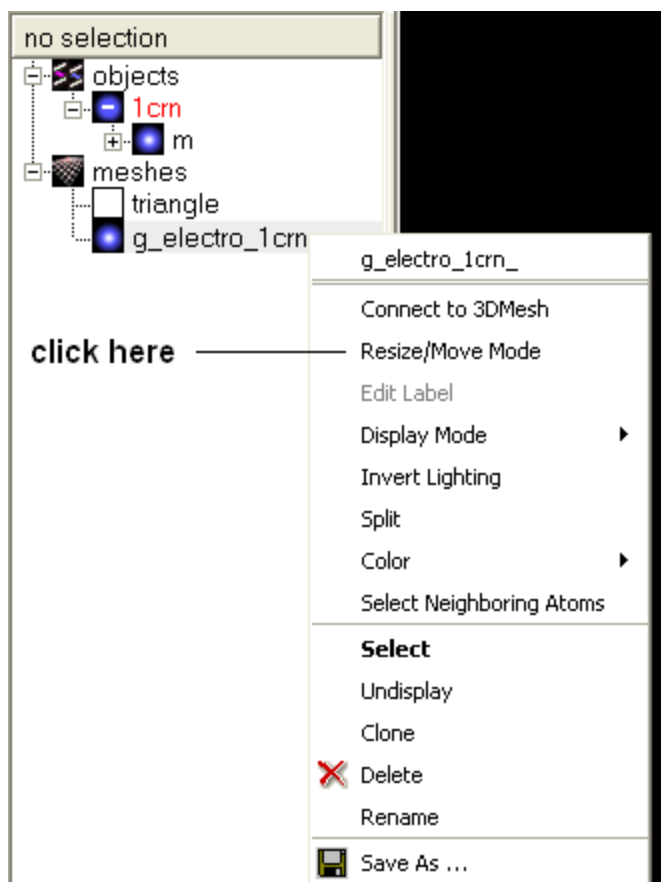
### 3.4.5.5 Mesh Options.

A number of options relating to meshes can be used by right clicking on the mesh in the ICM Workspace. This section describes some of these options.



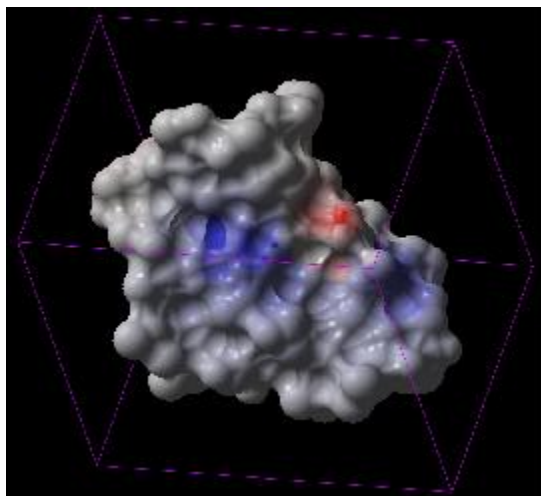
### 3.4.5.6 Move and Resize Mesh

Once a mesh has been created you can move it and resize it. To do this, locate the mesh you wish to either move or resize in the ICM Workspace and right click on it as shown below.

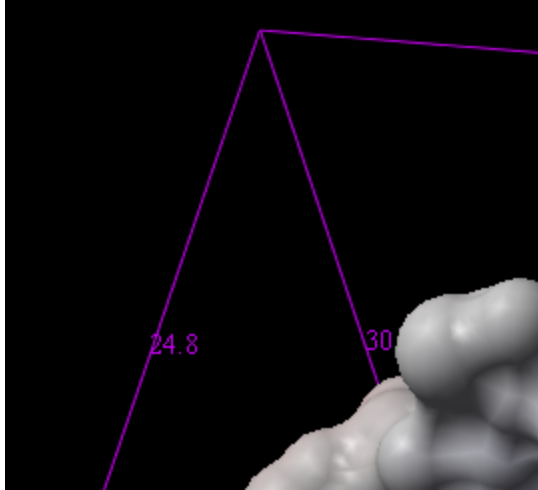


- Select the **Resize/Move Mode** in the menu.

A purple box as shown below will surround the molecule.



To resize the mesh click on one of the corners of the box and drag to the required size. The number displayed on the edges of the box represent the dimensions.

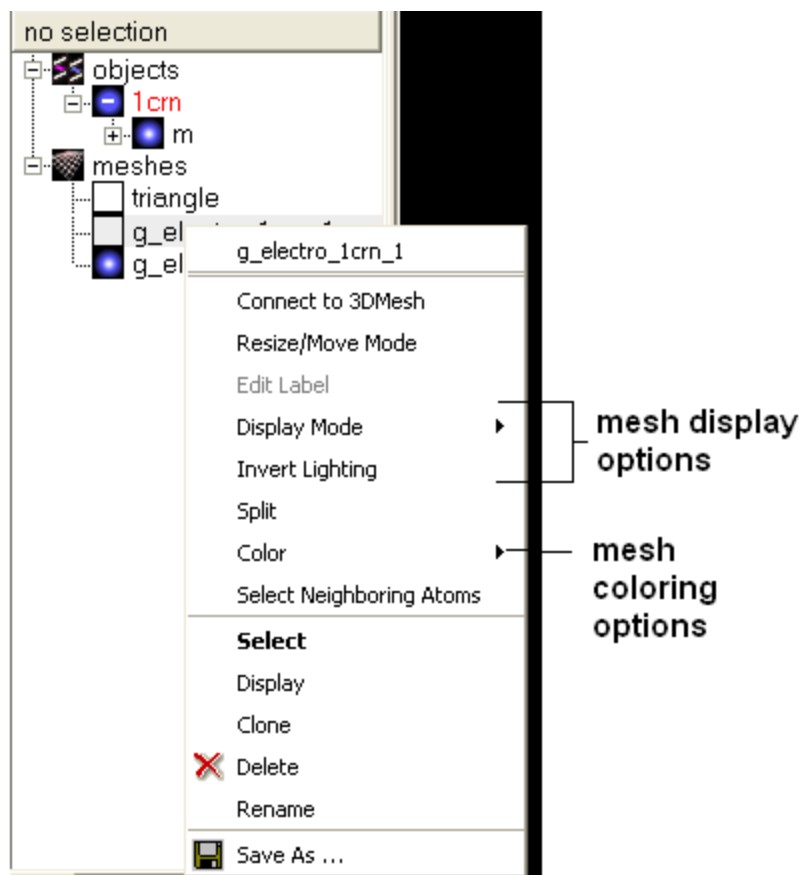


To move the mesh click on it with the center mouse button or select the connect option.

### **3.4.5.7 Color and Mesh Display**

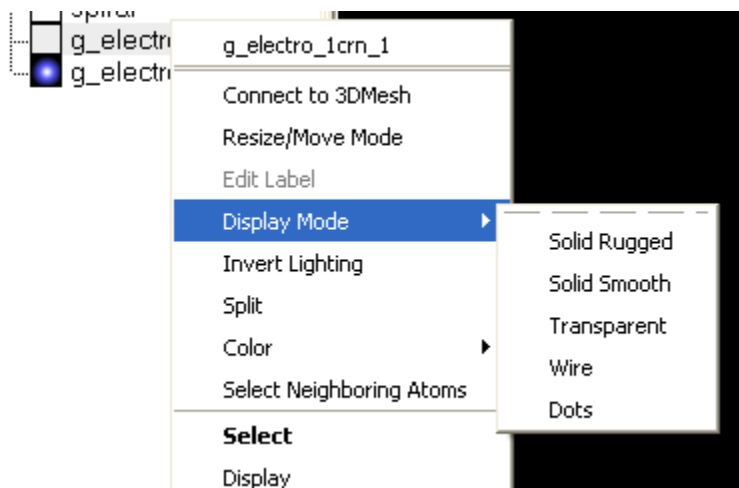
There are a number of options to color and change the display of the mesh. These options can be accessed simply by right clicking on the mesh name in the ICM Workspace as shown below.





The lighting and display can be changed by selecting the options 'Display Mode' or 'Invert Lighting'.

There are five different display modes as shown below:



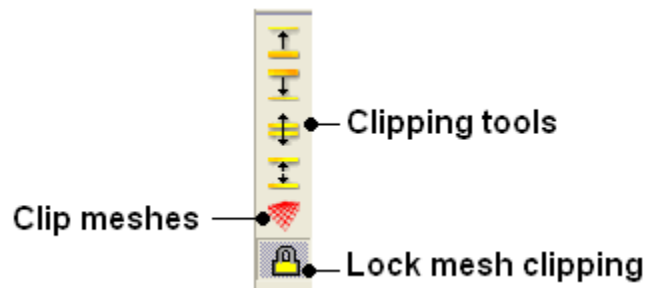
To change the lighting effects select 'Invert Lighting'.

The mesh colors can be changed by using the 'Color' option in the menu.

### 3.4.5.8 Mesh Clipping

Clipping tools can be used to adjust the frames of the mesh independently of other objects.

The buttons shown below can be used for this purpose.



The buttons used for clipping are described in the section entitled *Clipping Tools*.

### 3.4.5.9 Save Mesh

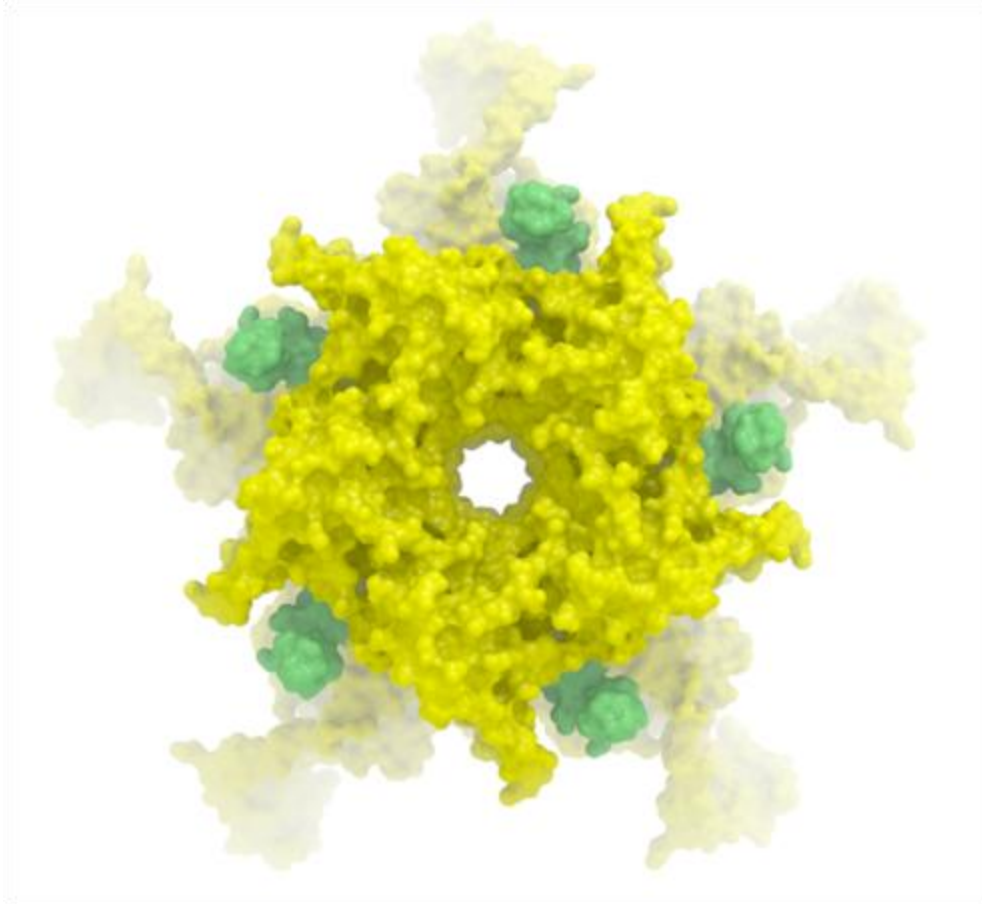
You can save a mesh as a wavefront object by right clicking on the mesh in the ICM Workspace and selecting **SaveAs**.

### 3.4.5.10 Occlusion Shading

The occlusion shading option provides better representation of depth within a cavity. The color of each surface element of a grob (mesh) is changed by mixing its own color with the background depending on the burial of the surface element

*To add occlusion shading:*

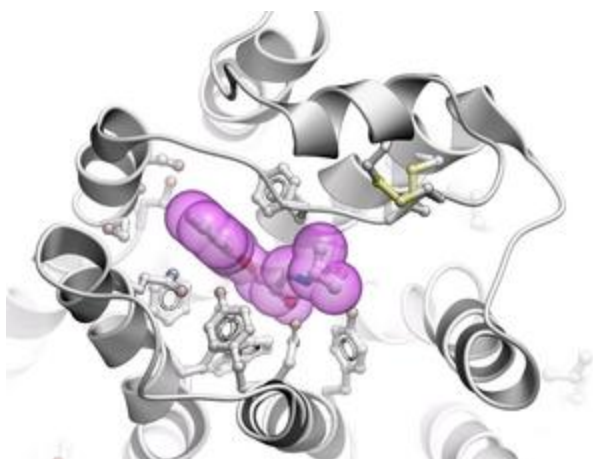
- Right click on the mesh in the ICM Workspace and select **Occlusion Shading**.
- Enter a depth value - default is 0.8. Higher values will generate a more dramatic shading.



---

## 4 Working with Protein Structures

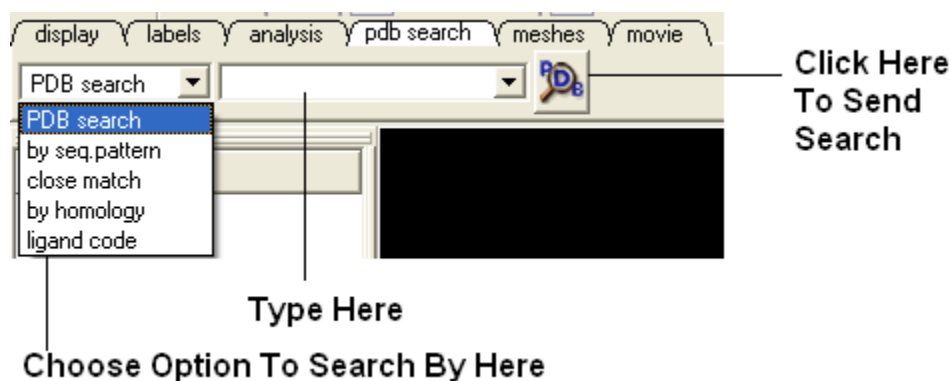
**Note:** Click **Next** (top right hand corner) to navigate through this chapter. Headings are listed on the left hand side (web version) or by clicking the **Contents** button on the left-hand-side of the help window in the graphical user interface.



In this chapter we describe how to work with protein structures. How to read them into ICM and display key aspects of the structure such as the ligand binding pocket and hydrogen bonds. We also teach how to convert a PDB file into an ICM object which is a critical operation if you want to perform any energy related task such as docking, displaying h-bonds etc...

## 4.1 Searching the PDB

The **PDB search tab** provides easy access to the PDB database. You can use keyword searching or type in the PDB code you are interested in. An asterisk (\*) wildcard can be used to list all the pdb files currently available in the protein databank. Different fields can be searched by using the drop down arrow as shown below. More advanced PDB search tools and how to use the PDB search result table are described in the section entitled *Searching the PDB*.



Once a search is complete a table of PDB files relating to your search query will be displayed. To view the PDB file in 3D in the graphical display double click on a row in the PDBSearchResults table.

**NOTE:** If you have a PDB structure already saved you can read it into ICM by going to the File Menu and selecting Open. PDB files that have been viewed previously can be loaded using File/

Recent PDB Codes.

### 4.1.1 Searching the PDB

Protein structures solved by X-ray crystallography, NMR or other experimental methods are stored in the Protein Data Bank (PDB). These structures can be easily accessed, displayed and analyzed using ICM.

There are four ways to find a structure from the PDB database and load it into ICM:

1. Query by keyword or PDB code.
2. Query by sequence pattern.
3. Query by sensitive similarity search.
4. Load the PDB file directly from FTP, http, local drive.

### 4.1.2 Querying PDB by Keyword or PDB Code

There are four ways of querying the PDB using ICM and keywords. OPTION 3 allows for a much more refined search.

#### *OPTION 1:*

- Select **Edit/PDB** search and the "Find PDB Entries by Keyword" data entry window will be displayed.
- Enter a keyword or PDB code into the Keywords data entry field.

**NOTE:** If a keyword has been entered previously it will be available by clicking on the drop-down button.

- Click the **OK** button and a list of related PDB entries will be displayed in the `PDBSearchResults` table of the graphical userinterface.

#### *OPTION 2:*

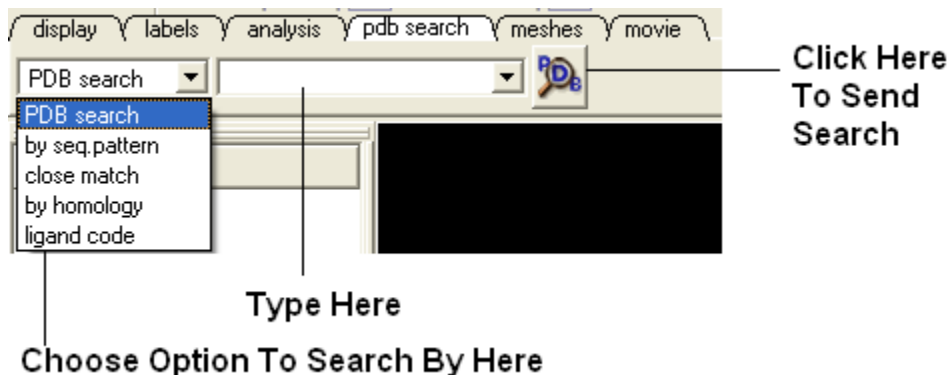
Use the pdb search tab on the tool bar. Select which parameter you wish to search by. Enter some text and this will be searched against the PDB.

Seq Pattern- Enter a protein sequence and this option will tell you whether a protein structure exists in the PDB for that sequence.

Close Match - Enter a protein sequence and this option will tell you which sequences are similar to your entered sequence.

Homology - Enter a protein sequence and homologous proteins in the PDB will be displayed in a table.

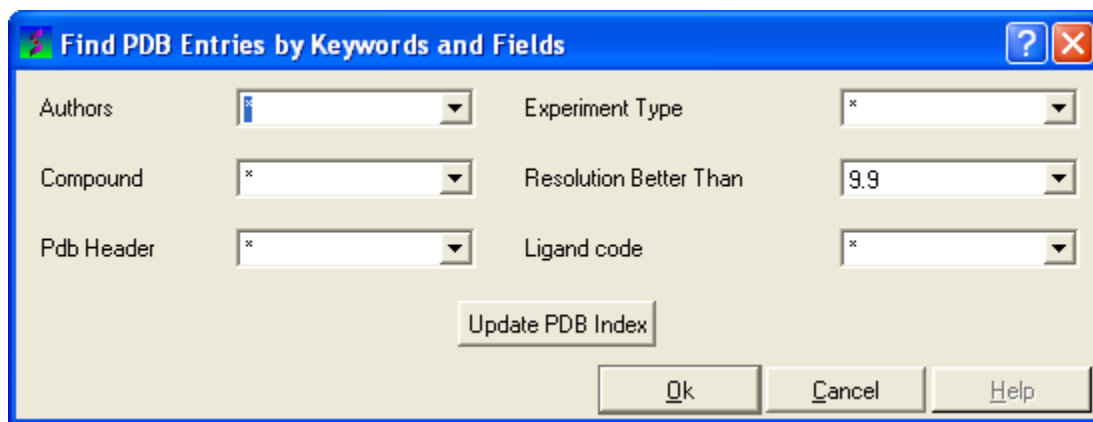
Ligand Code - Enter the PDB ligand code.(e.g. 1crn)



- Click the **OK** button and a list of related PDB entries will be displayed in the PDBSearchResults table of the graphical userinterface.

### OPTION 3:

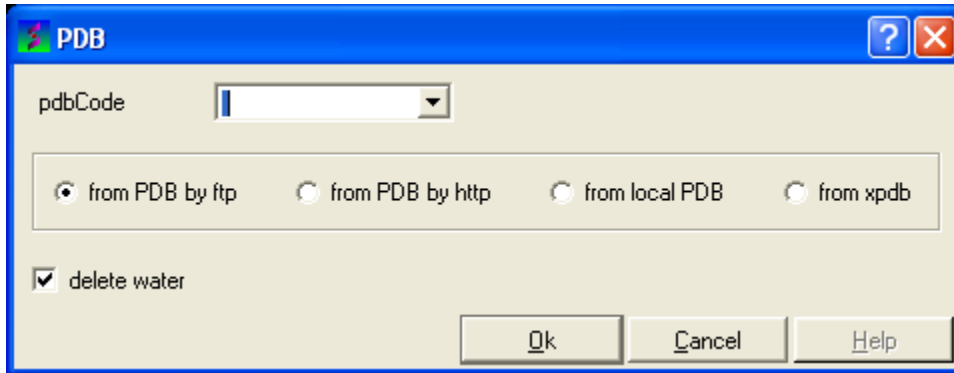
- Select **Edit/PDB** search by field and the **\*\* Find PDB Entries by Keywords and Fields \*\*** data entry window will be displayed.



- Enter your search words into the appropriate fields: **Author; Compound; PDB Header; Experiment Type; Resolution Better Than**
- Click the **OK** button and a list of related PDB entries will be displayed in the PDBSearchResults table of the graphical userinterface.

### OPTION 4:

- Select **File/Load** and the PDB data entry window will be displayed.
- Enter the PDB code and select the source of your PDB file.
- Click the **OK** button and a list of related PDB entries will be displayed in the PDBSearchResults table of the graphical userinterface.



### 4.1.3 PDB Search Results Table

- To load a pdb file double click on the search results table.
- Sort the table by right clicking on the column header. Other table manipulation options are described in the Working with Tables chapter.



### 4.1.4 Querying PDB by Sequence Pattern

There are two ways to query the PDB by sequence pattern.

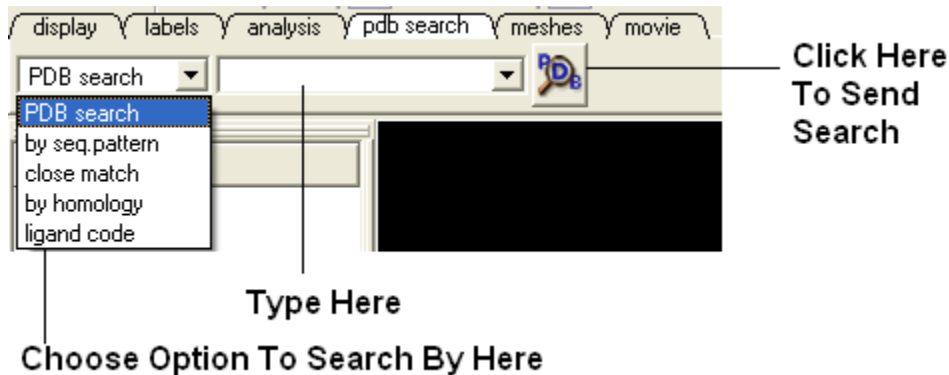
#### OPTION 1:

- Select **Edit/PDB Search by sequence pattern**
- Cut and paste or type your sequence into the Sequence data entry field.

- Choose whether you wish to display All entries or Entries with unique sequence by checking the appropriate button.
- Click the **OK** button.

**OPTION 2:**

Use the word search option on the tool bar



### 4.1.5 Sensitive PDB Similarity Searches

There are two ways to search a sequence against the PDB database.

**OPTION 1:**

If your sequence is already loaded into ICM:

- Select **Edit/PDB Search by sensitive similarity**
- Type the sequence name into the **Sequence name** field. Sequences which are already loaded into ICM can be seen by clicking the drop-down button
- Select the number of hits you wish to see by typing the number into the Limit field. A number can also be selected by clicking on the up and down arrows. (Default is 50)
- Select the sensitivity of your search by typing a value into the Expect field. This value is a database-size error estimate and the default value is 0.01.
- Choose whether you wish to display All entries or Entries with unique sequence by checking the appropriate button.
- If you wish to load the sequences leave the Load Sequences box checked.
- If you merely want to see the PDB codes which are similar to your sequence then uncheck the Load Sequences box.
- Click the **OK** button.

**OPTION 2:**

If your PDB sequence is not loaded into ICM:



- Select **Edit/Search with external sequence**
- Cut and paste or type (shown below) your sequence into the **Sequence** data entry field.
- Select the number of hits you wish to see by typing the number into the **Limit** field. A number can also be selected by clicking on the up and down arrows. (Default is 50)
- Select the sensitivity of your search by typing a value into the **Expect** field. This value is a database-size error estimate and the default value is 0.01.
- Choose whether you wish to display **All entries** or **\*\* Entries with unique sequence \*\*** by checking the appropriate button.
- If you wish to load the sequences leave the **Load Sequences** box checked.

**NOTE:** If you merely want to see the PDB codes which are similar to your sequence then uncheck the Load Sequences box.

- Click the **OK** button.

**NOTE:** You can also use the toolbar search option by homology if you wish.

#### 4.1.6 Working with PDB Search Results

Once you have searched for a PDB structure, a table with the search results will be displayed on the bottom of the ICM window. See the Tables section for more information on how to use ICM tables. See the next section loading your PDB file for information how to view the PDB file. More information about working with tables can be found in the Tables Section of this manual.

#### 4.1.7 Loading Your PDB File

- To load a pdb file double click on the search results table.
- Sort the table by right clicking on the column header. Other table manipulation options are described in the Working with Tables chapter.

Double click anywhere in the table to load the PDB file

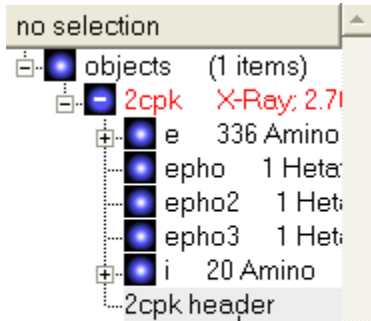
ID	name	date	title	source	auth	ins
1	1y4k TRANSFERASE	01/01/04	structure of hydroxyethylthiazole kinase protein from	PYROCOCCUS HOFKOSHE	Jayaraman, J., Telnov, T.H., RIKEN Structural	KR
2	1y4k TRANSFERASE (PHOSPHOTRANSFERASE)	01/02/05	crystal structure of the tyrosine kinase domain of the human	HOMO SAPIENS	Hubbard, S.R., Wu, L., Ellis, L., Hendrickson, W.A.	KR
3	1y4l TRANSFERASE	01/03/02	crystal structure of mycobacterium tuberculosis mycolate	MYCOBACTERIUM TUBERCULOSIS	Urbay, T., Wisk, M., Florouzent, E., Delarue, M., Goeben, M., SN	SR
4	1y4j TRANSFERASE	01/04/01	Binding of nucleotides to rhlp kinase	DICTYOSTELIUM DISCOIDEUM	Cervoni, L., Lecoq, I., Xu, Y., Gonia, P., Mor, M., Menouen, M., SN	SR
5	2k49 TRANSFERASE	01/04/06	Human protein kinase c, eta	HOMO SAPIENS	Walker, J.R., Liffen, D.R., Finerty, Jr., P.J., MacFarlane, F.,	KR
6	3b42 TRANSFERASE	01/04/08	morpholino pyrimidinone p38 alpha map kinase inhibitor	HOMO SAPIENS	Seck, J.S.	KR
7	3b43 TRANSFERASE	01/04/08	morpholino pyrimidinone p38 alpha map kinase inhibitor	HOMO SAPIENS	Seck, J.S.	KR
8	1y4g PHOSPHOTRANSFERASE (CARBONYL ACCEPTOR)	01/04/06	gamma-phosphoglycerate kinase, mutation 45q	SACCHAROMYCES CEREVISIAE	Moghilip, T.M., Hsu, B.T., Shamen, M.A., Mes, M.T., Pares,	KR
9	1y4v TRANSFERASE	01/05/05	crystal structure of thiamine monophosphate kinase (thk)	ADUPEXIAEOLICUS	Eswaramoorthy, S., Swaminathan, S., Suley, S.K., New York	KR
10	1y4g TRANSFERASE	01/05/05	crystal structure of pyridoxal kinase in complex with	OVIS ARIES	Tang, L., Li, M.H., Cao, P., Wang, F., Chang, W.R., Beck, S.,	KR
11	1y4h TRANSFERASE	01/05/05	crystal structure of pyridoxal kinase in complex with	OVIS ARIES	Tang, L., Li, M.H., Cao, P., Wang, F., Chang, W.R., Beck, S.,	KR

Right click on column header for sort and other table options

## 4.1.8 Display PDB Header

To display the PDB Header for a PDB file.

- First load a PDB file into ICM (see `Load PDB`)
- Double click on the word header in the ICM Workspace.



- The PDB Header information will be displayed.

2cpk header

PDB link: [Open PDB home Structure Explorer page for 2cpk](#)

Deposition Date: 21-oct-92

Resolution: 2.7 Å

Unit Cell  
 length: a= 73.62 Å b= 76.52 Å c= 80.14 Å  
 angles: α= 90.00° β= 90.00° γ= 90.00°

Molecule:  $\gamma$ -irradiation-induced protein kinase [e.c.2.7.1.37] (catalytic subunit)

Functional Class: transferase(phosphotransferase)

Chemical ID: pho

Chemical Name: phosphate group bonded to ser e 139

Chemical Formula: 3(o3 p1 -)

Species: recombinant mouse (*mus musculus*) "alpha" isoenzyme expressed in (*escherichia coli*)

Latest Update: 15-jan-93 2cpk 0

Refinement Programs: refinement. molecular dynamics refinement by the method of a. brunger, j. kuriyan, and m. karplus (program \*xplor\*, v. 3.0). the r value is 0.18 for reflections in the resolution range 10.0 to 2.7 angstroms with fobs .gt. 2.0\*sigma(fobs). the rms deviation from ideality of the bond lengths is 0.018 angstroms. the rms deviation from ideality of the bond angles is 3.6 degrees.

Refinement Format: secondary structure assignments in this entry were done by the use of program "dssp" of w.kabsch and c.sander. these assignments differ in some cases from those reported in the papers cited as references 1 and 2 above, which were derived from visual inspection.

WARNINGS: there is no electron density for the 14 n-terminal residues of the catalytic subunit, which are presumed disordered.

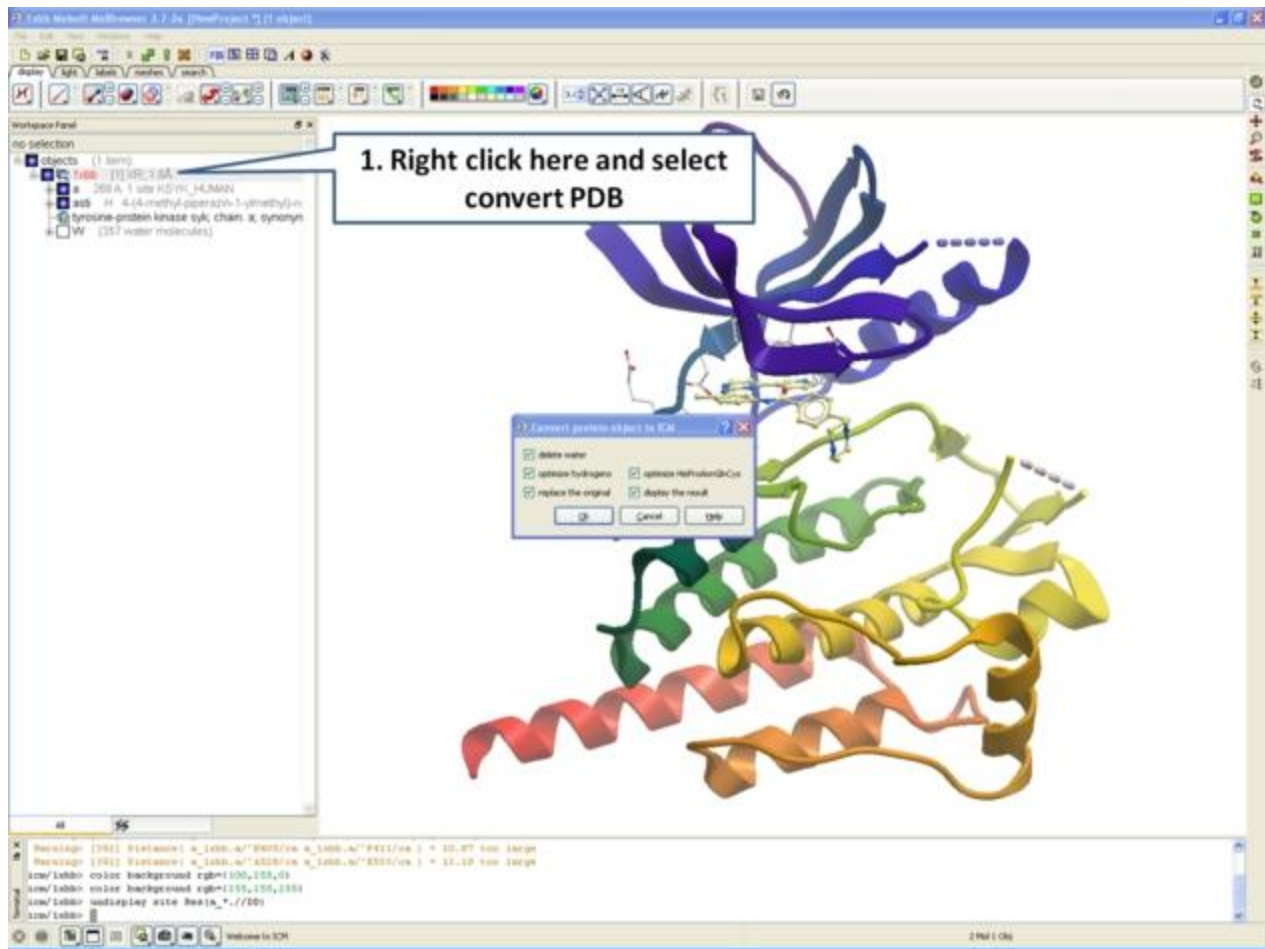
- Click on the blue hyperlinked text to link to external web pages for additional information if needed.

## 4.2 Converting PDB Files Into ICM Objects

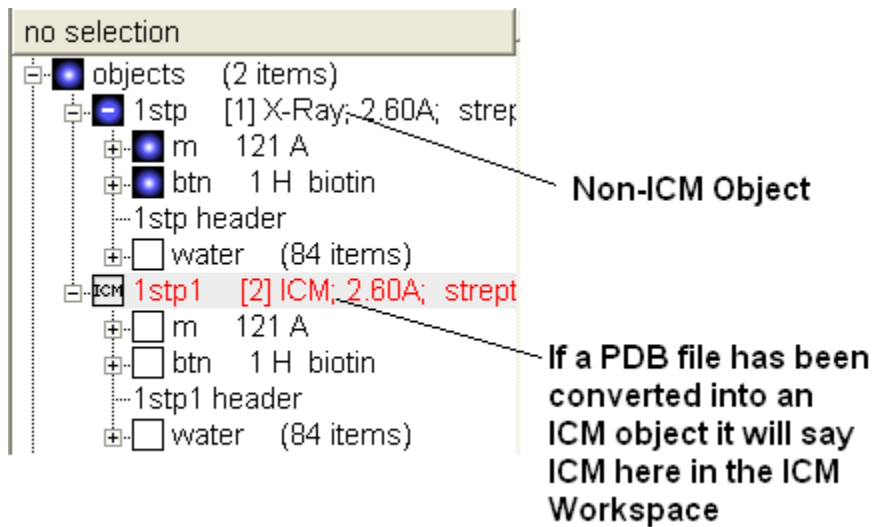
If you are going to make any energy calculation in ICM (eg docking, display H-bonds, display electrostatic and binding property surfaces etc..) it is necessary to convert a protein or chemical into an ICM object.

*To convert a PDB structure into an ICM object follow the steps shown below:*

- Right click on the name of the protein you wish to convert in the ICM Workspace.
- A dialog box will be displayed. Check the boxes as desired. If you are performing important calculations then it is necessary to optimize all hydrogens and ASN, GLU, PRO, and CYS.



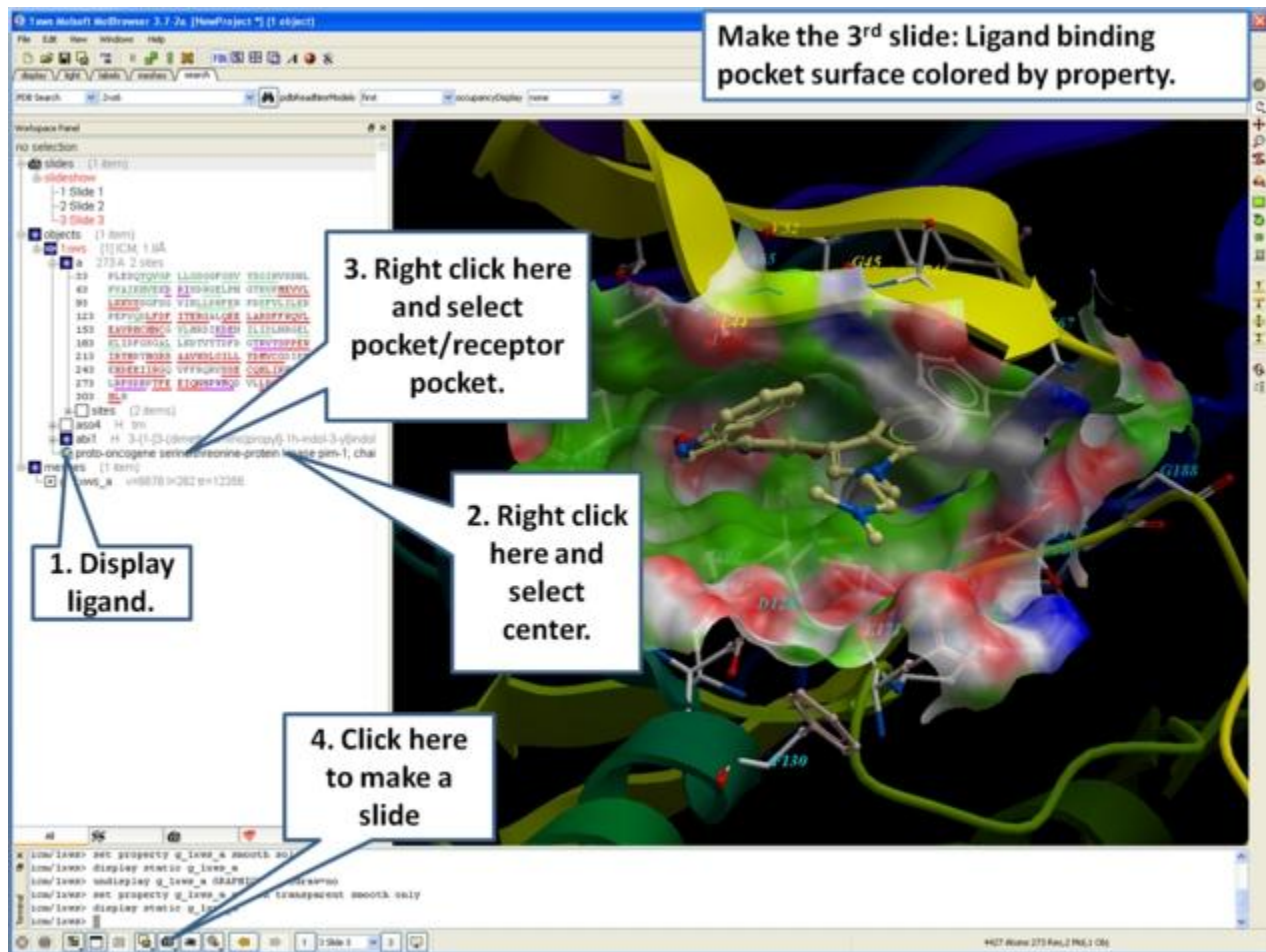
If your object is an ICM object it will tell you in the ICM Workspace:



### 4.3 How to Display the Ligand Binding Pocket Surface and

## Neighboring Residues.

- As an example we will use the PDB structure 1STP. Type 1STP in the pdb search tab and press return.
- Convert the protein to an ICM object.
- Right click on the ligand "btn" and select "Ligand Pocket"
- To remove the ribbon display and display only the residues in the pocket. Select the "display" tab and click on the ribbon button which will undisplay the ribbon representation and leave only the residues surrounding the pocket.



## 4.4 How to Display Hydrogen Bonds

**NOTE:** The method by which hydrogen bonds are calculated is described [here](#) in the command

line manual. The GRAPHICS.hbondMinStrength parameter determines the hbond strength threshold for hbond display. The strength value is between 0. and 2. By changing 1. to 0.2 you will see more weak hydrogen bonds.

- As an example we will use the PDB structure 1STP. Type 1STP in the pdb search tab and press return.
- In order to display energy related properties we need to convert the PDB file into an ICM object. Convert 1STP into an ICM object. In this example, the option "Replace the Original" was selected.
- Display the receptor in wire format and the ligand in xstick.
- Right click on the ligand and select "Neighbors" - Enter 3 Angstroms and Type = Visible. Do not exclude source (the ligand) therefore remove tick from box entitled "exclude source".
- Select the display tab and then select the Display H-Bond button.

**2. Display all hydrogens and the residues/ligands**

**3. Click on the hydrogen button in the Display tab. Click and hold for more options**

**4. Left click = display/undisplay hbonds  
Right click = change hbond representation  
Click on + to see all hbond in list**

**1. Right click here and select convert PDB**

**Note: Right click on hbondpairs in ICM workspace to select residues making a hbond and also export to table**

```

icm/latp: make hbond refresh Resid_"/301 Resid_"/301 name="Hbondpairs"
  info: 01 hydrogen bonds 'Hbondpairs' (a_not) created. aTotal(1) out(1)*01
icm/latp: 12 Red (Hbondpairs)>> display Hbondpairs Resid_"/301
icm/latp: color background rgb=(155,155,155)
icm/latp: color background rgb=(155,155,155)
icm/latp:
  
```

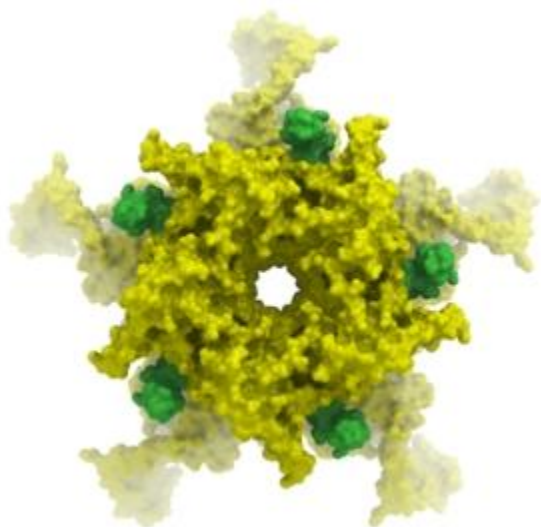
123 Res 2 PA, 1 On

**NOTE:** Different options for displaying the H-bond can be accessed by clicking and holding on the H-bond button in the "Display" tab. The coloring of the H-bonds are red (strong - thick spheres) to blue (weak - thin spheres). Once the hydrogen bonds have been displayed they can be displayed and undisplayed in the 3D labels section of the ICM Workspace (left hand side of graphical window).

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## 5 Molecular Graphics

**Note:** Click **Next** (top right hand corner) to navigate through this chapter or use the links below. Headings are listed on the left hand side (web version) or by clicking the **Contents** button on the left-hand-side of the help window in the graphical user interface.



In this chapter we describe the methods to make beautiful graphical representations of molecules and manipulate them in the 3D graphics window. This includes changing coloring, lighting, representation, clipping planes, and built in graphics effects. We also teach how to annotate your molecule with labeling.

### 5.1 Molecule Representation

To change the molecule display representation:

- Select the atoms, residues, molecules, or objects you wish to change in the graphical display or in the ICM Workspace.
- Then use the molecule representation (e.g. wire, ribbon) options in the `Display` Tab.

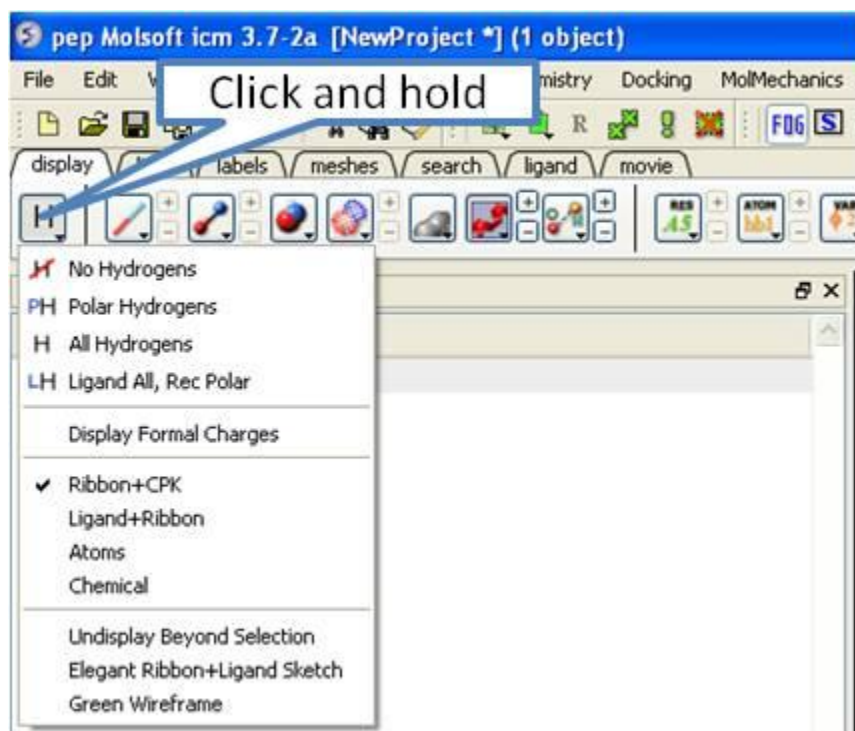
The display tab contains tools for a variety of functions including - structural representations, coloring, labeling and superposition. This tab is shown below.



### 5.1.1 Display and Undisplay Hydrogens

To display and undisplay hydrogens. Click and hold on the "**Change Hydrogen Display**" button shown below. Multiple single clicks will toggle through the hydrogen display options.

- Display Tab
- Click and hold on the "**Change Hydrogen Display**" button shown below.



### 5.1.2 Display Formal Charges

You can display formal charges by clicking and holding on the "**Change Hydrogen Display**" button in the **Display** tab.

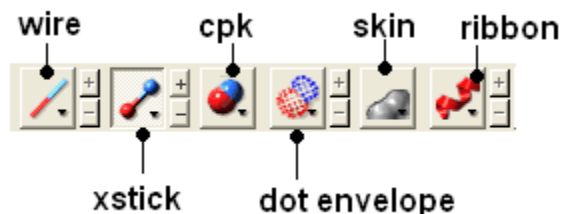
### 5.1.3 Structure Representation



There are six main types of structural representation in ICM. They are wire, ball and stick (Xstick), ribbon, skin, CPK and dot envelope (surface).

*To display one of these representations:*

- Click on the representation button you desire in the **display** tab.

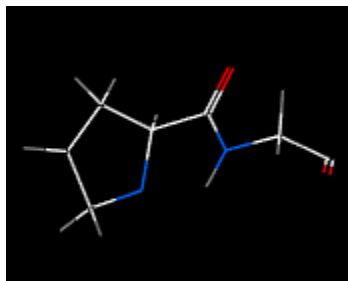


*To remove a displayed representation or to toggle between display and undisplay:*

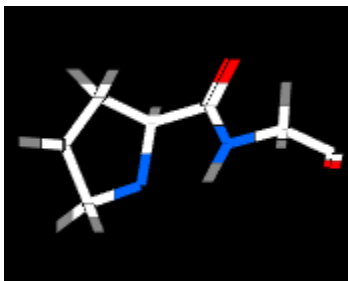
- Click on the corresponding representation button in the **display** tab.

**NOTE:** The button display will change appearance (shaded) when pressed. This makes it easier to identify which representations are currently being displayed. Many characteristics of the graphical representation such as color can be changed by clicking and holding on the button or by clicking the plus(+) and minus(-) buttons next to them.

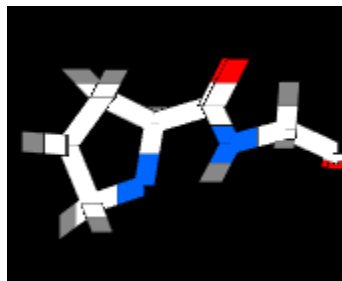
*Some examples of the representations you can choose:*



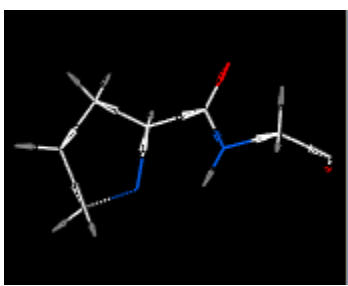
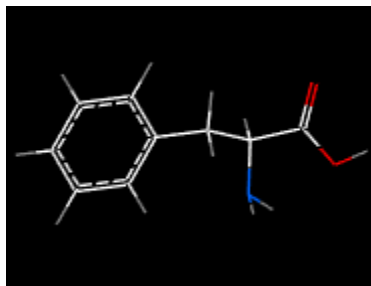
Wire : Thin



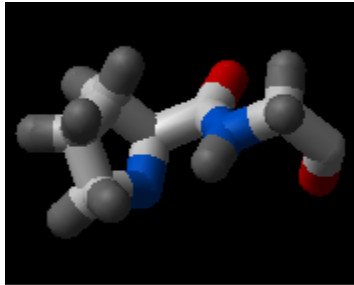
Wire : Normal



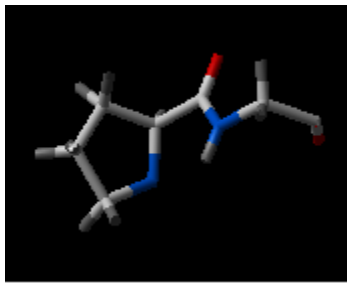
Wire : Thick



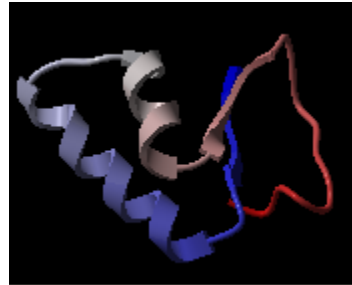
Wire : Chemistry



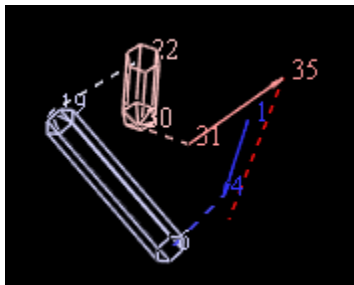
Wire : Tree



Xstick- Thin



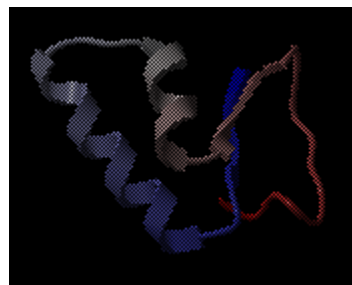
Xstick : Thick



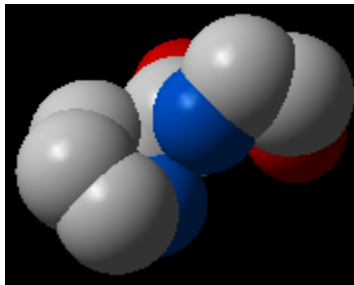
Xstick : Stick / Ball



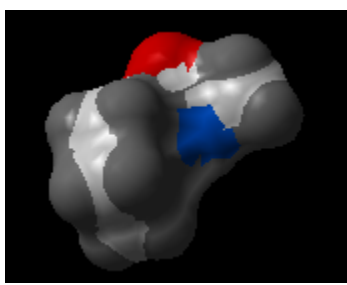
Ribbon : Ribbon



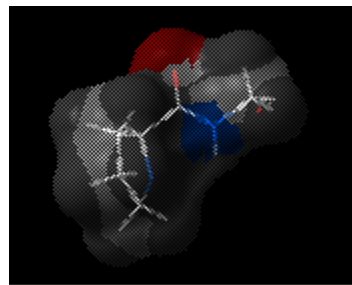
Ribbon : Segment



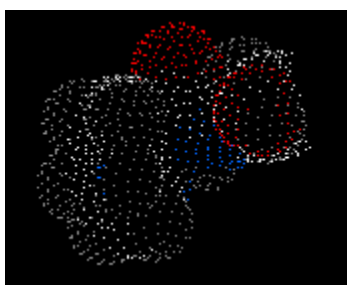
Ribbon : Protein Worm



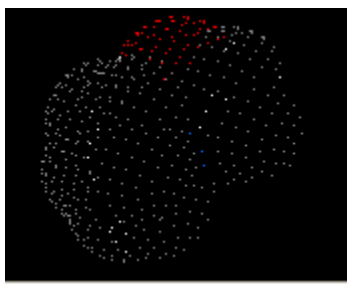
Ribbon : Transparent



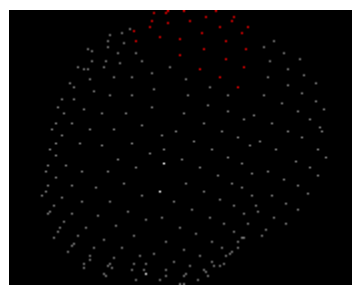
CPK : Default



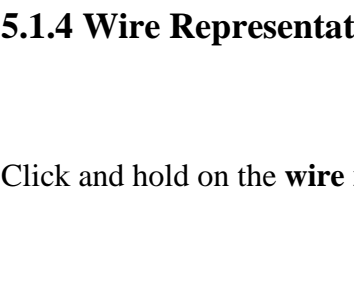
Skin : Default



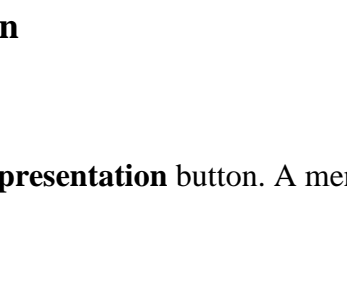
Skin : Transparent



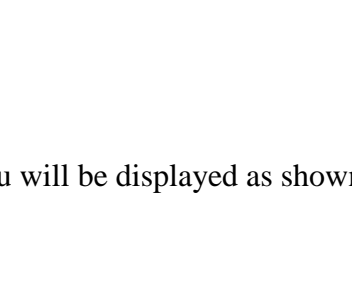
Surface : Tight



Surface : Normal

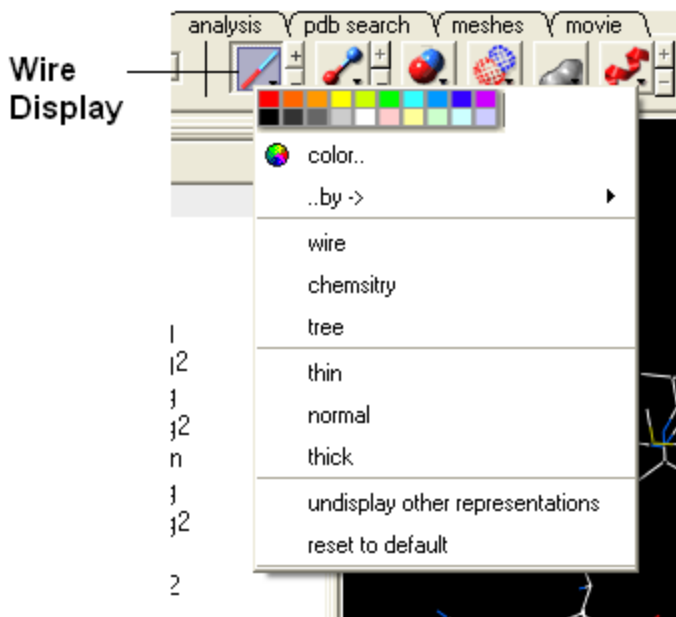


Surface - Sparse



### 5.1.4 Wire Representation

Click and hold on the **wire representation** button. A menu will be displayed as shown below.



*To change the wire style:*

- Click and hold on the **wire representation** button and then click on **wire**, **chemistry** or **tree**.

*To change the size of the wire representation:*

- Click and hold on the **wire representation** button and then click on **thin**, **normal** or **thick**.

**NOTE:** Clicking on the +/- next to the **wire representation** button also changes the thickness of the wire representation.

*To undisplay representations other than wire:*

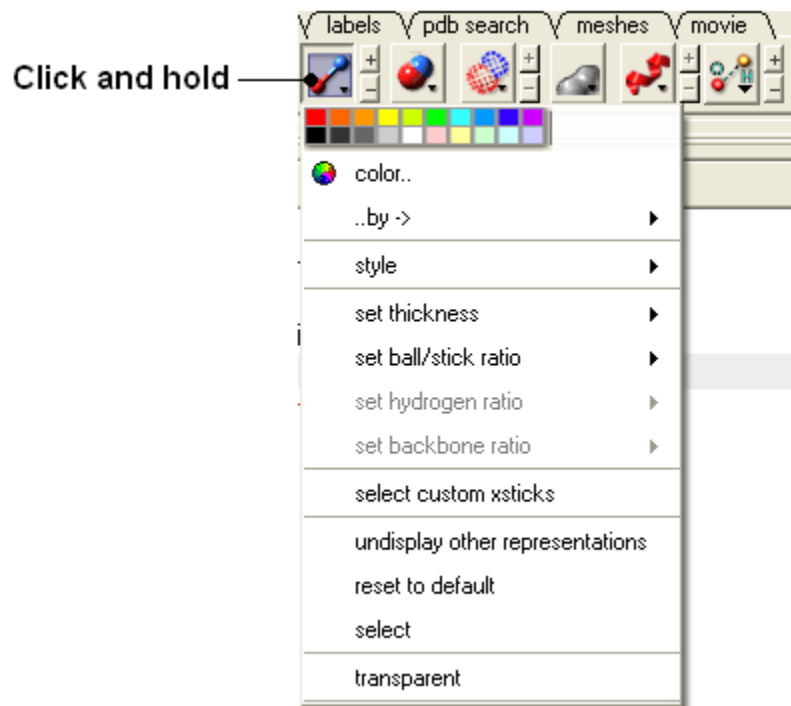
- Click and hold on the **wire representation** button and then click on undisplay other representations.

If you make a mistake or you are not happy with the way your structure is displayed with the wire representation:

- Click and hold on the **wire representation** button and then click on reset to default.

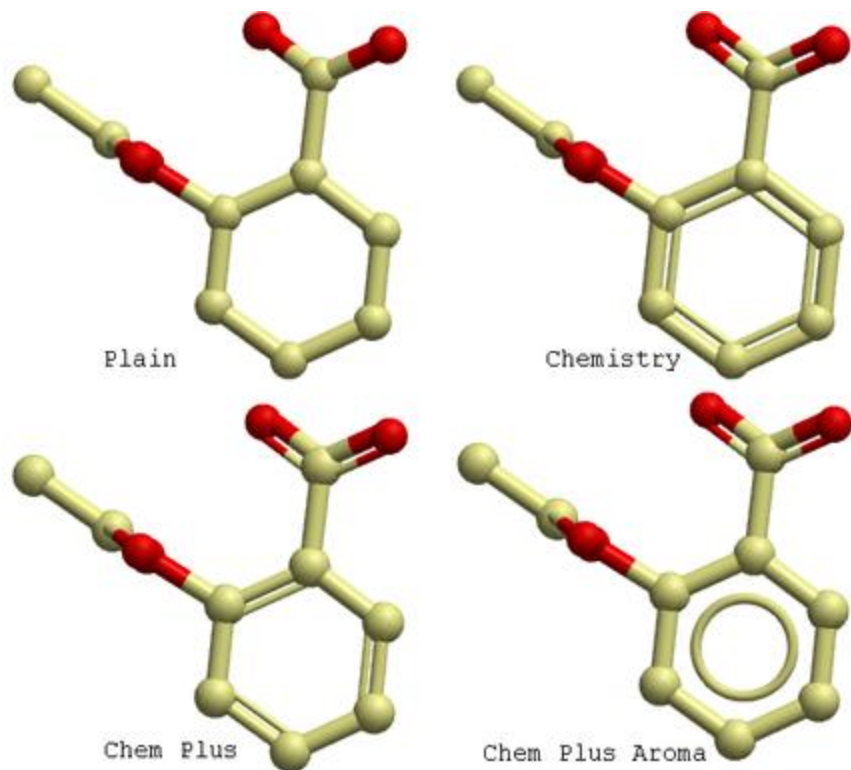
### 5.1.5 Stick and Ball (Xstick) Representation

Click and hold on the **stick and ball representation** button. A menu will be displayed as shown below.



***To change the style of the Xstick representation:***

- Click and hold on the **stick and ball representation** button and then click on style. Choose a style as shown below.



*To change the size of the Xstick representation:*

- Click and hold on the **stick and ball representation** button and then click on **set thickness**, **set ball/stick ratio**, **set hydrogen ratio**, and **set backbone ration**.

**NOTE:** Clicking on the +/- next to the **xstick representation** button also changes the thickness of the xstick representation.

*In order to make some parts of your picture clearer, the xstick representation can be set to transparent:*

- Click and hold on the **stick and ball representation** button and then click on transparent.

*To undisplay representations other than xstick:*

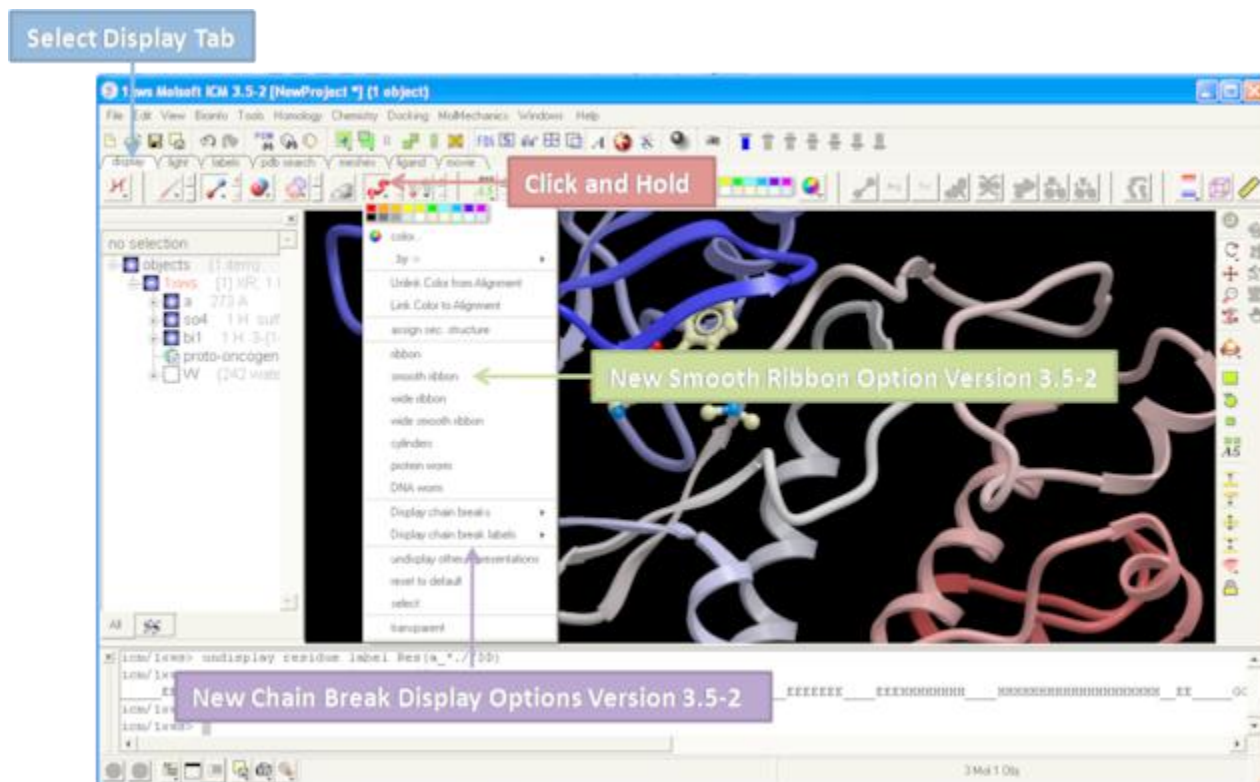
- Click and hold on the **stick and ball representation button** and then click on undisplay other representations.

*If you make a mistake or you are not happy with the way your structure is displayed with the xstick representation:*

- Click and hold on the **stick and ball representation** button and then click on reset to default.

## 5.1.6 Ribbon Representation

Click and hold on the ribbon representation button. A menu will be displayed as shown below.



*To change the style of the Ribbon representation:*

- Click and hold on the **ribbon representation button** and then click on a style option.

To accurately represent the secondary structure of the molecule in ribbon representation you may wish to assign secondary structure:

- Click and hold on the **ribbon representation button** and then click on **assign sec. structure**. New in version 3.5-2 is the smooth ribbon style.

*To make some parts of your picture clearer, the ribbon representation can be set to transparent:*

- Click and hold on the **ribbon representation button** and then click on **transparent**.

*To undisplay representations other than ribbon:*

- Click and hold on the **ribbon representation** button and then click on undisplay other representations.

*If you make a mistake or you are not happy with the way your structure is displayed with the ribbon representation:*

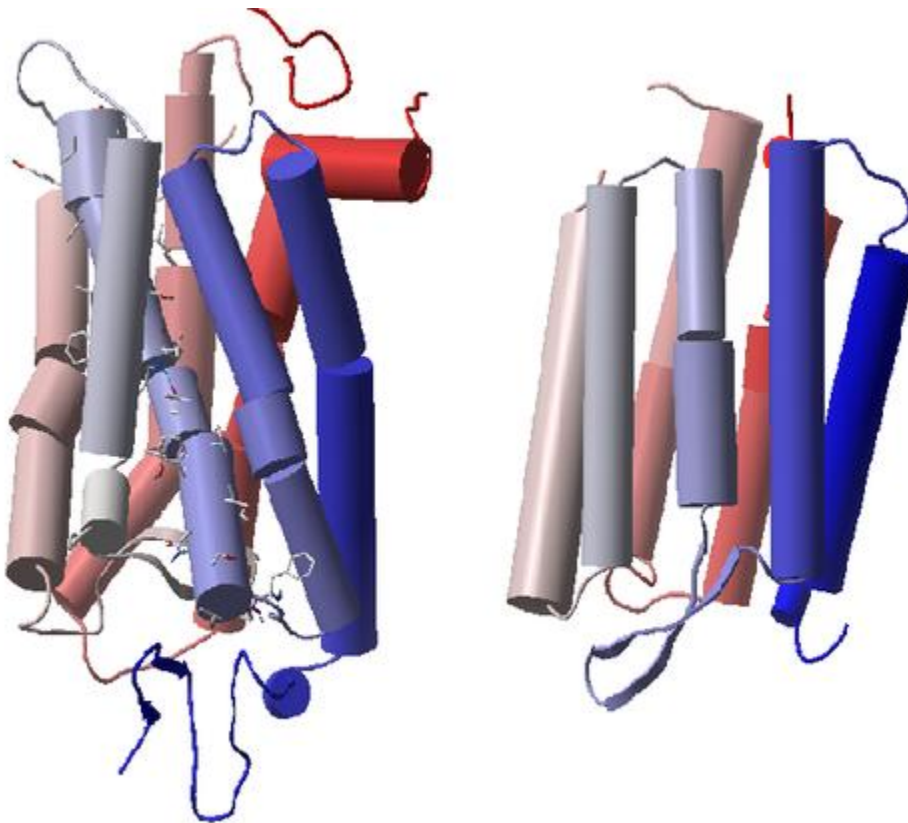
- Click and hold on the **ribbon representation button** and then click on **reset to default**.

**NOTE:** Always use the **ICM** assign sec.\*\* structure tool in the ribbon right click menu to get accurate secondary structure assignment. This is particularly important when studying helices which may have non-cannonical elements within them such as 3/10 or pi. To view non-cannonical helix segments use the segment option in the ribbon right click menu.

*To change the display of chain breaks (dotted lines):*

- Click and hold on the ribbon representation button.
- Select the options Display Chain Breaks or Display Chain Break label.

The helices in rhodopsin and bacteriorhodopsin are shown below in segment representation. Non-cannonical regions are represented as breaks in the helix segment.



### 5.1.7 Skin Representation

Click and hold on the **skin representation button**. A menu will be displayed as shown below.



*To make some parts of your picture clearer, the skin representation can be set to tight, normal or sparse:*

- Click and hold on the **skin representation button** and then click on either tight, normal or sparse.

*To undisplay representations other than skin:*

- Click and hold on the **skin representation button** and then click on **undisplay other representations**.

*If you make a mistake or you are not happy with the way your structure is displayed with the skin representation:*

- Click and hold on the **skin representation button** and then click on **\*\* reset to default\*\***.

**NOTE:** Sometimes due to singularity problems holes may appear within the skin surface. To cure this affliction select atoms nearby and right click select Advanced->RandomizeAtoms

### 5.1.8 CPK Representation

Click and hold on the **CPK representation button**. A menu will be displayed as shown below.





*To undisplay representations other than CPK:*

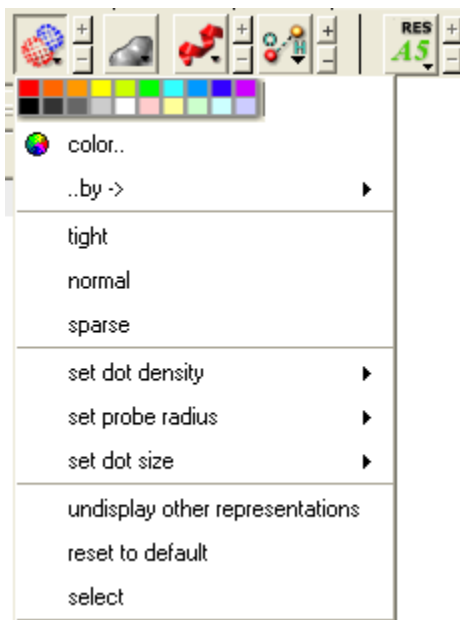
- Click and hold on the **CPK representation button** and then click on **undisplay other representations**.

*If you make a mistake or you are not happy with the way your structure is displayed with the cpk representation.*

- Click and hold on the **CPK representation button** and then click on **reset to default**.

### 5.1.9 Surface Representation

*Click and hold on the surface representation button. A menu will be displayed as shown below.*



*To change the style of the surface representation:*

- Click and hold on the **surface representation button** and then click on **tight, normal, or surface**.

*To undisplay representations other than surface:*

- Click and hold on the **surface representation button** and then click on undisplay other representations.

*If you make a mistake or you are not happy with the way your structure is displayed with the surface representation:*

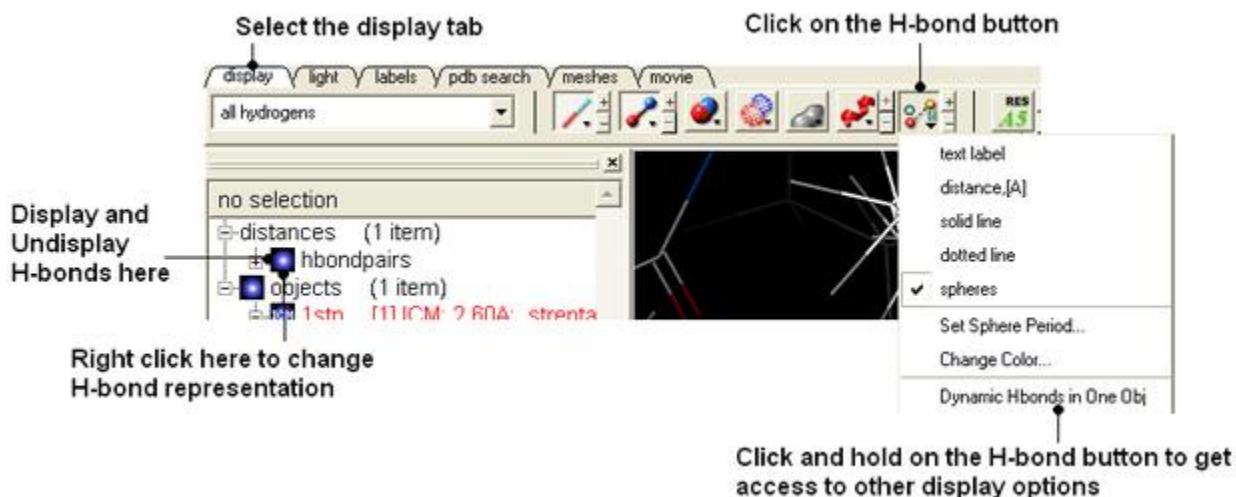
- Click and hold on the **surface representation button** and then click on **reset to default**.

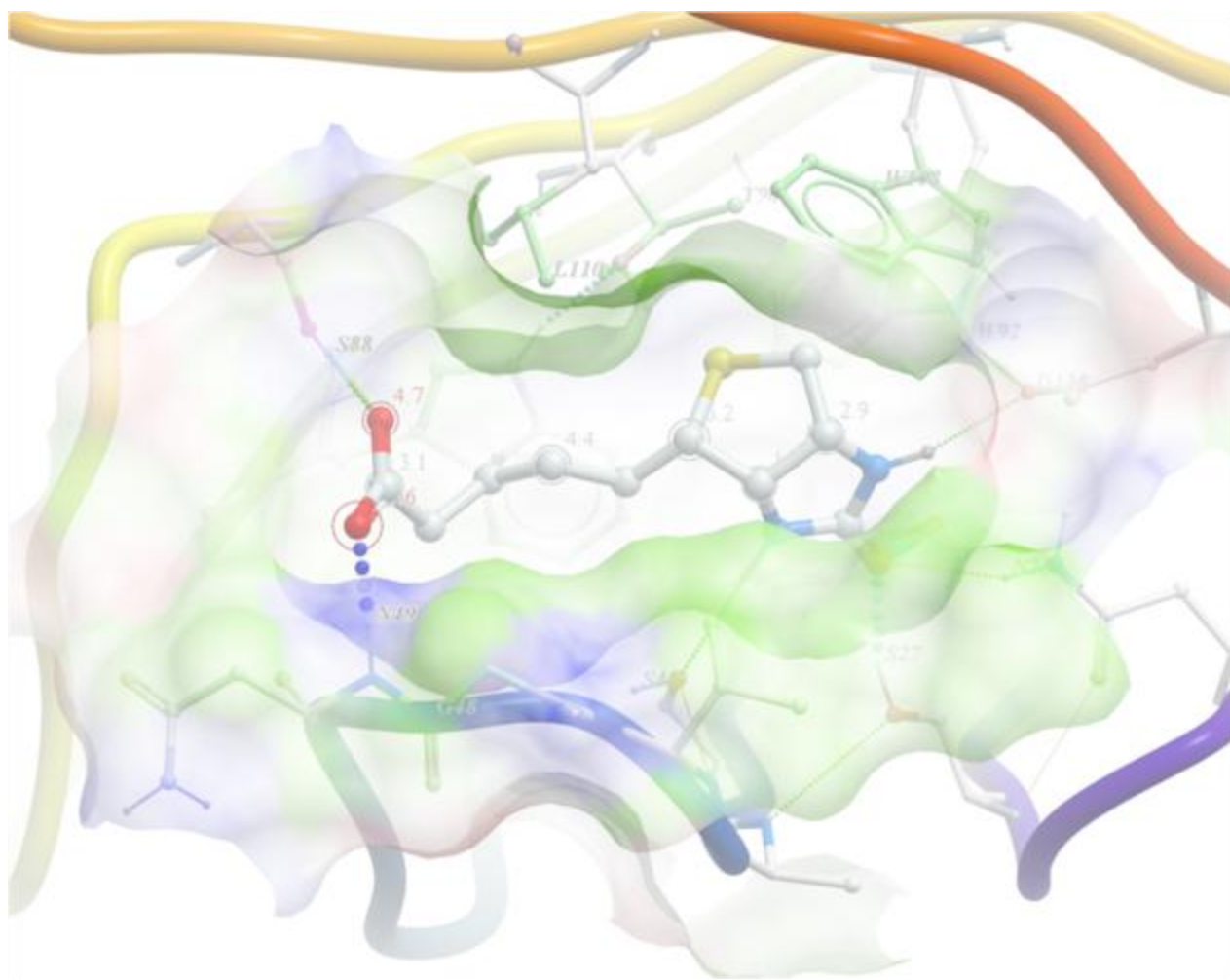
### 5.1.10 Hydrogen Bonding

**NOTE:** The method by which hydrogen bonds are calculated is described [here](#) in the command line manual. The GRAPHICS.hbondMinStrength parameter determines the hbond strength threshold for hbond display. The strength value is between 0. and 2. By changing 1. to 0.2 you will see more weak hydrogen bonds.

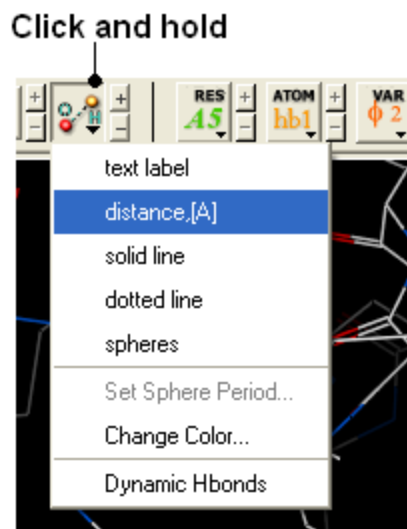
In order to display potential hydrogen bonds in your structure:

- Convert to an ICM Object
- Make a selection - if you are trying to display the H-bonds between a ligand and the receptor make sure the ligand is part of the selection.
- Click the Display Tab.
- Click on the **Toggle H-bonds** icon in the **display** tab.





- Click the +/- on the right of the H-Bond button to change thickness of H-bond representation.
- Click and hold the button to change representation or use the **hbondpairs** option in the ICM Workspace.



### What do the default coloring of the H-bond represent?

Longer and shorter H-X distances in the hydrogen bond are color-coded, from red to blue, respectively.

**NOTE** Dynamic hydrogen bonds can be set by clicking and holding on the **H-bond toggle** button in the **Display** tab. Hydrogen bonds will then respond to any changes made to the ligand.

## 5.2 Coloring

To change the coloring of the molecules:

- Select the atoms, residues, molecules, or objects you wish to color in the graphical display or in the ICM Workspace.
- Then use the color options in the `Display` Tab.

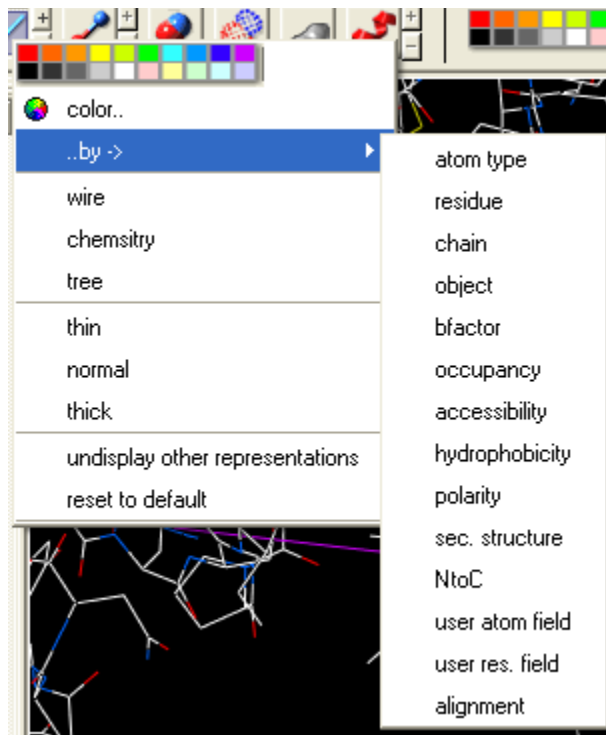
### 5.2.1 Coloring

*To change the color of a structural representation such as CPK, Xstick, wire or ribbon.*

- Click and hold on the structural representation buttons in the `Display` tab.
- Select a color by clicking color.

OR, if you wish to color by a particular parameter such as atom type, b-factor etc...

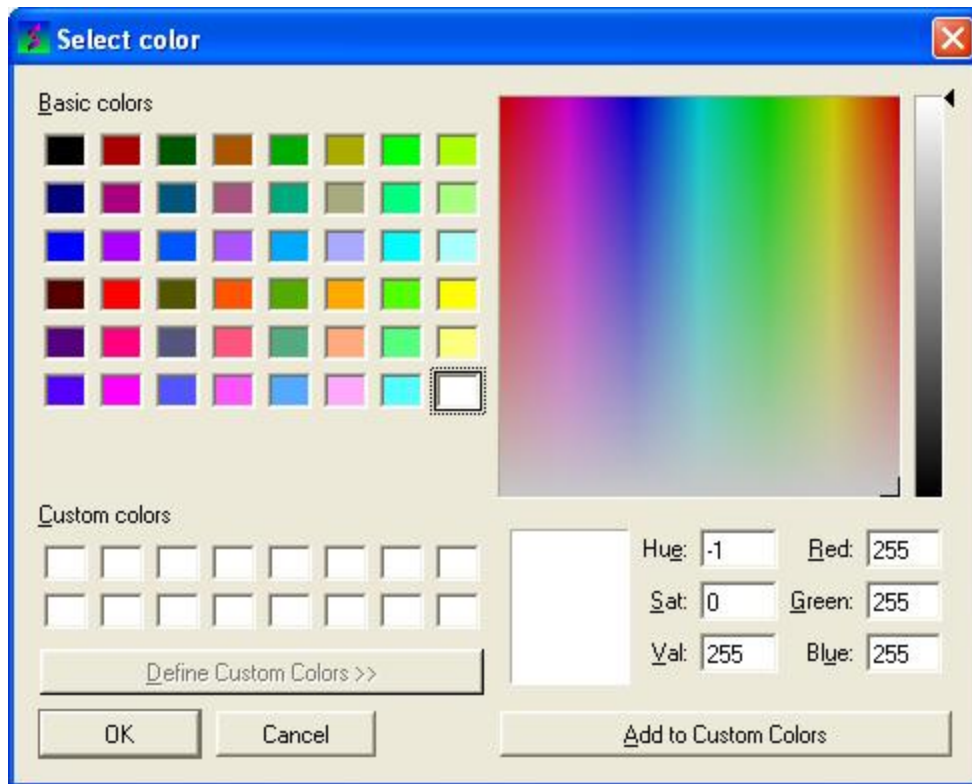
- Right click on the structural representation buttons in the Display tab.
- Select ..by-> option



*To change the color of the whole of your displayed structure:*



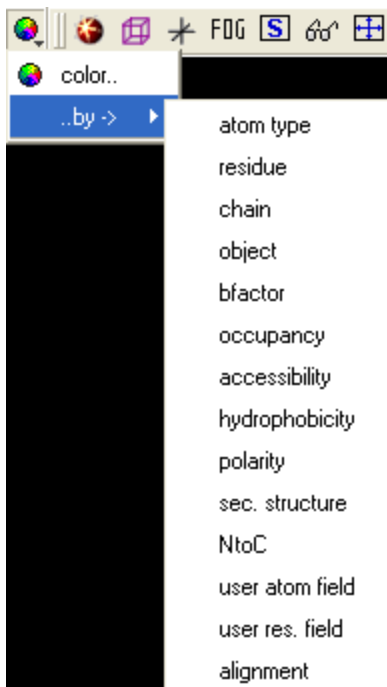
- Click on the color palate displayed on the toolbar.
- If you are not satisfied with these colors, click on the color wheel on the toolbar. A window as shown below will be displayed. Select the desired color by either clicking on one of the basic colors or by selecting the desired color on the right hand side of the window.



- Once the desired color has been selected it can be added to custom colors for future use by clicking on the Add to Custom Colors button.
- Click the **OK** button and the color will be applied to the structure.

*To change the color of the desired representation by a defined structural characteristic:*

- Click and hold on the **wire representation button** and then click **..by->**. A menu as shown below will be displayed.

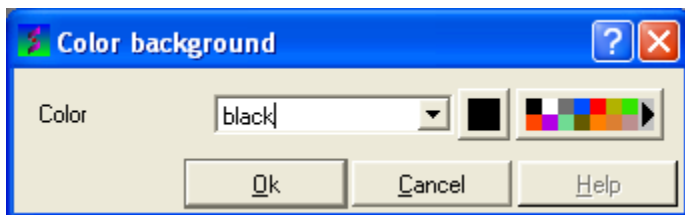


- Select the characteristic that you wish to color by and click on it.

### h3- Coloring Background {Color/BG}

*In order to change the color of your background:*

- Select **View/Color** background.



- Click on the square of your desired color. If you are not satisfied with the color palate, click on the arrow next to the colors to customize a color.

OR

- Right click on a color in the colors panel in the display tab.



Right click here in the display panel to set the background color.

## 5.2.2 Background Image

REQ\_352

A background image can be added to the graphical display. This can be useful for making cool images or for comparing structures (e.g. compare displayed object with background image of object).

*To add a background image from an image file (png or jpeg):*

- File/Open Image
- Right click on the image in the ICM Workspace and select "Set as Background in Graphics."

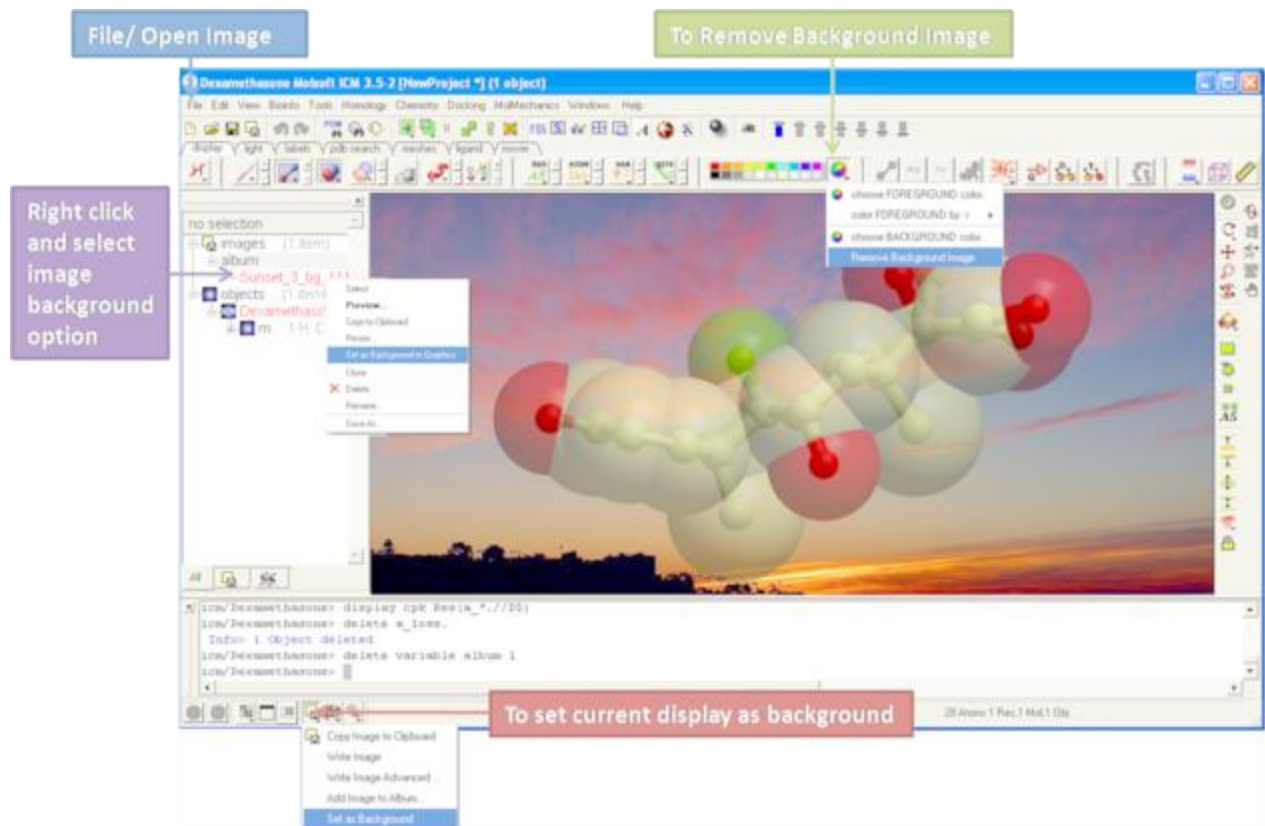
*To set currently display as background image:*

- Click and hold on the "Copy Image to Clipboard" button at the bottom of the gui and select the "Set as Background" option.

*To remove a background image:*

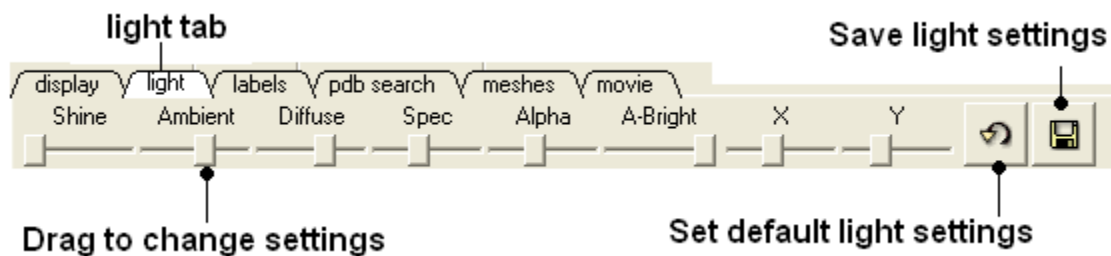
- Select the **display** tab and then click and hold on the color sphere button and select "Remove Background Image".





## 5.3 Lighting

These options are in the light-tab{light tab}



Click and drag the sliders to change the lighting. You can also save your preferred lighting settings and return to default.

**Shine** - shininess property of the solid material

**Ambient** - ambient light intensity of RGB for ambient light

**Diffuse** - diffuse light intensity of RGB for diffuse light

**Spec** - specular light intensity of RGB for specular light

**Alpha** - transparency setting for grob

**A-Bright** - light intensity shining on grob

**X and Y** - Change the position of the light source in the graphics window

## 5.4 Labeling and Annotation

To add labels or display or undisplay pre-defined annotation:

- Select the atoms, residues, molecules, or objects you wish to label in the graphical display or in the ICM Workspace.
- Then use the label options in the `Display Tab`.

To add new user-defined annotation:

- Select the atoms, residues, molecules, or objects you wish to label in the graphical display or in the ICM Workspace.
- Right click on the selection and choose "Annotate Selection".

### 5.4.1 Labeling

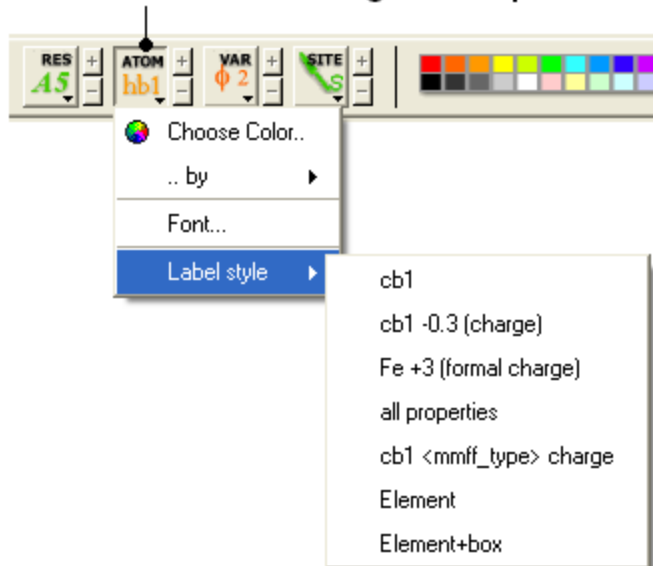
Labeling options are contained within the Labels or Display Tab. In many cases clicking and holding a label button will allow you to view more options.

### 5.4.2 Labeling Atoms

Select the atoms you wish to label (see `display structure` or `selection toolbar`).

- Select the **display** tab.
- Click the **label ATOM** button.

Click and hold to change label options



*To change the level of label detail:*

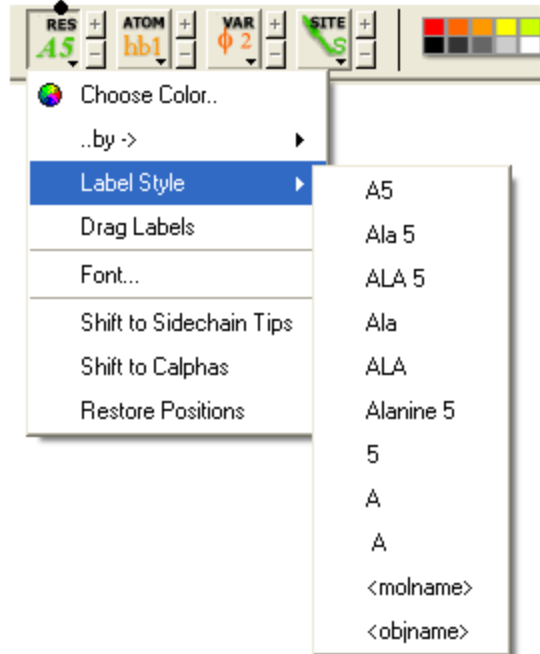
- Click and hold the **label ATOM** button and select the desired level of label detail, color or style.

### 5.4.3 Labeling Residues

*To label residues:*

- Select the **display** tab.
- Select the residues you wish to label (see `display structure` OR `selection toolbar`).
- Click the **label RES** button.

Click and hold for more options



*To change the level of label detail:*

- Click and hold the **label RES** button and select the desired level of label detail or style.

#### 5.4.4 Move Residue Label

*To change the location of your residue label:*

- Select View/Drag res labels.
- If your mouse has a middle mouse button, then click on handle (as shown) of the label you wish to move, and drag it to your desired area.

Click on  
this area  
to drag  
your  
label.



- If your mouse has no middle mouse button, then click on the Translation icon on the toolbar, and click on the handle (as shown) of the label you wish to move, and drag it to your desired area.

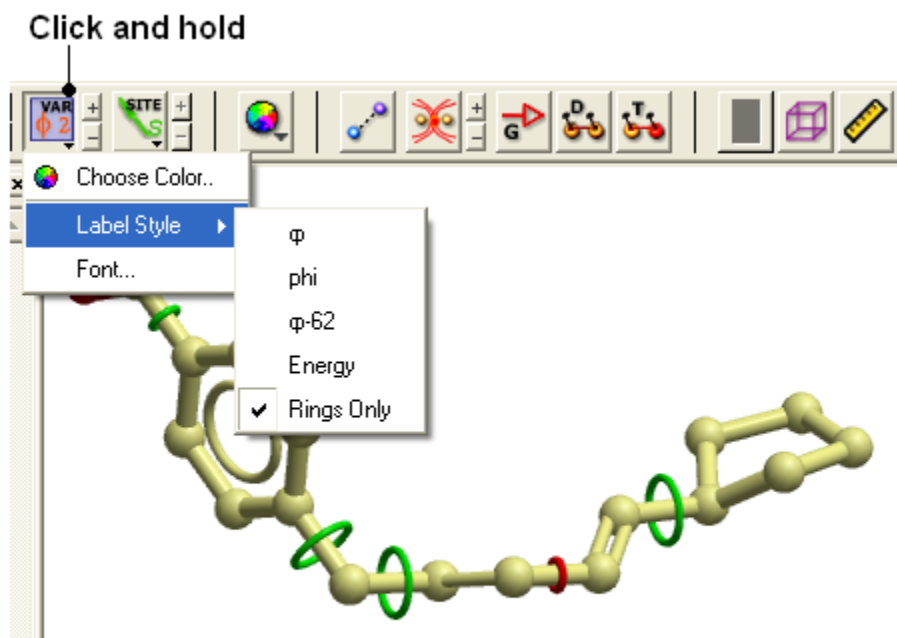
The +/- buttons on the side of the Residue and Atom buttons will shift the label. There are also other **residue label move** options available when you click and hold the residue label button. These options include **Shift to Sidechain Tips**, **Shift to Calphas**, and **Restore Positions**

## 5.4.5 Label Variables

*To label variable angles (dihedral-torsion, planar and phase angle) the molecule needs to be converted into an ICM object.*

- Convert the molecule to an ICM object.
- Select the atoms for which you would like to display the variables (see `display structure` or `selection toolbar`).
- Click on the **toggle variable label** button shown above located in the **display** tab.
- Change the font size by using the +/- buttons.
- Change the font and color by clicking and holding on the variable atom label button.

To change the variable label style click and hold the variable atom label button as shown below.

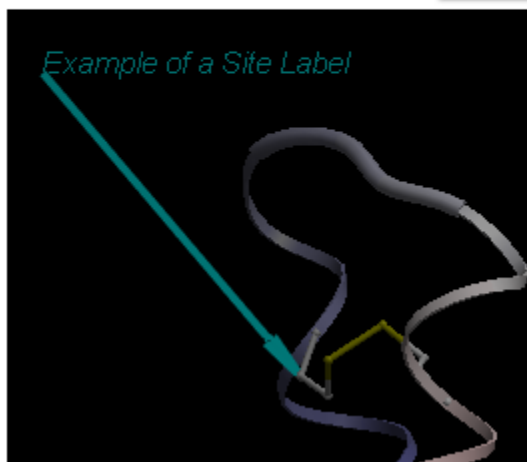
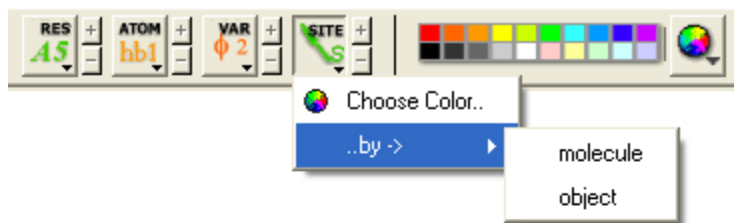


**Green rings = rotatable**  
**Red rings = constrained**

Rings of varying diameter and color are superimposed on rotatable bonds. Green rings with large diameter are considered less constrained than rings with small green rings. Red rings are highly constrained and non-rotatable. When the **Label Style/Energy** option is selected the first number displayed represents the bond angle, the second the energy and the third the worst energy that could be achieved by rotating the bond.

## 5.4.6 Labeling Sites

*To display and undisplay sites use the Toggle Site Label button shown below*



- Click the **label SITE** button.

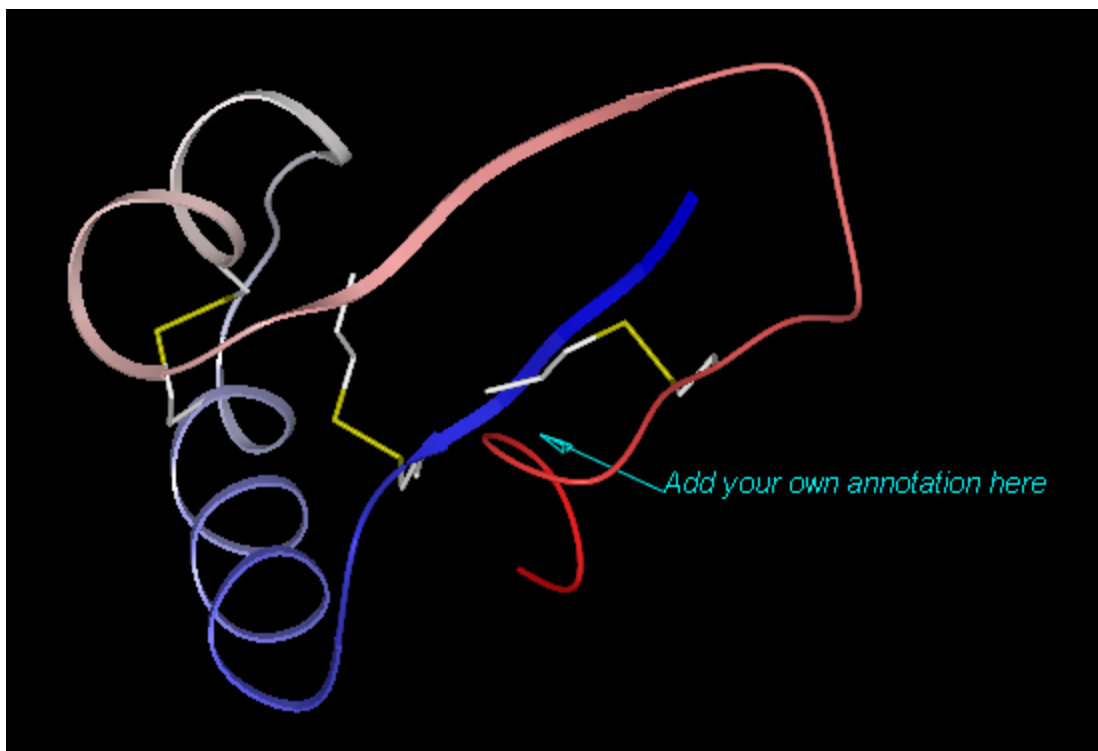
*To change the level of label detail:*

- Click and hold the **label SITE** button and select the desired level of label detail or style.

**NOTE:** To create your own site labels see the [Label Annotation](#) section.

## 5.4.7 Annotation

To annotate a protein structure. Select the region you wish to annotate (see [Selection Toolbar](#)).



- Right click on the selection.
- Select the option **Annotate Selection**.
- Enter the annotation into the text box and select ok

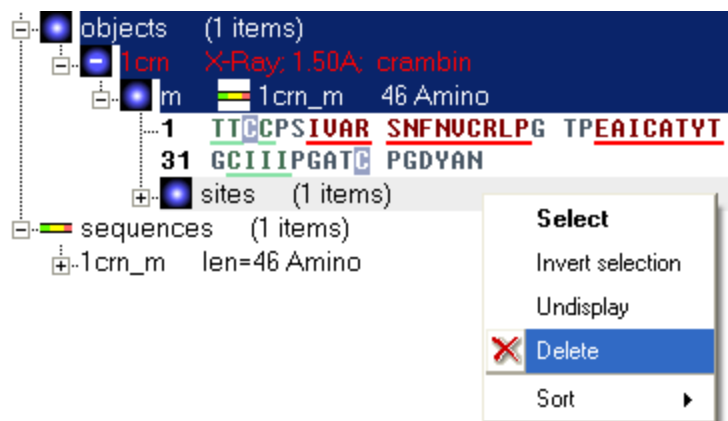
To change the detail (such as residue number) contained within the annotation.

- Click in the bottom left hand corner of your annotation.

To undisplay an annotation click on the site button in the Display tab.

To permanently delete an annotation.

- Right click on the Sites box in the ICM Workspace and select delete (see below).



To change the direction the arrow is pointing or move the arrow.

- Click on the translation button (or use the middle mouse button).
- Click on the end of the arrow and drag to the desired position.

## 5.4.8 Changing Label Colors

*To change the color of any label:*

- Click and hold down the required label button and a menu as shown below will be displayed.



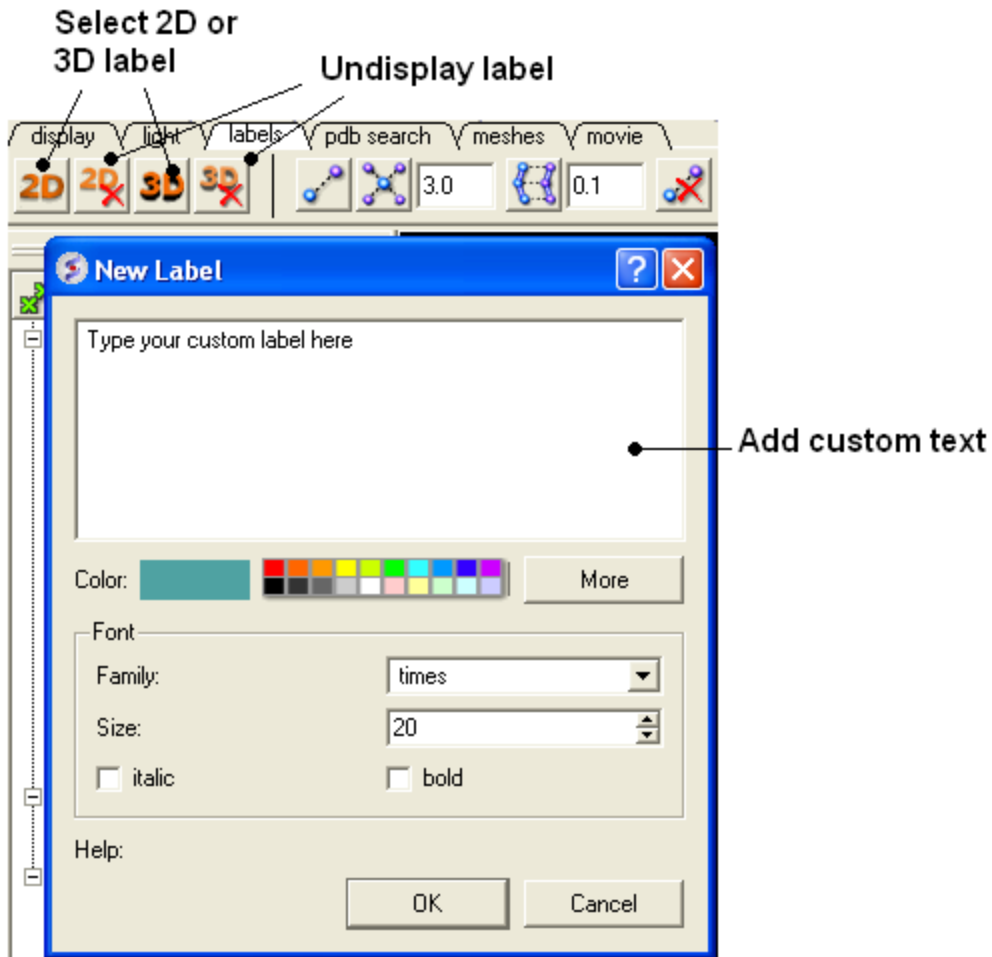
- Select **color**.

## 5.4.9 Customized Label 2D or 3D

To generate a customized a label:

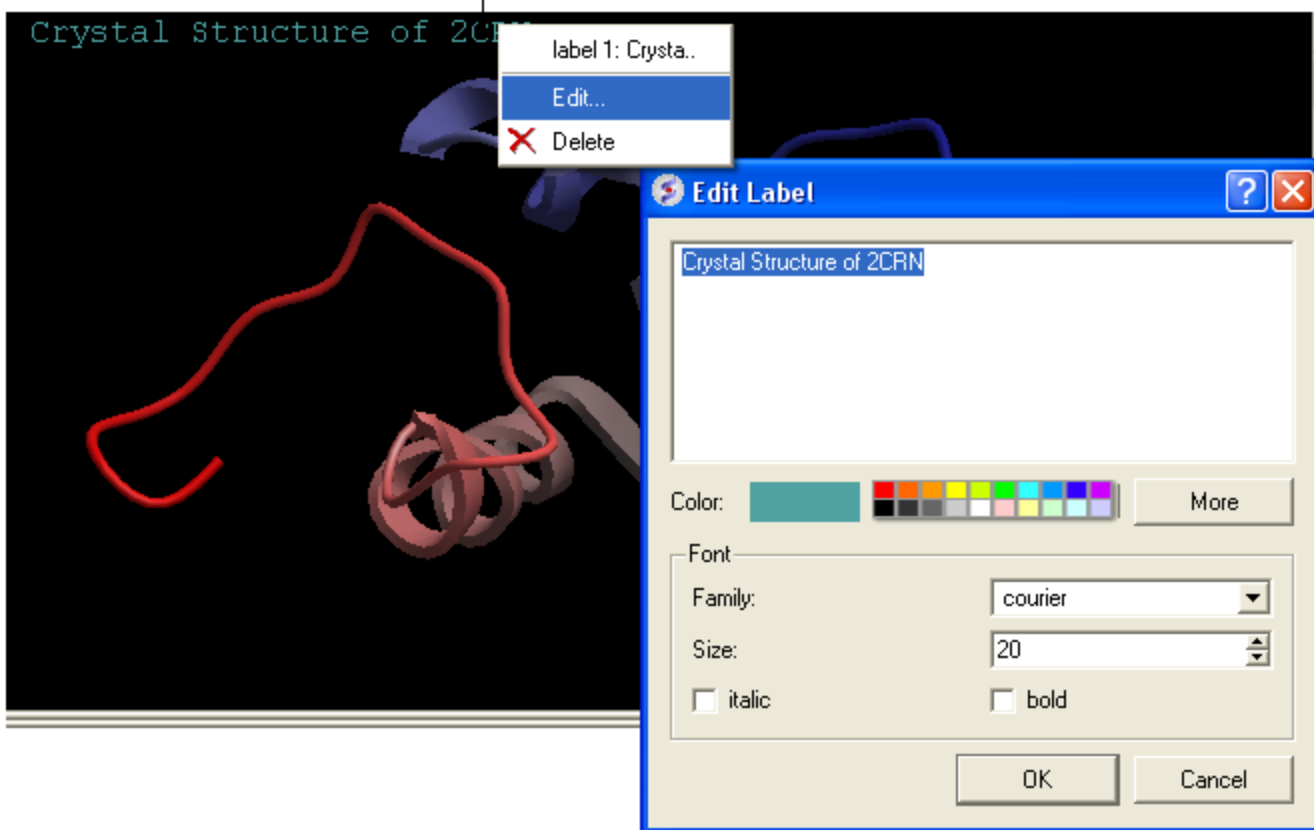
- Select the **labels** tab.
- Select either 2D or 3D button.
- Enter your label and select the desired color, font and size.





To **edit** or **delete** a label - right click on the label in the graphical display as shown below.

Right click here to Edit or Delete label



#### 5.4.10 Undisplay Customized Label

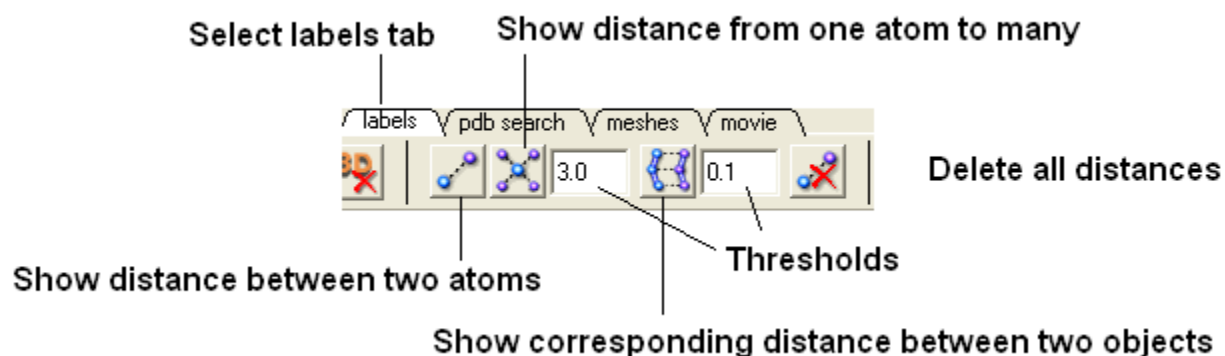
**Undisplay Residue, Atom, and Variable Label** Any label that is displayed can be undisplayed by selecting the region of the molecule related to the label and clicking on the corresponding label button in the labels tab. For example if you wish to undisplay an atom label - click the atom label button. If a label is displayed the corresponding button in the **display** tab will be shaded blue. When you delete the button will return to grey. 2D and 3D labels have an undisplay button (red cross on the button see `customized label` section).

**Undisplay 2D or 3D label** Click on the undisplay label button in **labels** tab.

**NOTE:** A label can also be deleted by right clicking on the label in the graphical display and selecting **delete**.

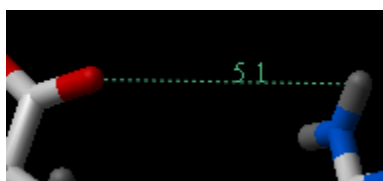
#### 5.4.11 Labeling Distances

Within the **labels** tab there are tools for calculating and displaying distances. These tools can also be found in the Tools/Analysis menu.



*To display distance between two atoms:*

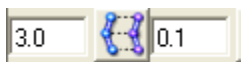
- Click on the labels tab (previously called advanced tab).
- Select the atoms between which you would like to find the distance. (See *selection toolbar*)
- Click on the 'Show Distances Between Two Atoms' Button
- The distance will be displayed in angstroms, in green.



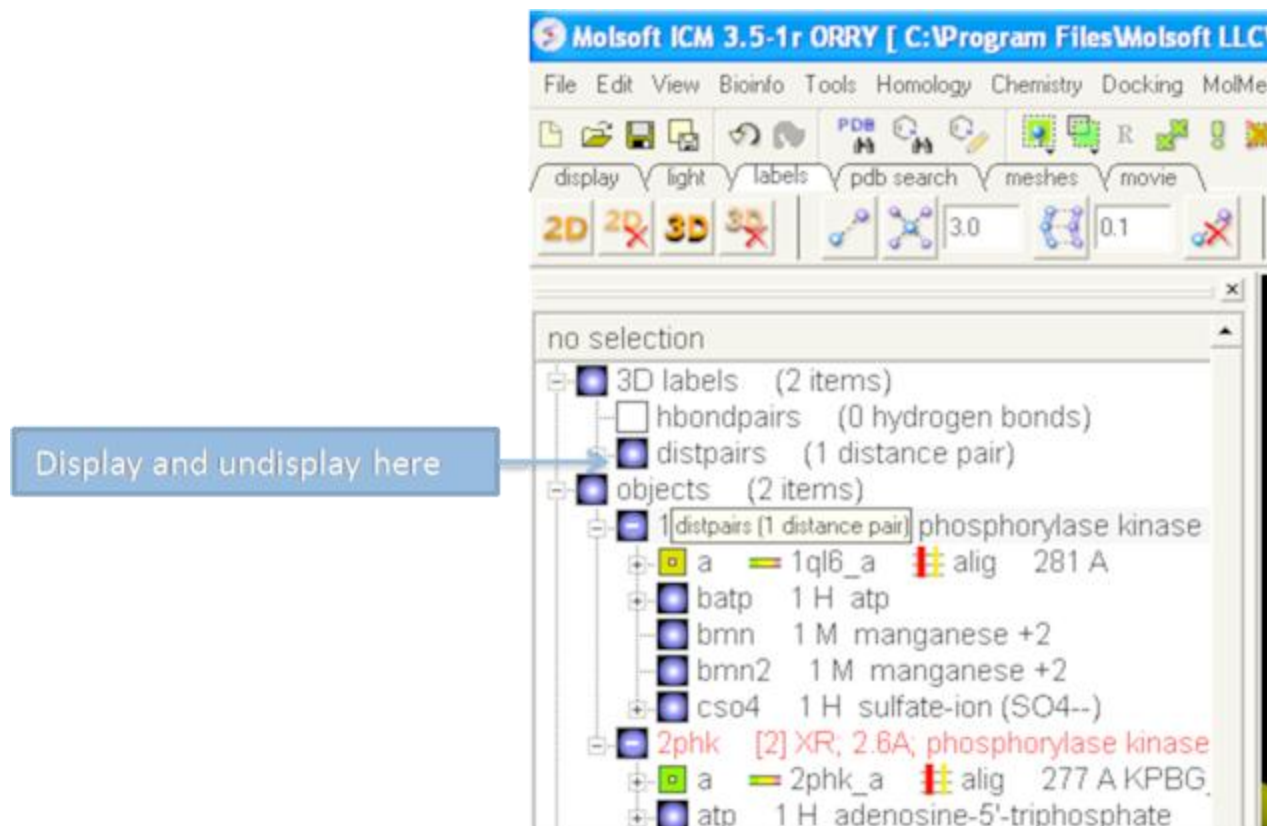
*To find the distance from one atom to many:*

- Click on the labels tab (previously called advanced tab).
- Select the atom from which you wish to measure the distance from (See *selection toolbar*)
- Click on the 'Show Distances From One Atom To Many' button.
- The distances will be displayed in green.

The maximal and minimal distances can be selected by entering values in the boxes shown here (below) in the labels tab (previously called Advanced tab).



**NOTE:** Distances can be displayed and undisplayed in the 3D labels section of the ICM Workspace. See image below.



***To change the color of the distance label***

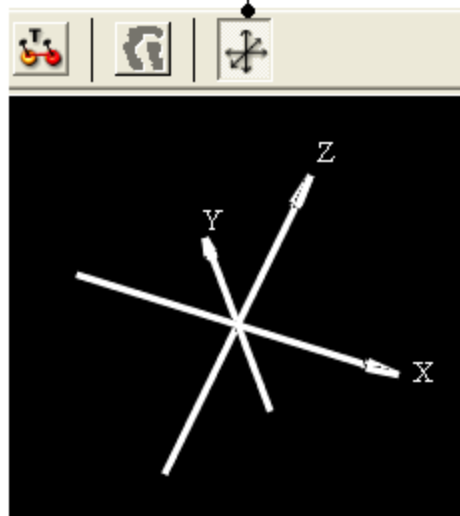
- Right click on the **distpairs** under the **3D labels** section of the ICM workspace and select **Change Color**.

**5.4.12 (Un)display Origin**

***To display and undisplay the axis of the coordinate frame (origin):***

- Select the **labels** tab and select the **toggle origin** button.

Display or undisplay origin button - located in the labels tab



### 5.4.13 Displaying Tethers

#### *Theory*

A tether is a harmonic restraint pulling an atom in the current object to a static point in space. This point is represented by an atom in another object. Typically, it is used to relate the geometry of an ICM molecular object with that of, say, an X-ray structure whose geometry is considered as a target. Tethers can be imposed between atoms of an ICM-object and atoms belonging to another object, which is static and may be a non-ICM-object. You cannot create tethers in ICM-Browser, however, if the project that you have loaded contains tethers between two objects, then they can be displayed:

- Click on the **display tab** (previously called advanced tab).
- Click on the 'Toggle Tethers' button.

### 5.4.14 Displaying Distance Restraints

#### *Theory*

A distance restraint imposes a penalty function on the distance between two atoms in the same object. You cannot create distance restraints in ICM-Browser, however, if the project that you have loaded contains distance restraints, then they can be displayed:

- Click on the **display tab** (previously called advanced tab).

- Click on the 'Toggle distance restraints' button.

### 5.4.15 Display Clash

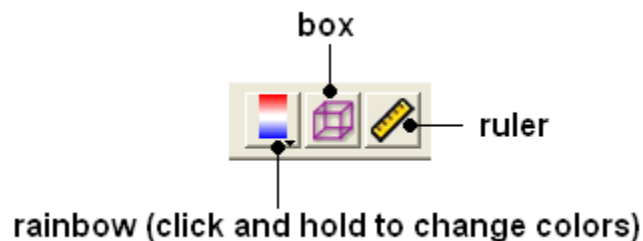
To display a clash the file needs to be an ICM Object.

- Select the region around which you would like to identify clashes.
- Select the display tabs and the "toggle clashes" button shown below.



### 5.4.16 Display Rainbow, Box, Ruler

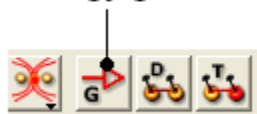
To (un)display a rainbow key, box or ruler use the buttons shown below located in the **display** tab.



### 5.4.17 Display Gradient

This button is located in the **display** tab.

Toggle energy gradient button

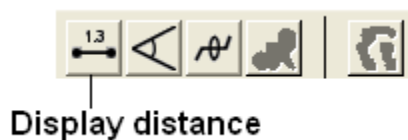


This option is described in detail in the language manual <http://www.molsoft.com/man/icm-commands.html#display-gradient>

## 5.5 Display Distances and Angles

### 5.5.1 Display Distance Between Two Atoms - the quick way

- Click on the **Display** tab
- Click on the **Distance between two atoms** button shown below.
- Click on the atoms you wish to measure.
- Distance will be displayed in the graphical display. You can turn this on and off in the ICM Workspace panel under the heading **3D labels**.



### 5.5.2 Display Planar Angle

- Select the **display** tab.
- Select three atoms.
- Select the button shown below.

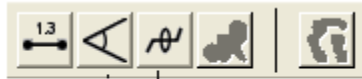


**NOTE:** This option is also available in the Tools/Analysis menu.

### 5.5.3 Display Dihedral Angle

- Select the **display** tab.
- Select four atoms.

- Select the button shown below.



Dihedral angle

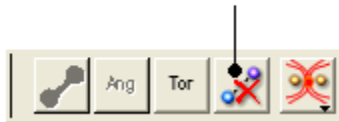
**NOTE:** This option is also available in the Tools/Analysis menu.

### 5.5.4 Delete Label

To delete distance or angle labels

- Select the **display** tab.
- Select the delete distance or angle label button shown below.

Delete distance or angle labels button in display tab



## 5.6 Graphics Effects

All the visual effects tools can be accessed by the View Menu or click on the corresponding button in the View Tools panel shown below.



### 5.6.1 Fog

**Fog Toggle**(Ctrl + D) : this feature creates a fog-like environment for your object, so that the part of your structure that is closer appears clear and the distant parts are faded as if they are in fog. The clipping planes control the point at which the fog begins.

- View/Fog



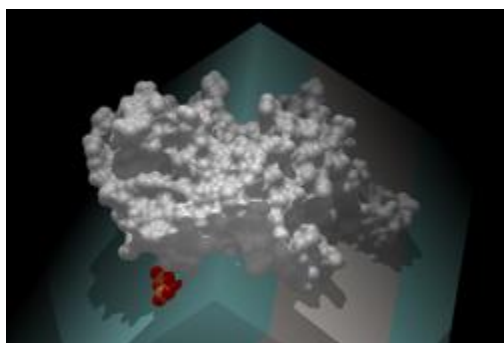
## 5.6.2 Shadows

- View/Shadows

OR

select the shadow button shown below.

Toggle shadow



## 5.6.3 Sketch Accents

*To make images as shown below use:*

- View/Sketch Accents

## 5.6.4 Elegant Ribbon & Ligand Sketch

- Display Tab
- Click and hold Hydrogen button
- Select Elegant Ribbon+Sketch



### 5.6.5 Perspective

**Toggle perspective Ctrl\_P** this will add perspective to your structure, enhancing depth in the graphical display.

- View/Perspective

### 5.6.6 Animate View

This tool is described in more detail in the [Molecular Animations and Transitions](#) section.

## 5.7 Graphics Shortcuts

The left mouse button can be mapped onto different graphics tools which can be selected from the right hand tool bar.

**Note: (1) You can access many non-rotation modes directly from the rotation mode by using Middle and Right-mouse buttons, as well as by using the right, top and left margins of the graphics window. (2) You can access the rotation mode from non-rotation modes by pressing Ctrl.**

- rotation ( **the default** , press Ctrl if you in the non-rotation modes )
- translation ( the middle mouse button in the rotation mode)
- zooming in and out by dragging the mouse up and down (the left margin in the rotation mode, or use the mouse **wheel**)
- Z-rotation ( the top margin in the rotation mode)
- selecting by box ( the right mouse click in the rotation mode )
- selecting by lasso ( Ctrl-draw lasso in the rotation mode )

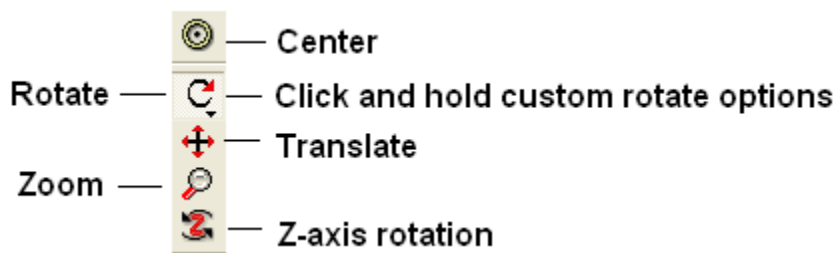
- picking out atoms ( a toggle )
- picking out and labeling residues (a toggle)
- moving the front clipping plane ( the top section of the right margin in the rotation mode)
- moving the rear clipping plane ( the bottom section of the right margin in the rotation mode)
- moving the slab ( the middle section of right margin in the rotation mode)
- unclipping ( Ctrl-U )
- rotating torsions (Ctrl-left-mouse-click in the rotation mode)
- connect and unconnect separate molecules to movement controls

Many useful graphics tips are summarized [here](#).

**NOTE:** Key mouse controls are summarized in the command line manual [here](http://www.molsoft.com/man/graphics-controls.html)

## 5.8 Molecule Move Buttons

To move your structure it must first be displayed in the graphics window (for instructions on how to display a structure see the `Display` Tab). All of the following options are displayed in the Move Tools toolbar (shown below).



### 5.8.1 Rotation

*In order to achieve the best pose for a picture or to enable the study of a certain region of your structure in more detail you may need to rotate the structure:*

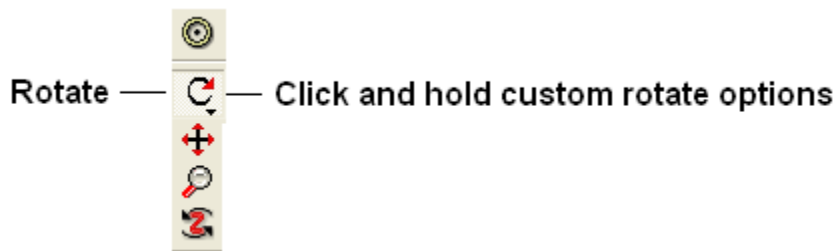
- Click on the **rotation** icon on the toolbar.



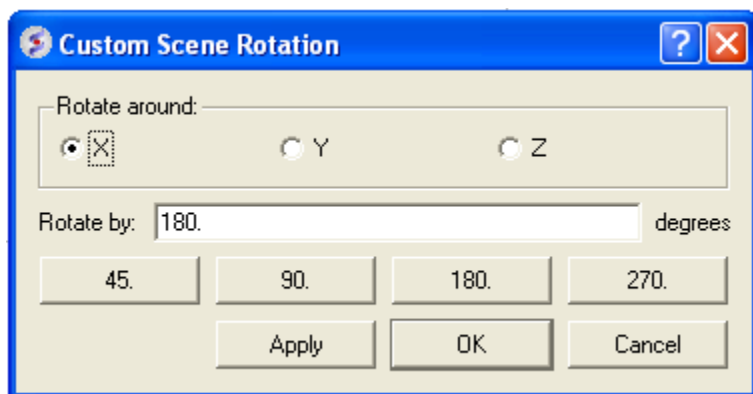
- Click and drag on your structure in the display window until it is in the desired position.

## 5.8.2 Custom Rotation

An option is provided to customize the rotation of the molecule. This allows exact rotation by a specified number of degrees.



- Click and hold down the rotation button and a data entry box as shown below will be displayed.
- Enter the number of degrees of rotation you require and in which X, Y or Z coordinate.



*To continuously rotate the picture:*

- Click on the **continuous rotation** icon on the toolbar.
- Click, hold, and slightly move your mouse anywhere on the graphical display window. The point at which you hold your mouse, is the direction to which the object will turn.
- Positioning the mouse towards the center of the display will move the object slower than if the mouse is positioned towards the edge of the graphical display.

In order to rotate your picture around the Z-axis:

- Click on the **Z-axis rotation** icon on the toolbar.

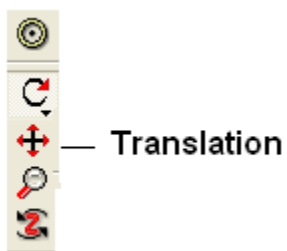


- Click and drag your object around the Z-axis until it is in the desired position.

### 5.8.3 Translation

To translate your structure up, down, left, or right:

- Click on the **translation** icon on the toolbar.



- Click and drag on your structure in the display window until it is in the desired position.

When you are displaying more than one object and you wish to translate one object in relation to the other on the Z-axis:

- Right click on the name of the object you wish to move in the ICM workspace and select connect to object. This object is now independent from the other object and can now be manipulated separately.
- Click on the **Z translate** icon on the toolbar.
- Click and drag your structure along the Z-axis, moving it closer or further from your unconnected structure.
- Once you are finished, right click on the name of the object which is connected, and click on disconnect.

### 5.8.4 Zoom

*To zoom in or out of your structure:*

- Click on the **zoom** icon on the toolbar.



- Click and drag your mouse up to zoom in and down to zoom out.

You can also zoom in and out directly with the right-mouse-button *without* explicitly switching to the zoom tool, if you use the **left 5%-margin** of the graphics window.

### 5.8.5 Center

*To restore your picture to the center of the graphical display window or to center on a selection:*

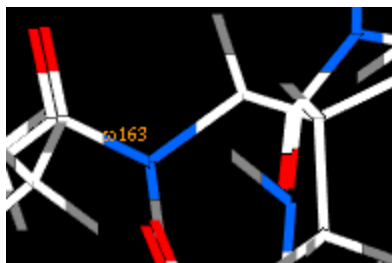
- Make a `selection` of the region you wish to zoom into - if no selection is made the whole structure will be centered.
- Click on the **center** icon on the toolbar.



### 5.8.6 Torsion Angles

*To alter the torsion angle of certain residues of your structure:*

- Convert your pdb structure into an ICM object.
- Click on the **change torsion angles** icon on the toolbar (see button key above).
- Click and drag on the atom around which you wish to rotate a residue. The changing angle will be displayed in orange.



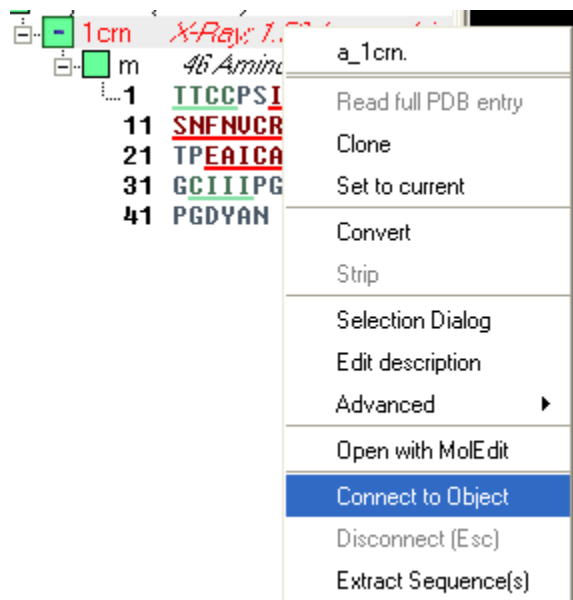
**NOTE:** This option can be used more effectively in conjunction with the `variable label` option.

### 5.8.7 Connect (Move)

When there is more than one object displayed in the graphical display window the objects are connected to one another. If you wish to move or manipulate one object independently from the others you need to **connect** to it

*To do this from the ICM Workspace:*

- Right click on the name of the object you wish to move in the ICM workspace and select **Connect to Object**. The object will now be colored yellow.

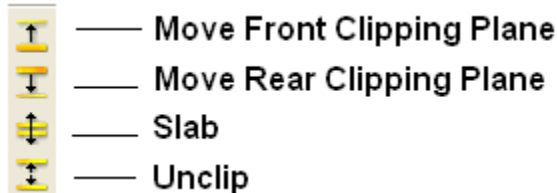


- The object is now controlled separately from the rest of your objects by your mouse.
- Disconnect your object by once again right clicking on the name of the object in the ICM Workspace and selecting disconnect in the drop down menu or **Press the ESCAPE key**.

**Note: you can temporarily switch to the global rotation in the connected state if you press Shift**

**Note: use the Escape button to disconnect**

## 5.9 Clipping Tools



The clipping tools allow you to adjust the frames of the ICM window, changing the clipping planes.

Clipping planes can also be moved *without* switching to the clipping tool, if you click the right hand margin of the graphics window:

- The top section of the right 5% margin of the graphics window: moves the back clipping plane
- The middle section of the right 5% margin of the graphics window: moves the slab (both clipping planes)
- The bottom section of the right 5% margin of the graphics window: moves the front clipping plane

In order to move the front or rear clipping planes of your screen:

- Click on the **Move front clipping plane** or **Move rear clipping plane** icons on the toolbar.
- Click and drag the respective plane frontward or backward, depending on how you wish to clip it.

You can also move the **slab** of viewing window, keeping the distance between the front and back clipping planes. In order to adjust the area of the structure where your viewing window is located:

- Click on the **Slab** icon on the toolbar.
- Click and drag the slab frontward or backward, depending on the desired area of the structure you wish to see.

If you have made changes to the clipping planes which you do not wish to keep or you wish to automatically fit your entire structure within the clipping planes:

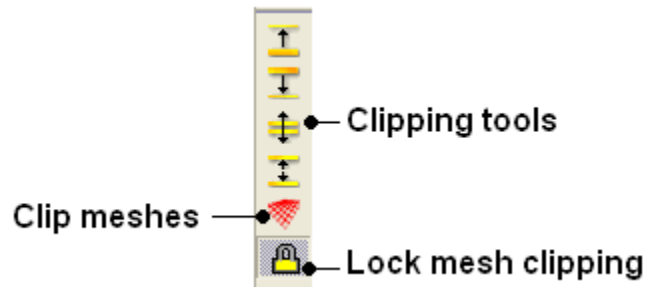


- Click on the **Unclip** icon on the toolbar. This will automatically set the clipping planes to fit your object.

## 5.9.1 Mesh Clipping

Clipping tools can be used to adjust the frames of the mesh independently of other objects.

The buttons shown below can be used for this purpose.



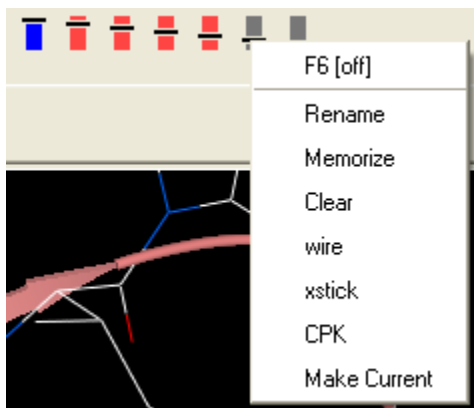
The buttons used for clipping are described in the section entitled `Clipping Tools`.

## 5.10 Graphic Layers

To display and undisplay layers of a structure you can use the buttons shown below. Seven layers can be created and within each layer different structural representations can be displayed.



Right click on one of the layer buttons and a number of options can be chosen as shown below.



To change the display in one of the layers:

- Right click on one of the layer buttons.
- Select a representation wire, xstick or CPK.
- You can do this for each of the seven layer buttons.
- Click on the layer button to display and undisplay. If the layer button is shaded red then the layer is not displayed. If the layer button is shaded light blue then it is displayed. You can switch between layers by clicking on the button or using the. You can use the **memorize** button to store a particular representation and **clear** to remove a memorized representation.

## 5.11 Make High Quality Publication Images

### 5.11.1 Write Image

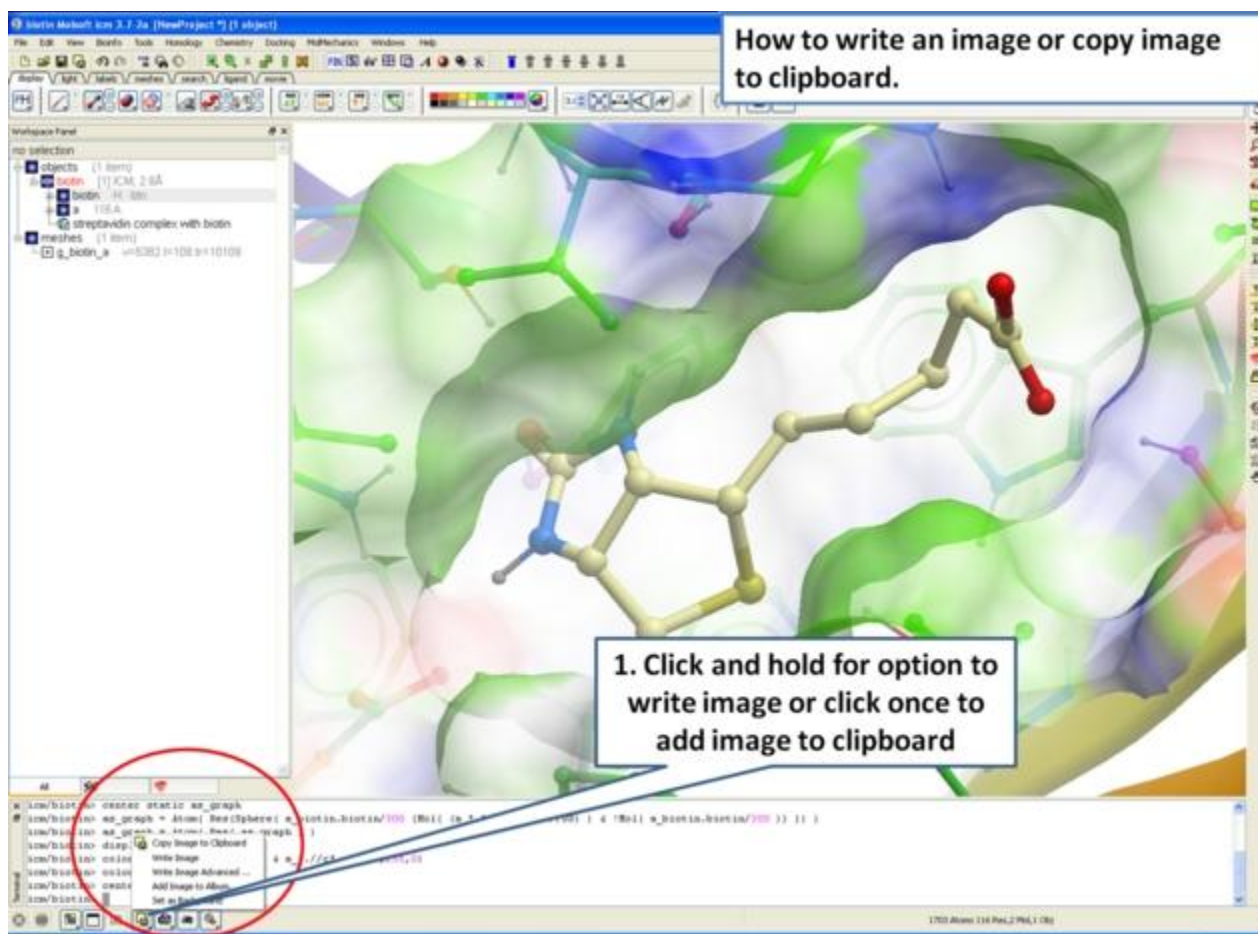
To make high quality publication images:

- File/Write Image

This is described in more detail [here](#).

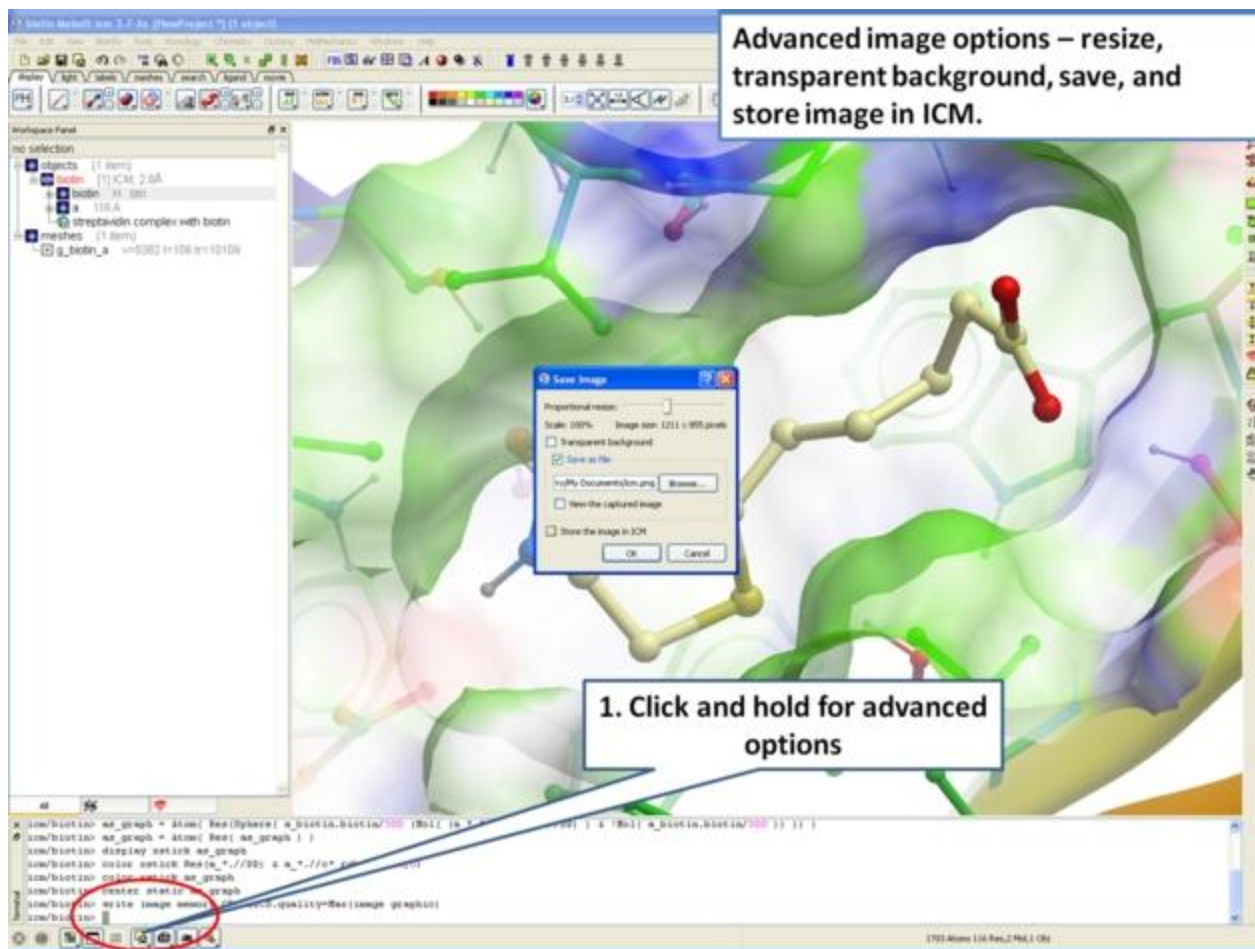
Or, use the button at the bottom of the graphical user interface (see images below).

### 5.11.2 How to Save an Image to the Clipboard



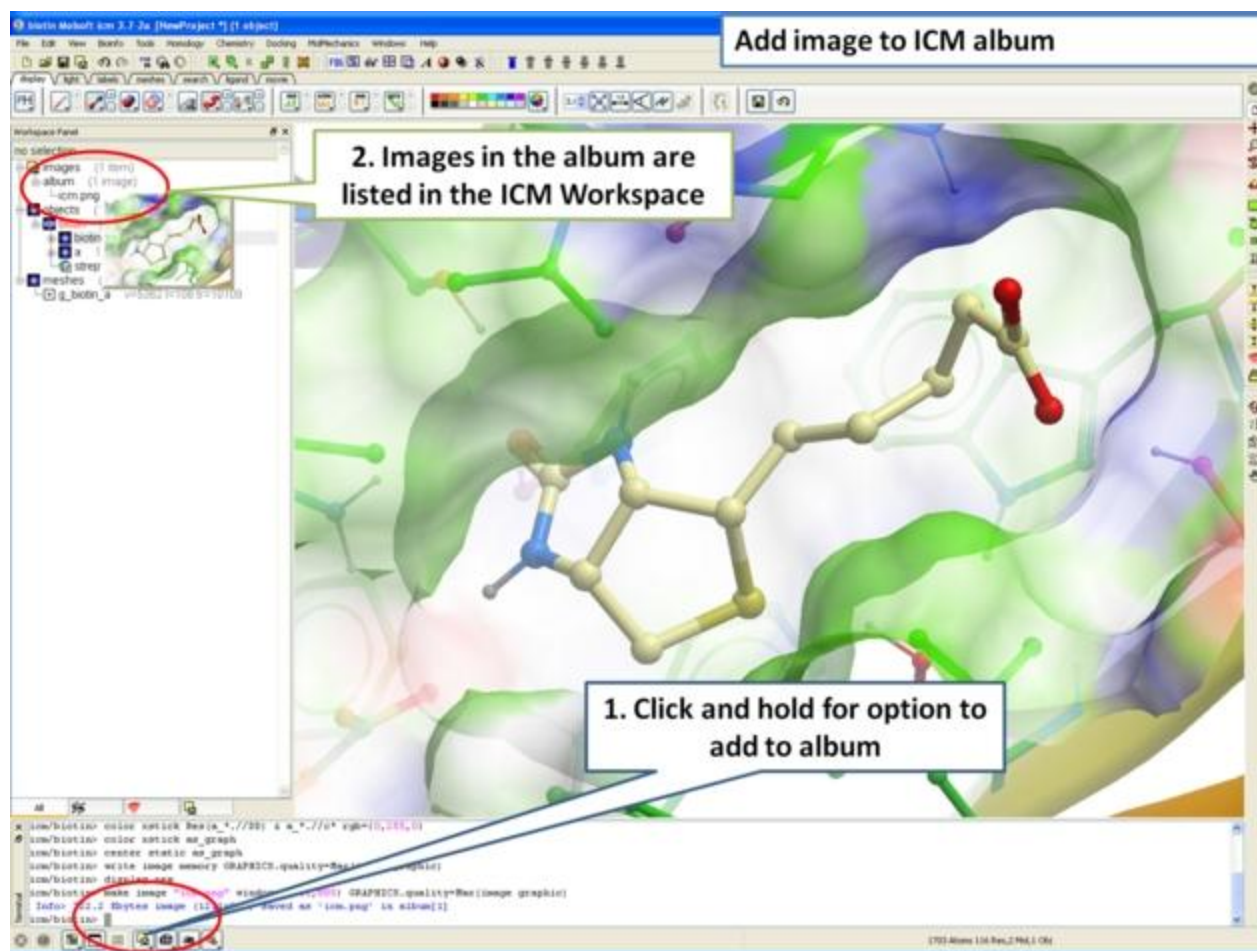
### 5.11.3 Advanced Image Options.

Click and hold the button shown below for options for resizing, transparent background, and storing an image in ICM.



### 5.11.4 Add Image to Album

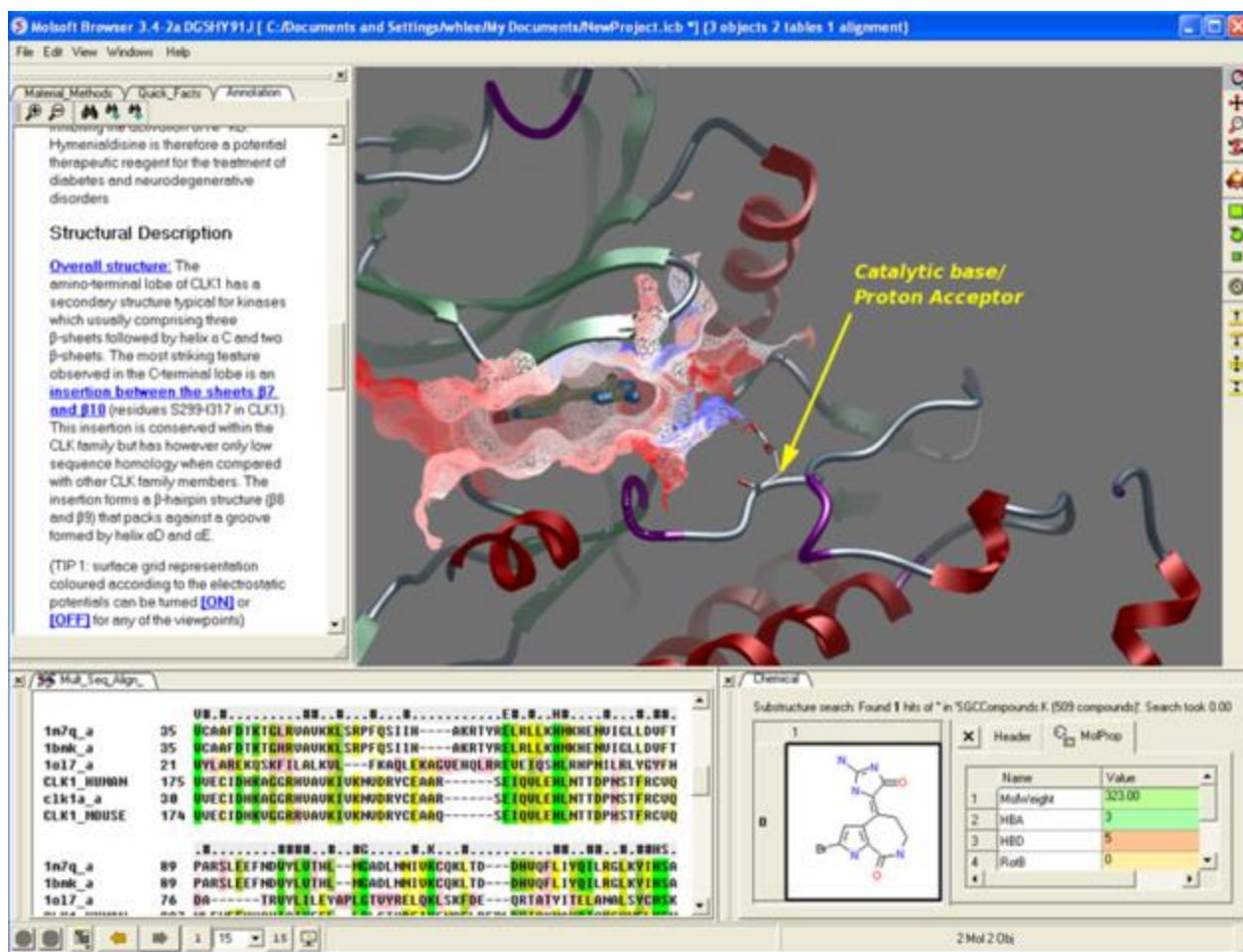
If you are making an ICM document you may want to store images inside ICM.



## 6 Molecular Animations, Slides, and Documents

**Note:** Click **Next** (top right hand corner) to navigate through this chapter or use the links below. Headings are listed on the left hand side (web version) or by clicking the **Contents** button on the left-hand-side of the help window in the graphical user interface.

Here you will find a description of the tools to produce and exchange interactive three-dimensional (3D) and two-dimensional (2D) information consisting of multiple interactive views and animations of molecular structures and objects in conjunction with related hyperlinked text, chemical, biological sequence, alignment and data views. These tools enable the user to produce small, easily transferable and quickly downloadable files. The files can be used for Molecular Presentations and Documents.



Highlights of these tools include:

- Construct molecular animations - including rock, rotation, and transition from one point to another.
- Fully-interruptable animations and transitions allow the user to stop an animation and alter the display. For example, stop and zoom into a particular region of a protein structure.
- Link hypertext to action.
- Construct fully-interactive molecular documents linking text and the graphical display.
- Build molecular slides incorporating static representations, animations and annotations.

For examples of ICM Molecular Documents please see the structures solved by the Structural Genomics Consortium in Oxford, UK <http://www.sgc.ox.ac.uk/>

*The following information can be stored in a slide.*

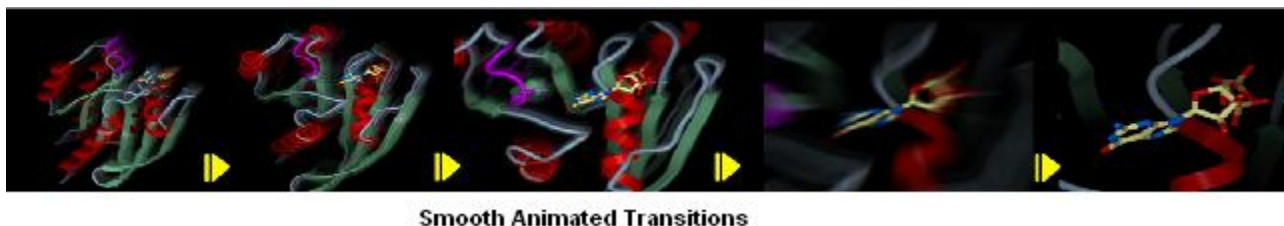
- Viewpoint
- Window layout
- Current table(s)

- Alignments
- Annotations, labels, user-defined
- HTML
- Preferences for GRAPHICS.quality, ruler style, rocking state information
- For each (mol.) object: representations and their colors, sites
- For each grob (mesh): representation and colors.

---

## 6.1 Molecular Animations and Transitions

Learn how to build fully-interruptible and interactive animations.



### 6.1.1 Make Animation

To quickly produce an ICM Molecular Animation:

- Click and hold down the "Begin rocking/rotation" button shown in the picture below.
- Choose from the following options - X-Rock, Y-Rock, Xy-Rock, xY-Rock, X-Rotate, and Y-Rotate.

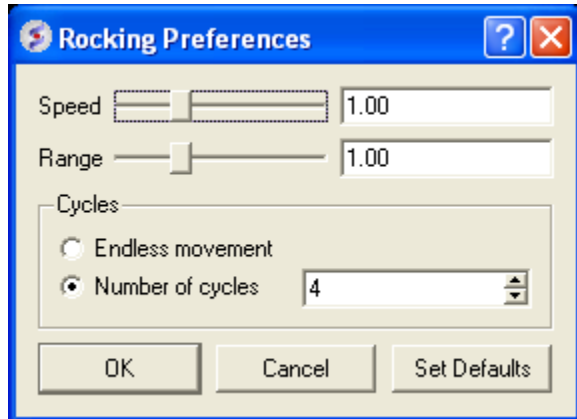


**NOTE:** Default rocking representation can be changed in the `File/Preferences/Gui` menu.

### 6.1.2 Change Speed, Range and Cycle Length of Animation

To change the speed, range and cycle length of the animation:

- Click and hold down the "Begin rocking/rotation" button shown in the picture above.
- Choose the set speed range option and change the speed and range using the drag bars. Any change will appear in the graphical display behind this box.
- If desired you can change the number of cycles of the animation. This is an ideal tool for screen-shot movie making.



**NOTE:** There is a return to default button in the Rocking Preferences dialog box shown above and default values can be changed in `File/Preferences/Gui`.

**NOTE:** Default rocking speed can be changed in the `File/Preferences/Gui` menu.

### 6.1.3 Interrupt Animation

An ICM Animation or Transition is fully interactive and is interrupted by a single click of the mouse.

To stop or change an animation or transition:

- Click the "Begin rocking/rotation" button shown in the picture below.

To temporarily halt an animation or transition:

- Click in the graphical display. Once you release the mouse button the animation will start again.

**NOTE:** If you click on the graphical display during an animation the animation will be



interrupted. Whilst clicking and holding the mouse button other operations can be performed such as zooming and selections.



Click in the graphical display window to temporarily interrupt an animation

### 6.1.4 Saving an Animation

An animation can be saved in an ICM project:

File/Save Project

Or

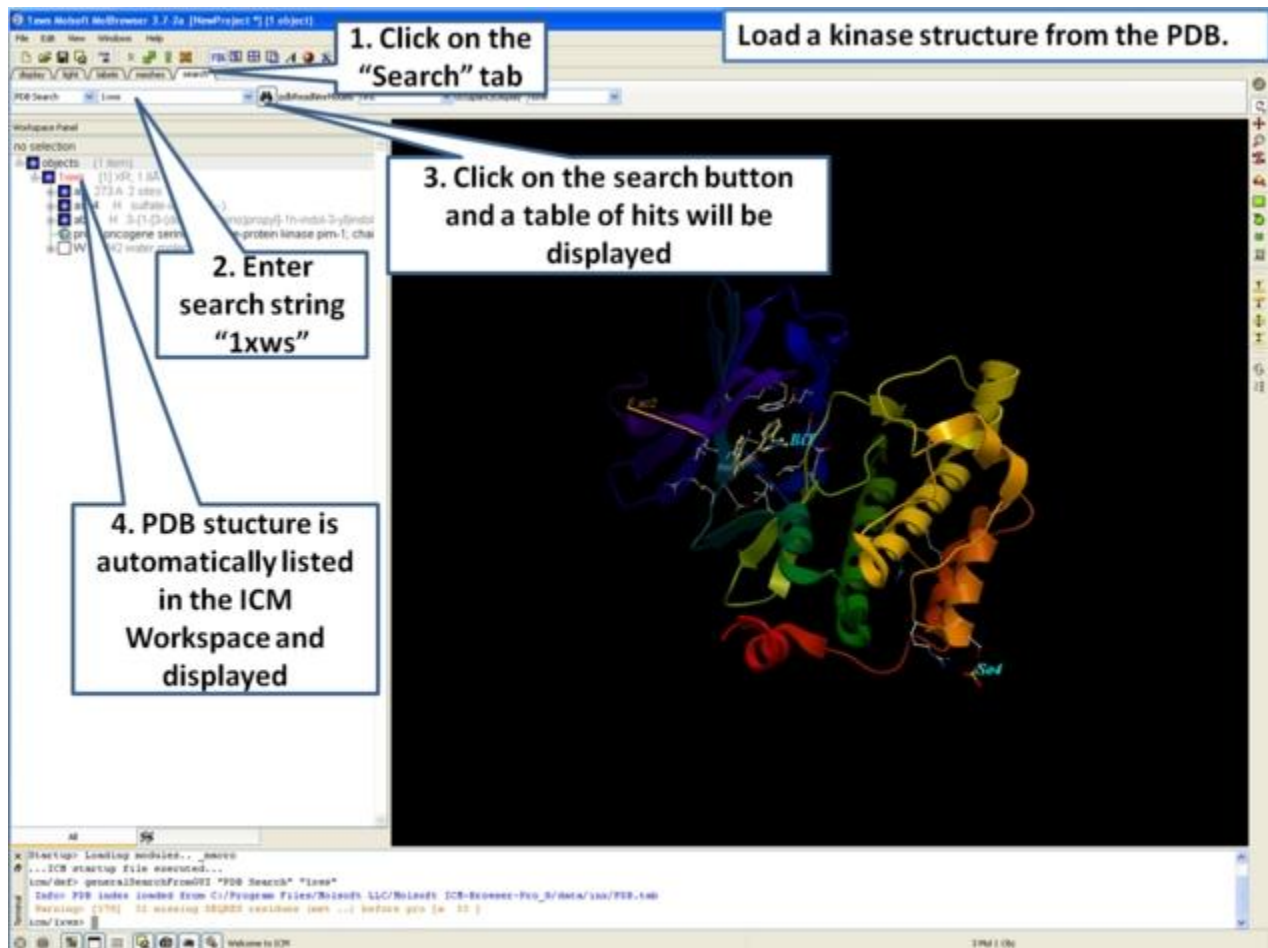
as a slide.

## 6.2 Making Molecular Slides

This tutorial takes you through the steps to create a series of fully interactive 3D slides. The slides can then be embedded into the web, or PowerPoint using ActiveICM or viewed in ICM-Browser (or ICM-Pro).

*To begin making ICM Molecular Slides:*

- First load the structure or structures you wish to display in your first slide. Additional structures, labels etc and text can be added at any point during the slide making process. In this example we will load the PDB file 1XWS a PIM1 kinase.



- Next, we will convert the PDB file to an ICM object so we can make slides of the ligand-receptor hydrogen bonds and binding pocket surface.

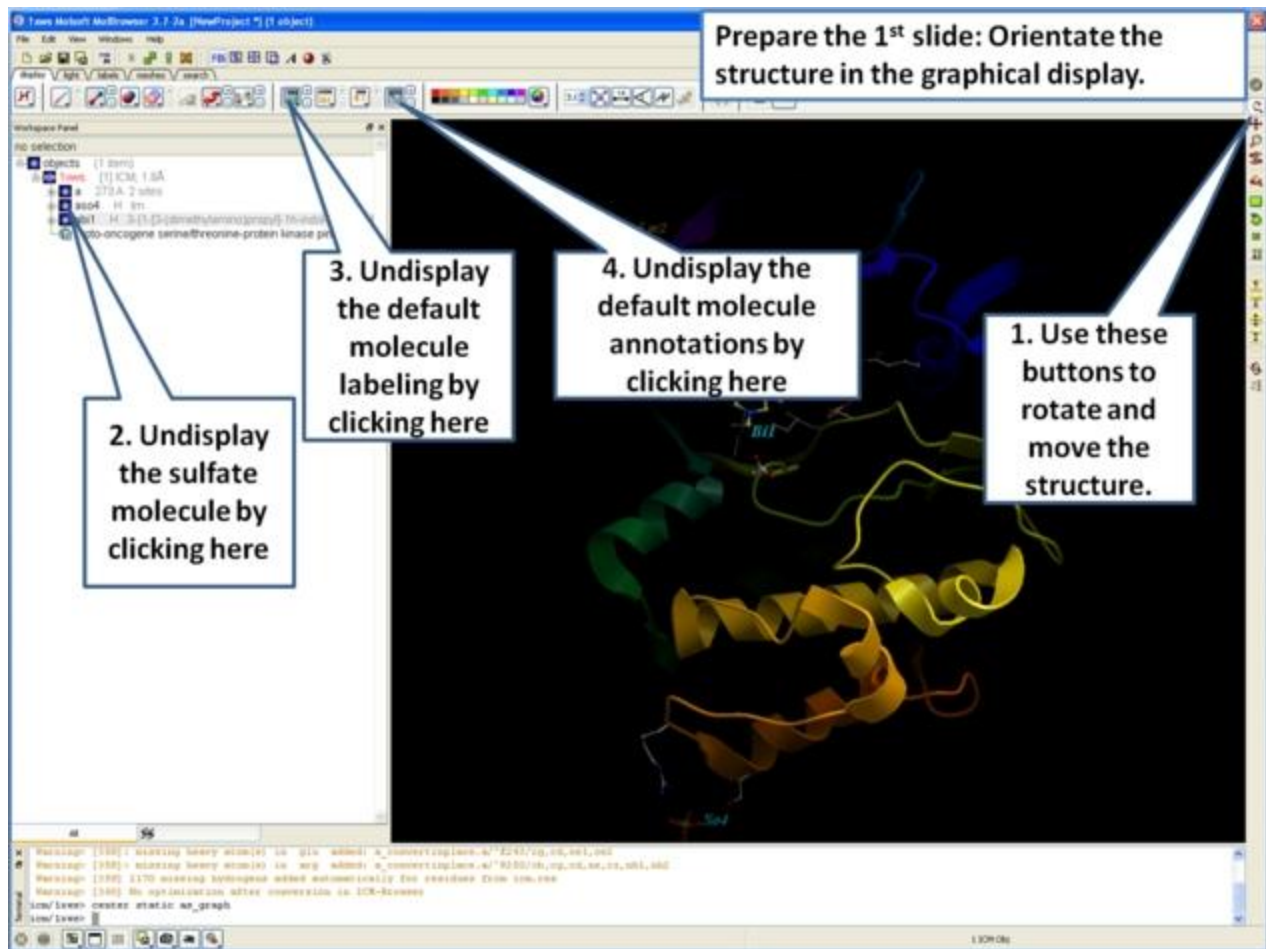
Convert the structure from PDB format into an ICM object.

The screenshot shows the ICM software interface. On the left, a tree view under 'no selection' lists objects: '1.000' (1.000), '273 A' (273 A), '273 B' (273 B), '273 C' (273 C), '273 D' (273 D), '273 E' (273 E), '273 F' (273 F), '273 G' (273 G), '273 H' (273 H), '273 I' (273 I), '273 J' (273 J), '273 K' (273 K), '273 L' (273 L), '273 M' (273 M), '273 N' (273 N), '273 O' (273 O), '273 P' (273 P), '273 Q' (273 Q), '273 R' (273 R), '273 S' (273 S), '273 T' (273 T), '273 U' (273 U), '273 V' (273 V), '273 W' (273 W), '273 X' (273 X), '273 Y' (273 Y), '273 Z' (273 Z). A callout box points to the '1.000' object with the text: '1. Right click here and select "Convert PDB"'. The main window displays a 3D protein structure with a callout box pointing to a 'Convert to ICM' dialog box with the text: '2. Enter the options as shown and press OK.' The dialog box has two checked options: 'delete water' and 'replace the original'. The 'OK' button is highlighted.

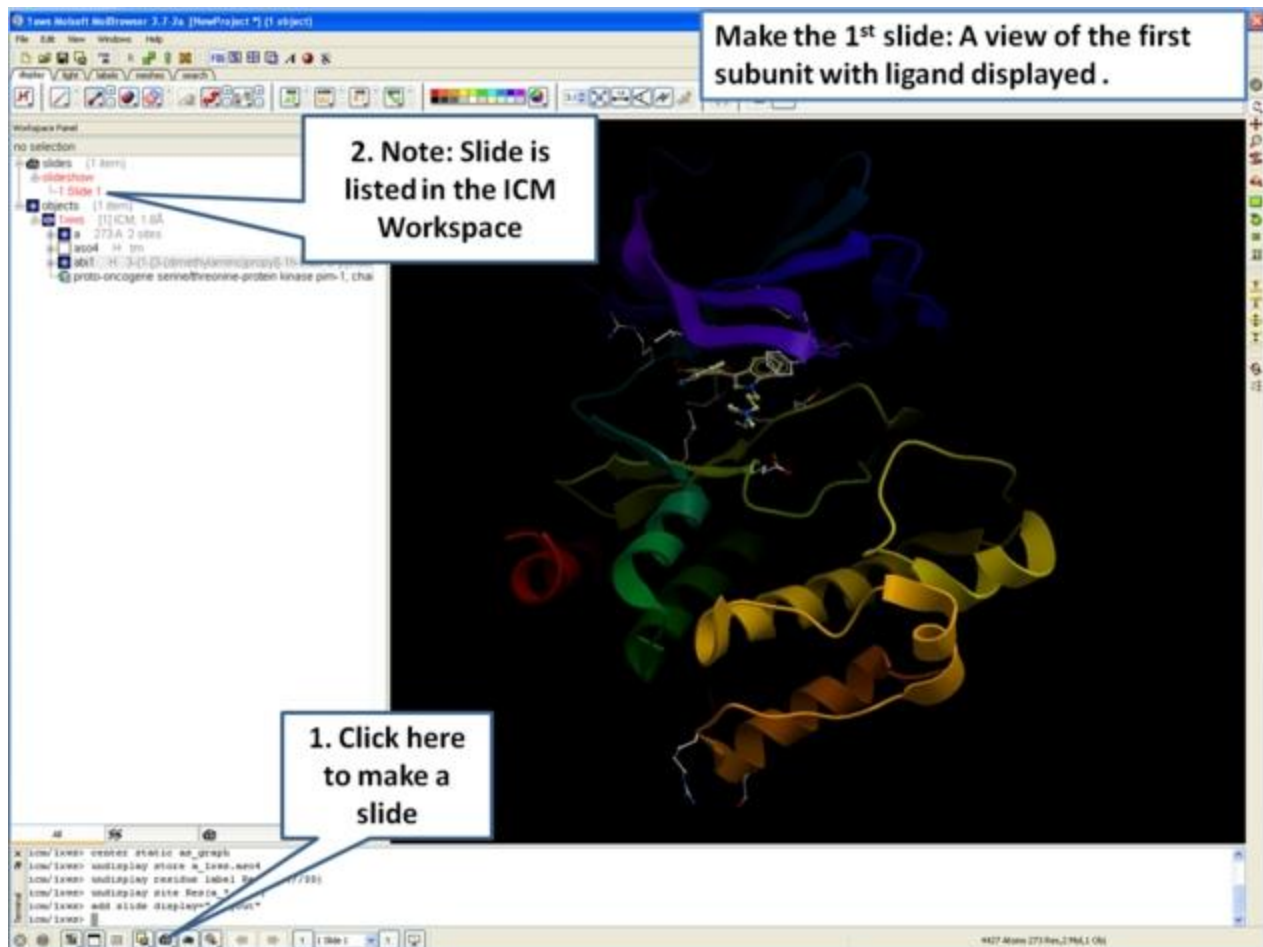
1. Right click here and select "Convert PDB"

2. Enter the options as shown and press OK.

- Now we are going to prepare the first slide by rotating the protein structure to an orientation which allows the viewer to see the key features of the kinase. For example the bulge in the hinge region (between the N- and C- lobes) which is unique to PIM proteins.

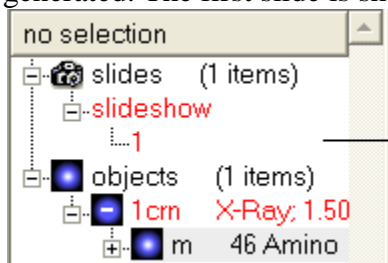


- Next, make the first slide by clicking on the camera button at the bottom of the graphical user interface.



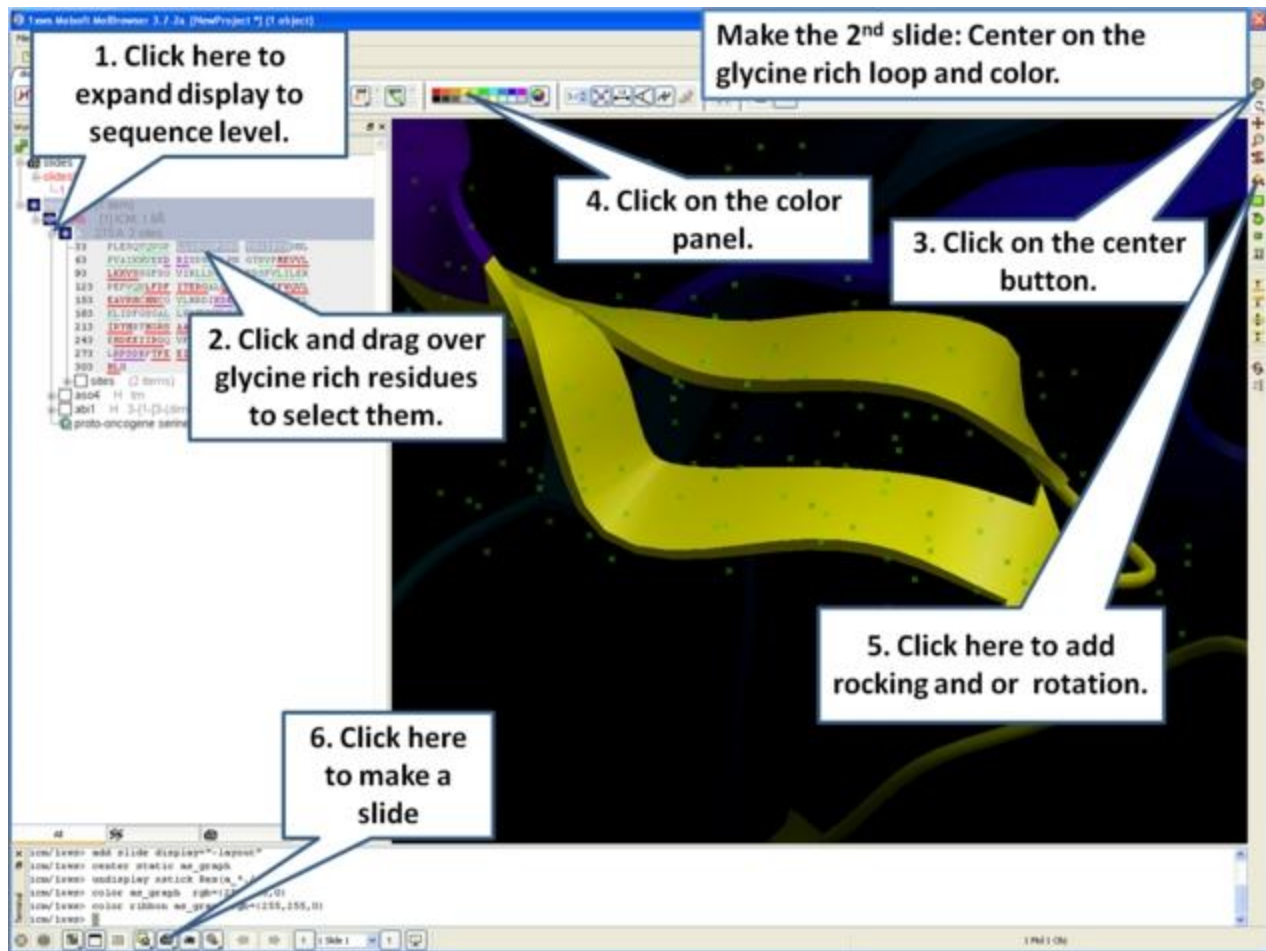
Click to add slide

- Once you have clicked on the camera button you will see that the first slide has been generated. The first slide is shown in the ICM Workspace window as shown below.

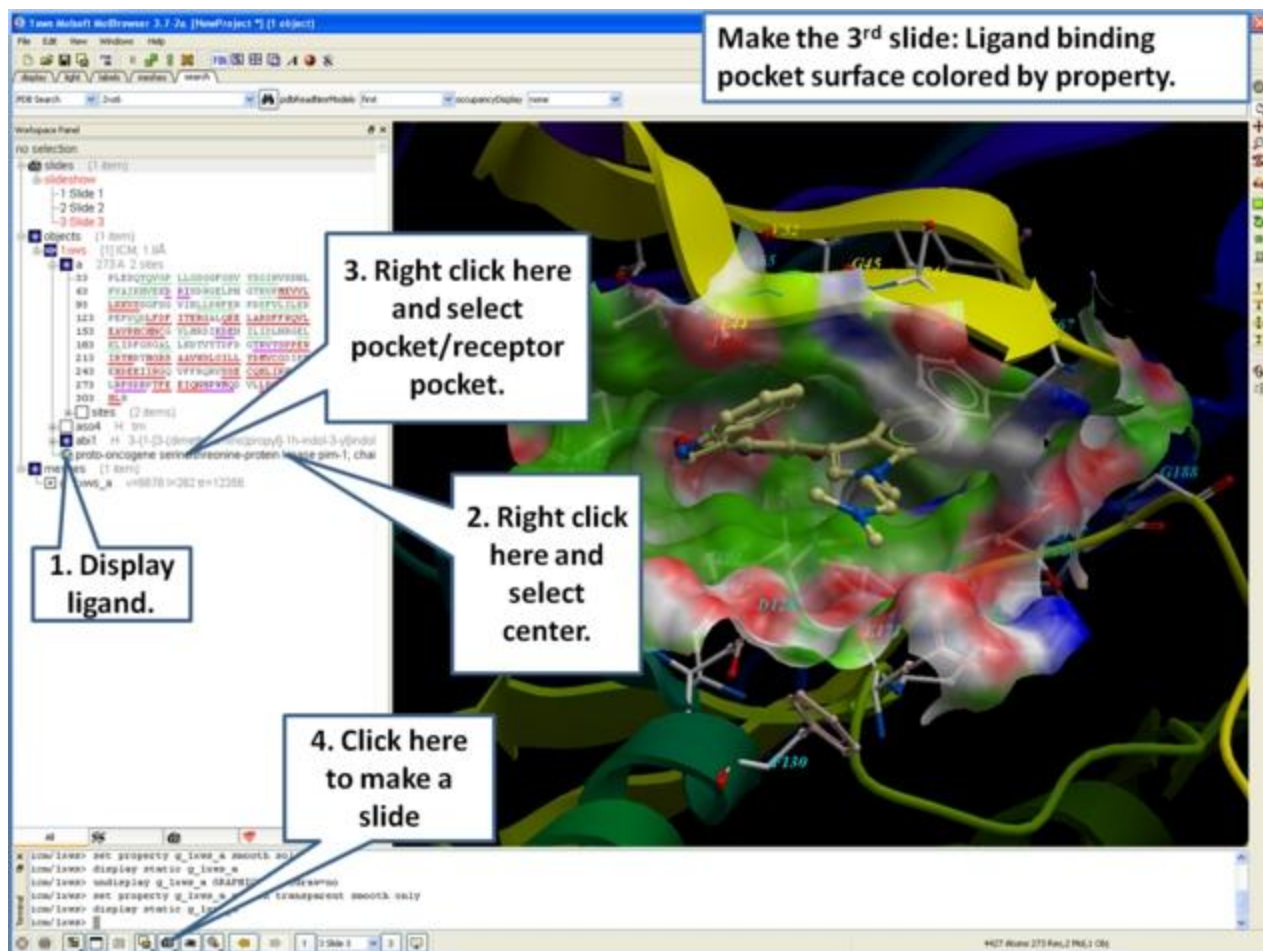


The number and name of the first slide is displayed in the ICM Workspace

- Slides can consist of Static views or Transitions and Animations. Here we will zoom into the flexible glycine rich region of the kinase which lays across the roof of the ATP-binding pocket. Click on the camera button and make the second slide



- Next, we will make a slide of the surface of the ligand binding pocket colored by binding property.

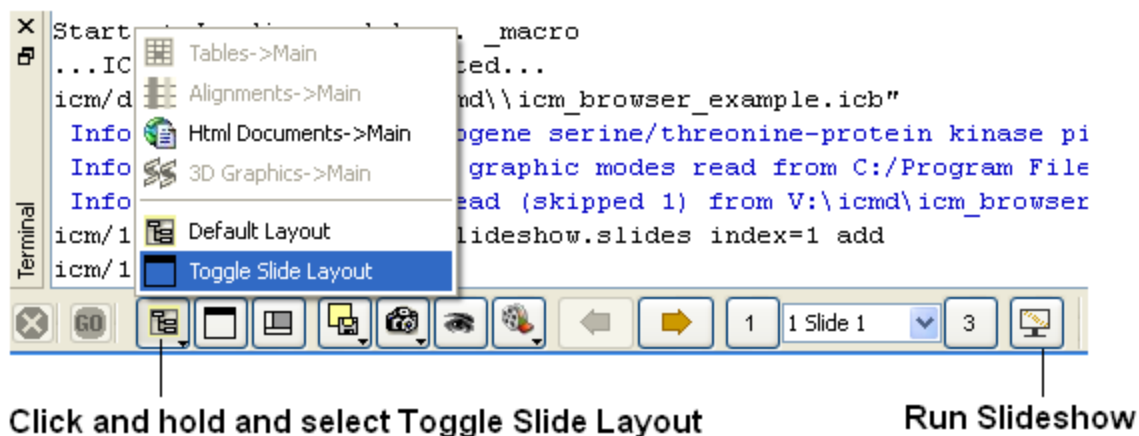


- Now save the document as an icb file. Go to File/Save as...

## 6.3 How to View and Navigate Slides

### *To run a slide show*

To view a slide show select the buttons shown below:



**NOTE:** Slides are associated with the objects currently loaded into ICM. Therefore if you delete an object then the slides will not work. However if you delete an object and then re-read the same object with the same name and structure the slides will be ok.

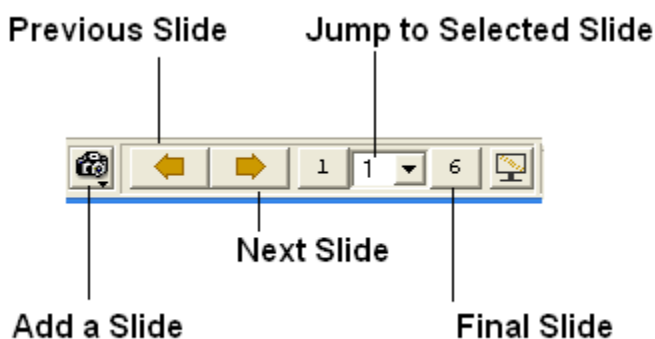
#### *To save a slide show*

- File/Save Project

### 6.3.1 Slide Navigation

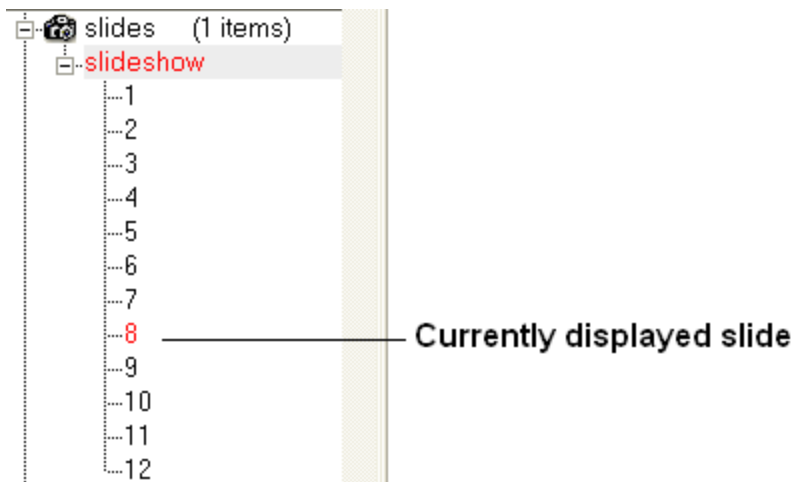
You can make as many slides as you wish as described in the [Making Molecular Slides](#) section.

To navigate through the slides you can use the buttons shown below, the cursor keys for some operations or the right click options in the ICM Workspace.



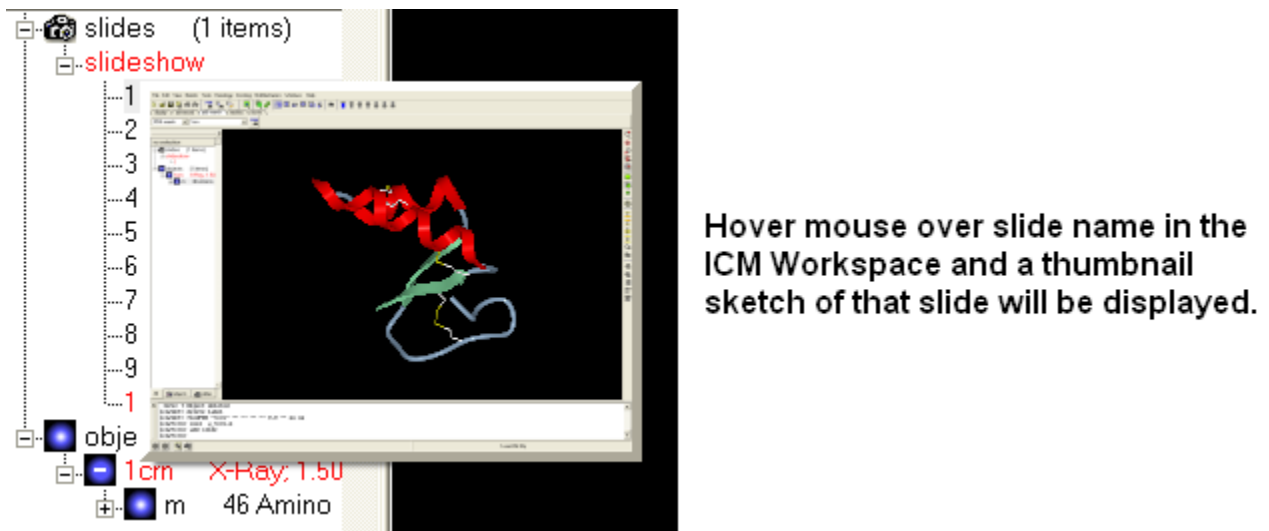
The slide currently displayed is highlighted in red in the ICM Workspace.



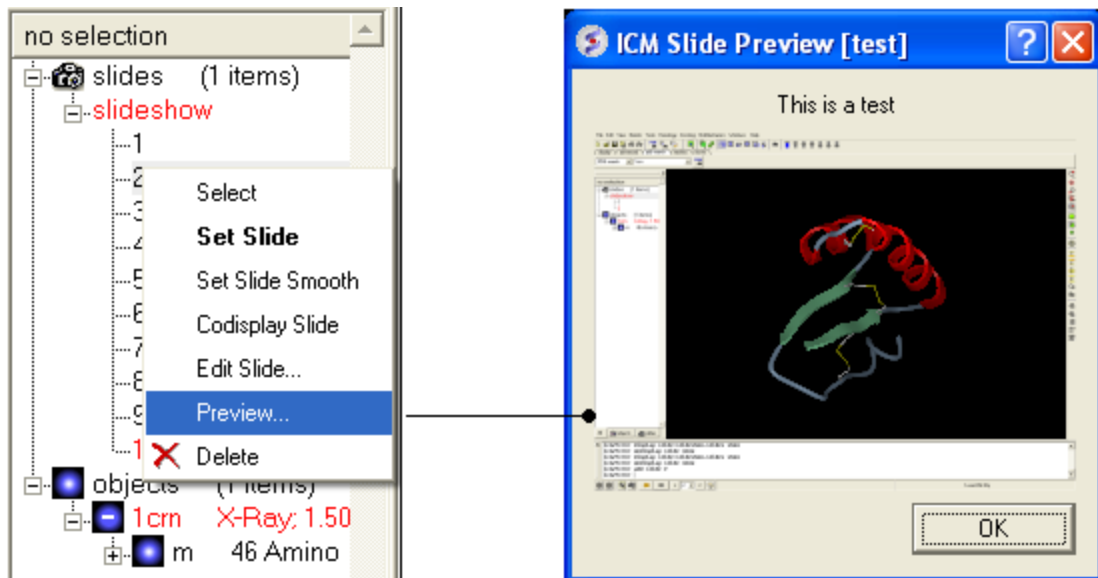


To jump to another slide right click and select "Set Slide".

All slides are displayed in the ICM Workspace. You can hover the mouse over a slide name in the ICM Workspace and a thumbnail sketch of the slide is displayed as shown below. This can be used for slide navigation purposes.



Or you can right click on the name of the slide in the ICM Workspace and select the option "Preview".

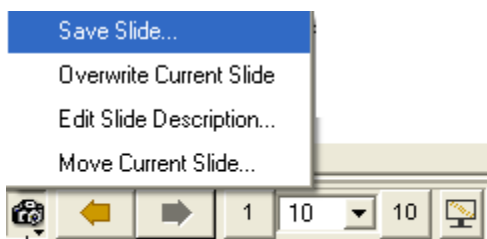


## 6.4 How to Edit Slides

You can jump to the slide you wish to edit by following the `slide navigation` instructions.

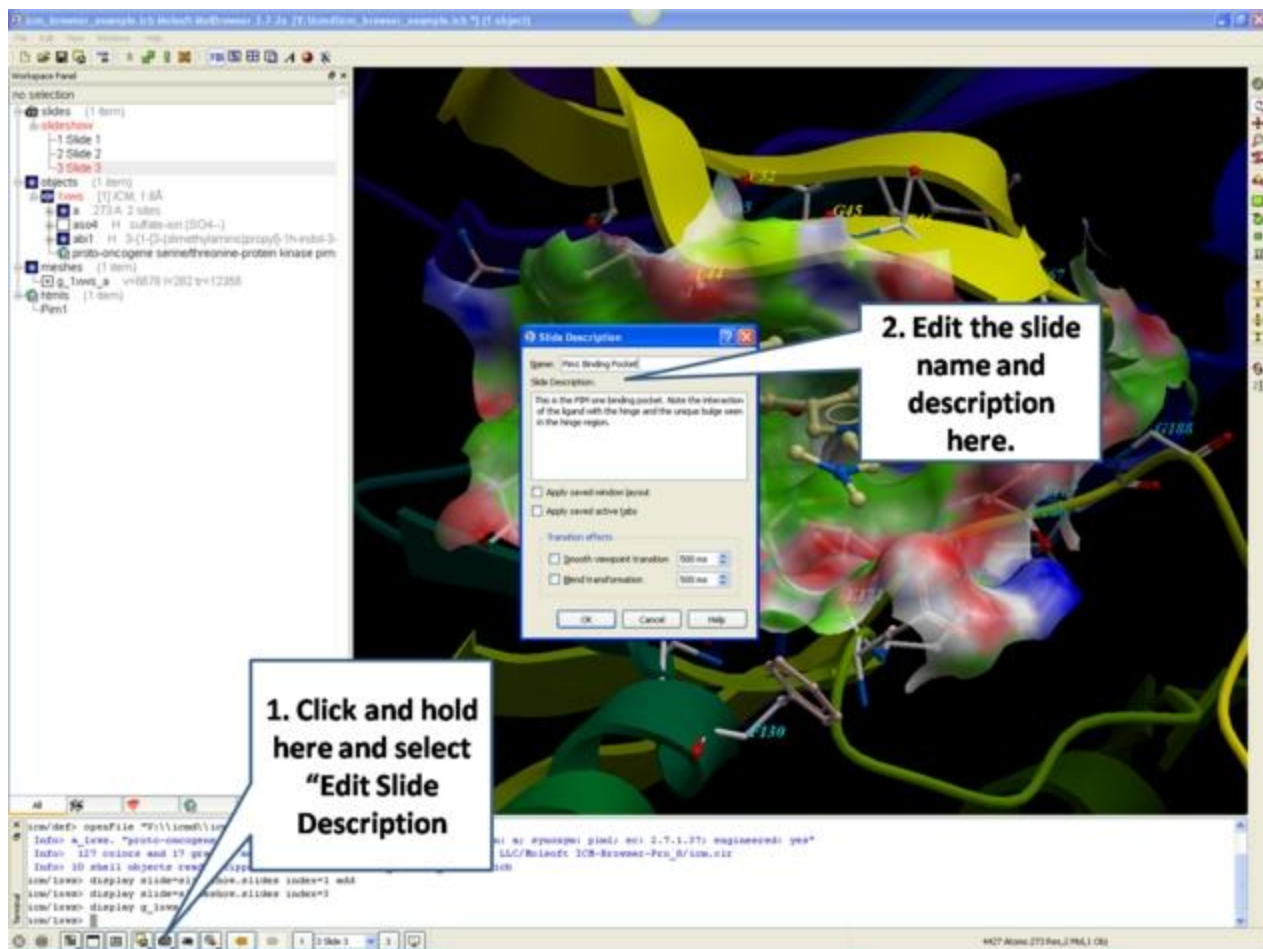
To edit the content of a slide the procedure is to add a new slide and then delete the old one or use the "overwrite current slide" option as shown below:

- Click and hold down on the camera button.



**Click and hold**

- To edit a slide description.
- Click and hold down on the camera button and select the option "Edit Slide Description".



- Enter the name of the slide
- Enter a description of the slide.
- If you wish to keep the current window layout or active tabs check the boxes provided

---

#### *To delete a slide:*

- Right click on the name of the slide in the ICM Workspace and select Delete.

---

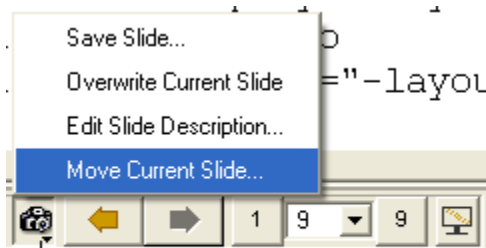
#### *To change the name of a slide*

- Right click on the name of the slide in the ICM Workspace and select Edit Slide.

### 6.4.1 Move Slide

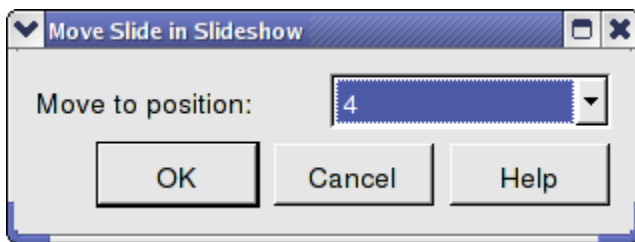
To change the slide's position in the slideshow use the Move Current Slide option and select the new position from the list.

- Click and hold on the "make slide button".
- Select Move Current Slide.



Click and hold

- Select the position in the slide show where you want to move the slide to.



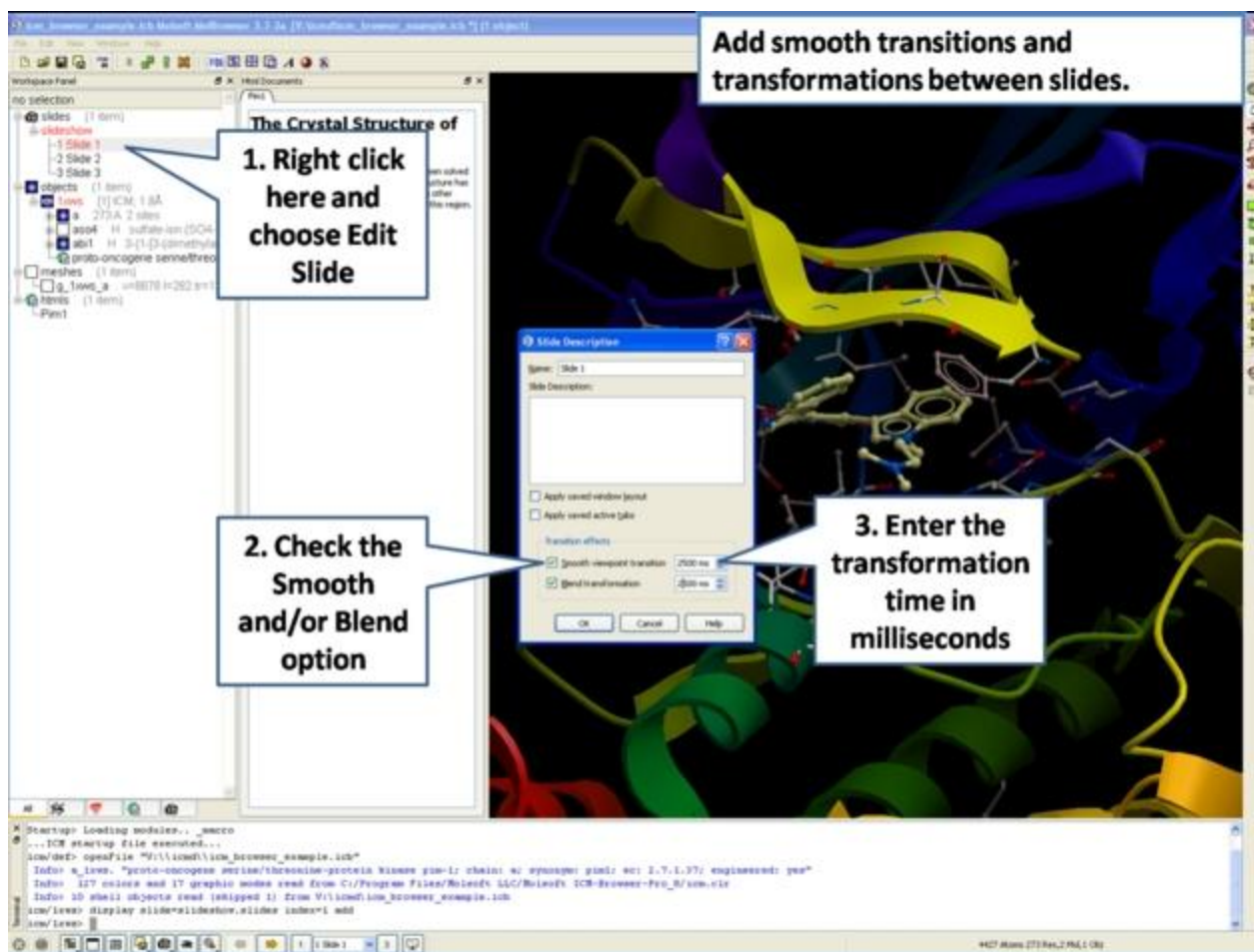
### *Co-display more than one slide*

- Right click on the name of the slide in the ICM Workspace you wish to co-display with the currently displayed slide.
- Select the option co-display slide.

## **6.5 How to Add Smooth Blending and Transition Effects Between Slides**

### *How to add smooth and blend transitions to a slide.*

- Right click on the name of the slide in the ICM Workspace.
- Select **Edit Slide**.
- Select the desired transition effect - **smooth** or **blend** as shown below.
- Select the length of the transition in milli seconds.

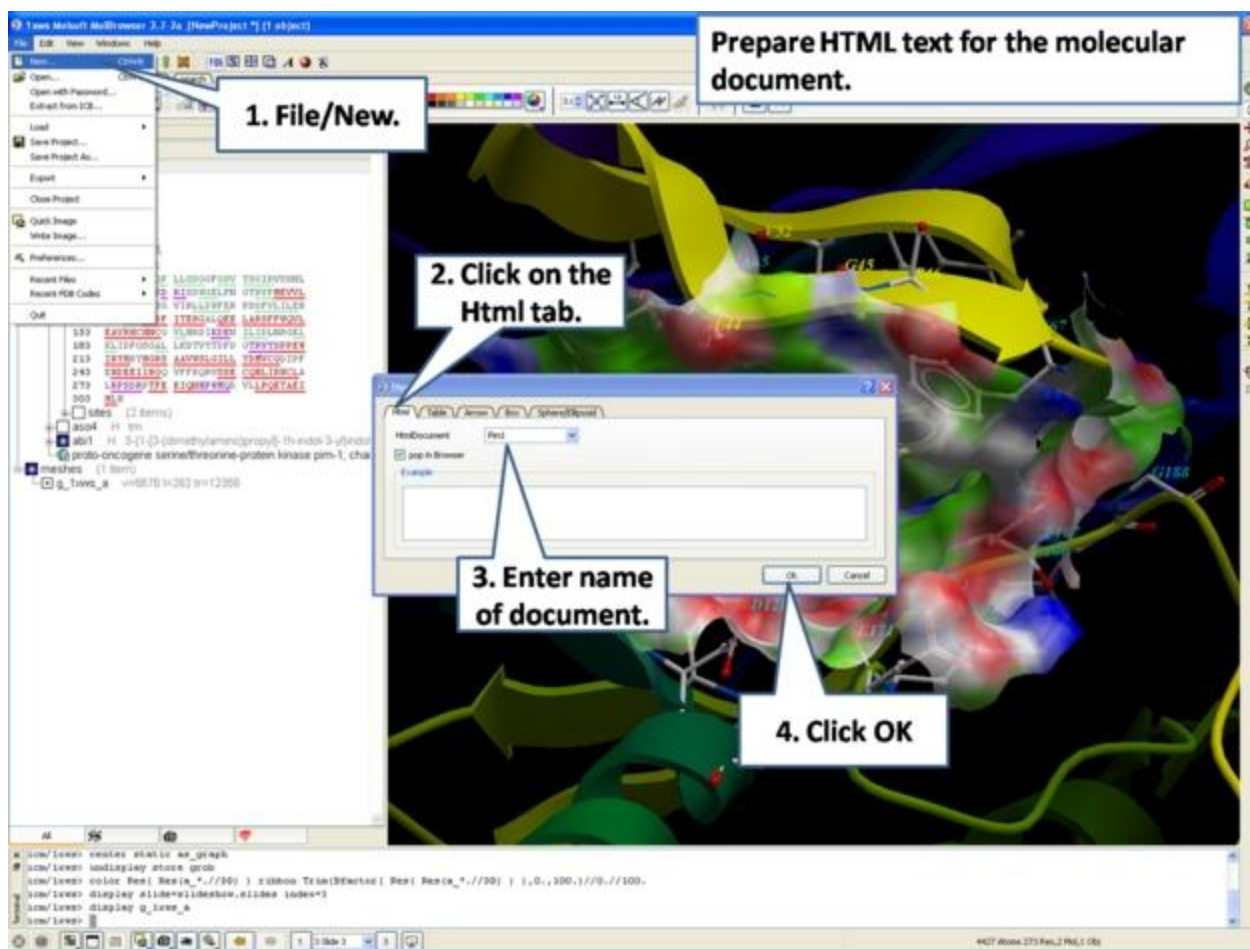


## 6.6 How to Make Molecular Documents - Link HTML Text to Slides

An ICM Molecular Document contains text and images which can be hyperlinked to the graphical display. Click on the hyperlinked text and then a fully-interactive 3D slide will be displayed. The hyperlinks are usually linked to a set of slides but can also be linked to a series of commands in a script, a web page, a table or alignment. Once a molecular document has been made you can view it in the ICM-Browser (File/Save Project .icb file) or download ActiveICM and view it in a web page or Powerpoint.

### *To begin creating an ICM document*

- File/New/ and click on the HTML tab.
- Enter some text. E.g the Name of the HTML document. Formatting can be changed as described in the edit section below.
- Click OK



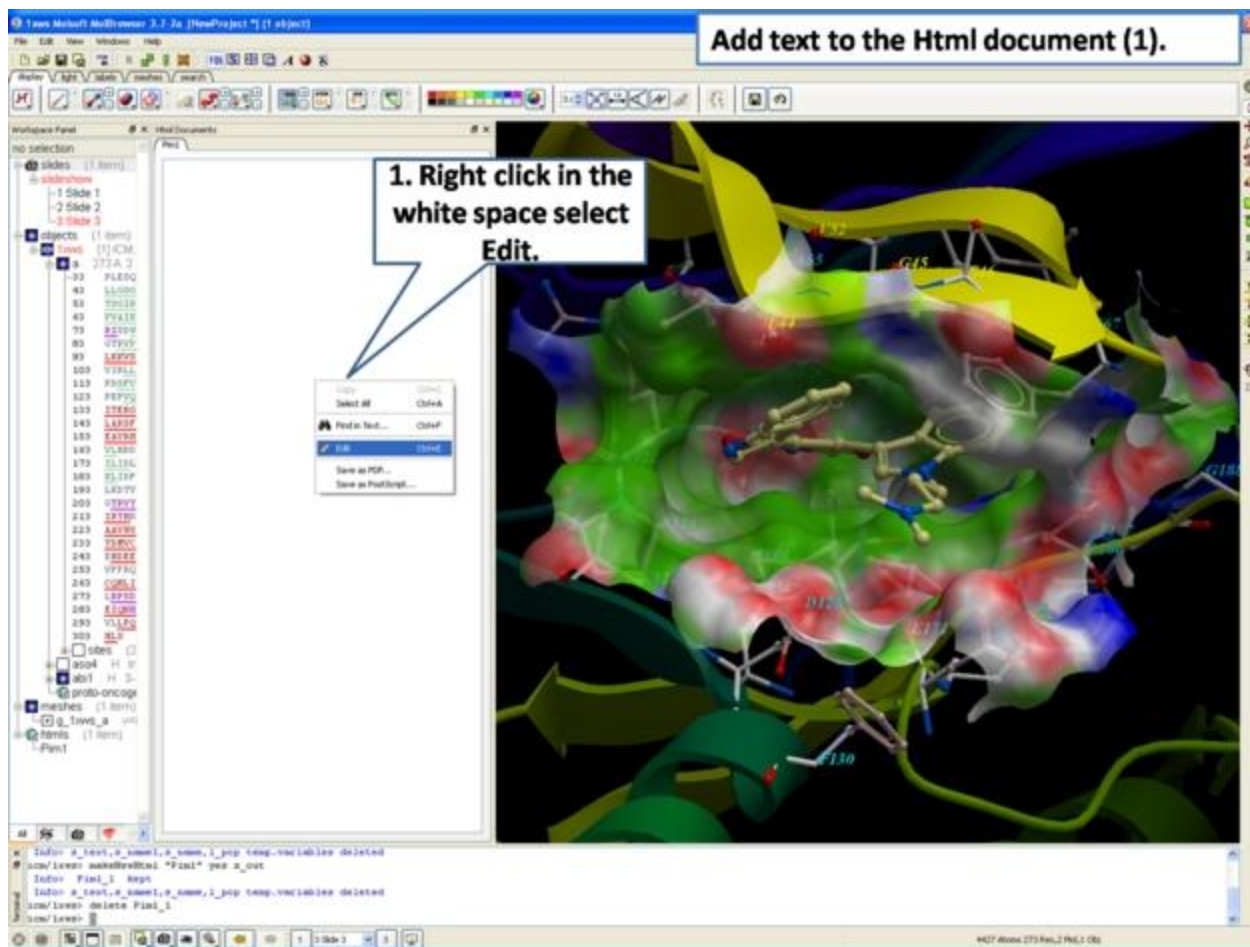
- A HTML text panel will be displayed in the graphical user interface.

**NOTE:** You can add multiple documents into a single file. The documents will be accessible via tabs at the top of the HTML panel.

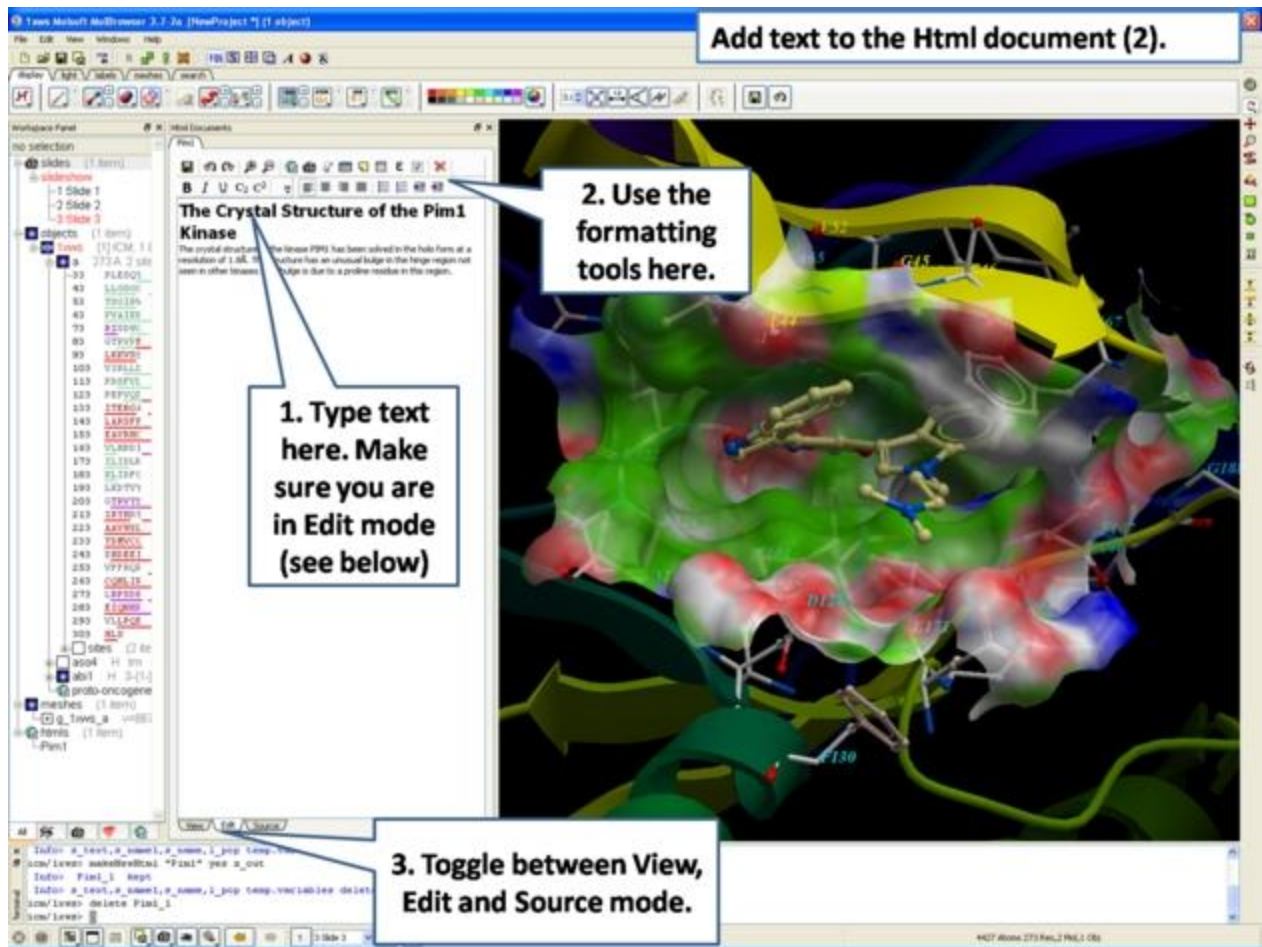
### 6.6.1 How to Add Text or Edit a Molecular Document

*To edit the HTML text in the graphical display*

- First create an HTML document and the text panel will be displayed in the graphical user interface.
- Right click in the body of the text display panel and select **Edit**.

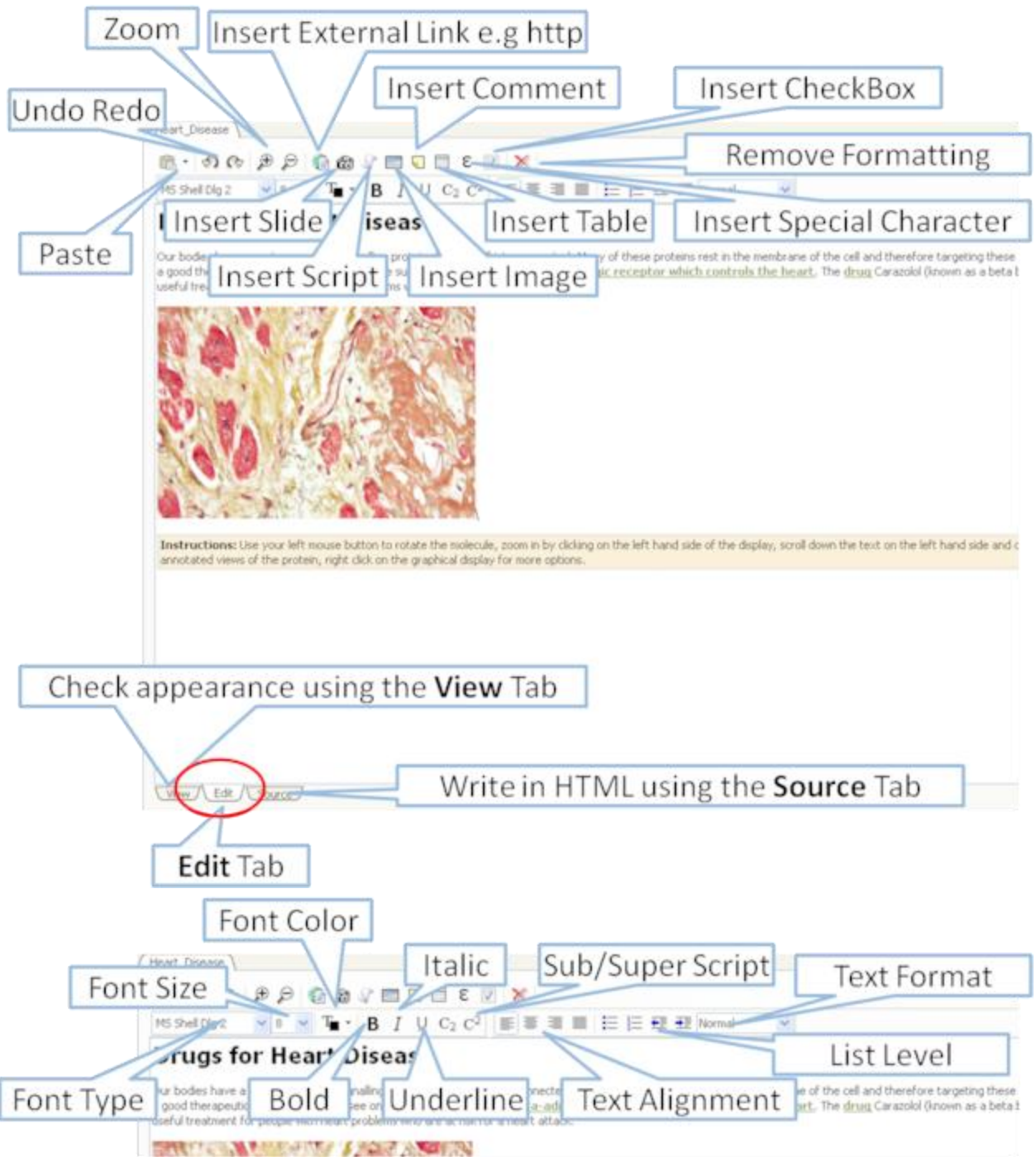


- Enter text and use the formatting tools provided in the panel above the text editor. Make sure you have selected the **Edit** tab in the HTML editor. You can see your page in the **View** tab or write directly in HTML in the **Source** tab.



The key formatting tools in the HTML editor are shown below.



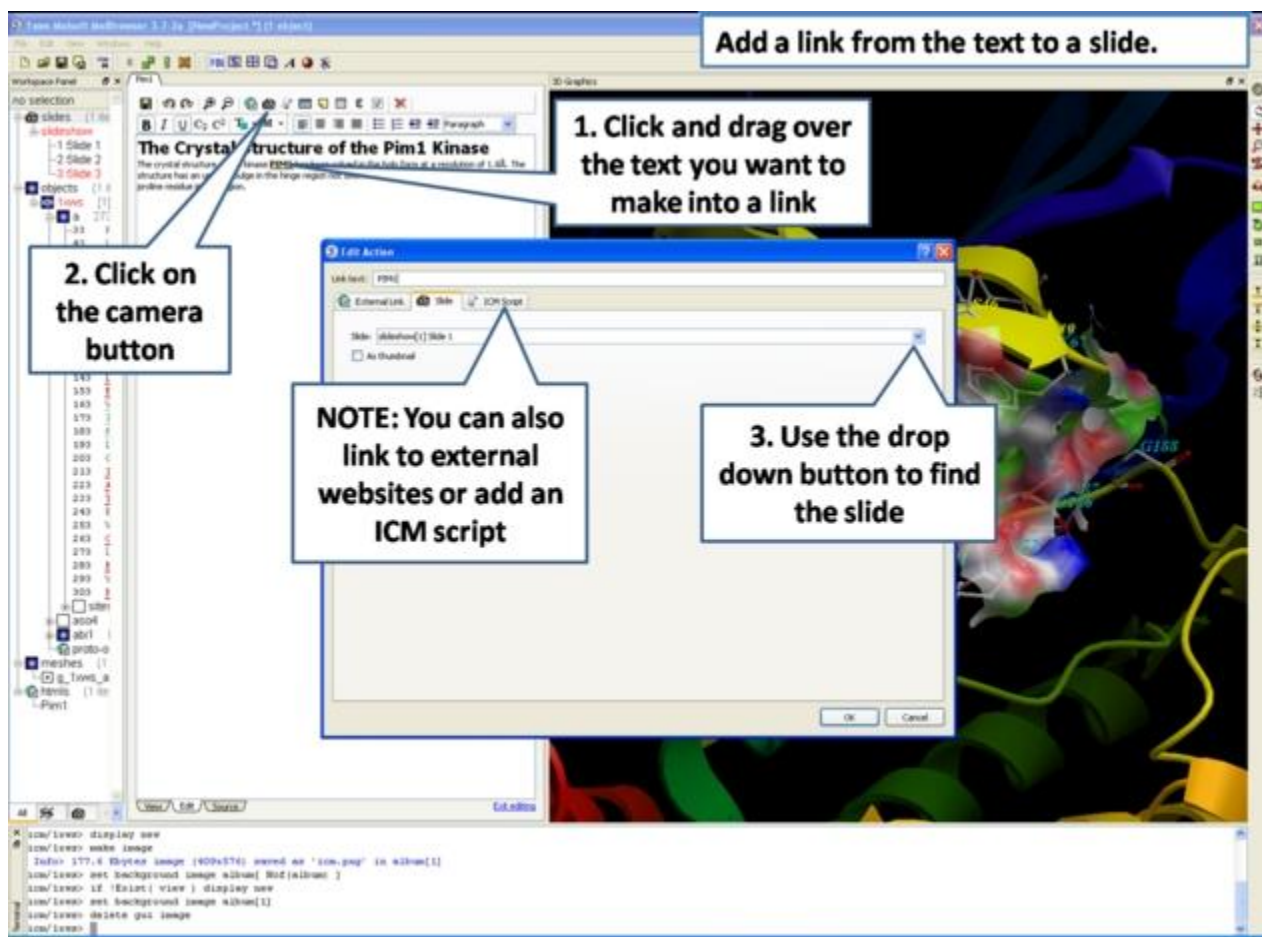


## 6.6.2 How to Make a Hyperlink Between Text and a Slide

*To make a hyperlink between the text and the graphical display (slide)*

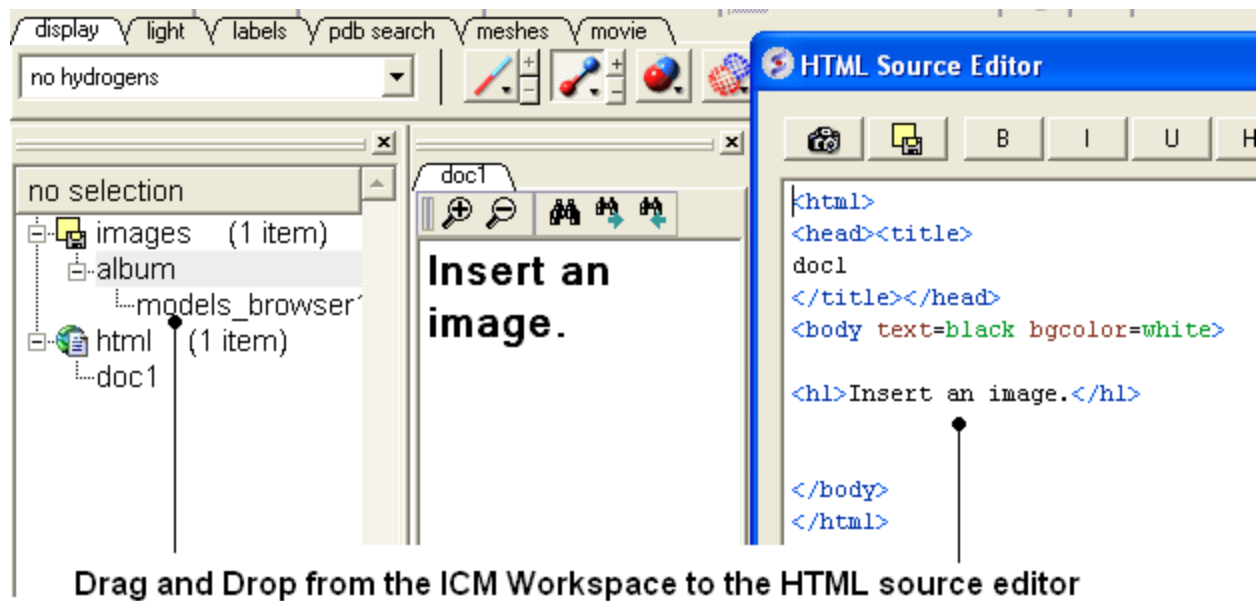
Make a slide or set of slides of the graphical display you wish to link to. See [Making Molecular Slides](#) for help on this. Once slides have been created:

- File/New/Html
- Right click in the body of the text display panel.
- Select Edit.
- Highlight the text you wish to link to a graphical display - you can do this by left clicking and dragging over the text (selected text will be highlighted in blue).
- Click on the "Camera button" in the HTML editor formatting tool panel.
- Select the **Slide** tab.
- Select which number slide you wish the text to be linked to from the drop down menu.
- There is an option to display the slide as a thumbnail image in the text document panel. Check if appropriate.



### 6.6.3 Insert Image

**NOTE:** The easiest way to add images (PNG or JPEG) into an ICM Document is to use drag and drop. You can drag and drop the image into the ICM Workspace or go to File/Open. Once the image is in the album in the ICM Workspace you can then drag it from the ICM workspace into the HTML editor.



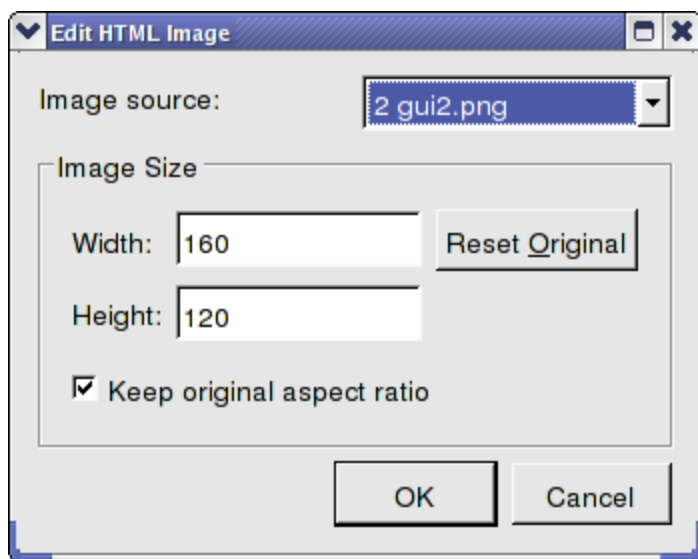
*Another way to insert a picture into the HTML text panel*

- First read the image into the ICM photo album File/Open OR Drag and Drop from directory into the ICM Workspace.

The image name and preview will then be displayed in the ICM Workspace.



- Create HTML text - File/New/HTML. Add text.
- Right click in the HTML window and select 'Edit Source'.
- Right click on the position in the ICM Script Editor where you would like to insert the image.
- Select 'Insert Image'



- Select the image name source.
- Choose the desired Width and Height.
- Click OK.
- Click Save in the ICM Script Editor.

## 6.6.4 Insert Script

### *How to insert a script to the text panel*

There are 3 ways to add a script - described in more detail below

1. Drag and drop script from ICM Workspace
2. In the HTML Source Editor - right click and select Insert Slide or Action
3. Create an "inline" script

These methods are described below:

### *Drag and Drop Method*

- Create a script File/New/Script
- The script will be displayed in the ICM Workspace.
- Right click in the HTML Text Panel (for instructions on how to create this panel see create molecular document) and select edit source and the HTML Source Editor will be displayed.
- Click-Drag and Drop the script into the HTML Source Editor

A line as shown below will be added.

```
<a href="#icm/script/script1">text placed here will be displayed as a link in the document</a>
```

***Another way to add a script to the document is to Insert Action:***

- Right click in the body of the text display panel.
- Select Edit Source
- Highlight the text you wish to link to a graphical display - you can do this by left clicking and dragging over the text (selected text will be highlighted in blue).
- Right click and select 'Insert Slide or Action' or select the button in the HTML Source Editor and a window as shown below will be displayed.

Internal Link Name

Highlighted text

Help: start script from #dialog{"name"} to generate a dialog

Display Slide :   As Thumbnail  Smooth Transition:  msec

[Arguments and] ICM commands

Add your script here

OK Cancel

- Select the option [Arguments and] ICM commands
- Add script in the editor provided
- Select ok

## ***Inline Script***

A script can be added to the HTML text in the following way

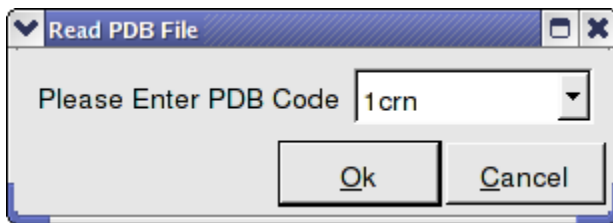
- Right click in the body of the text display panel.
- Select Edit Source
- Enter script in the format as shown below.

```
<!--icmscript name="script2"  
print $1 + $2  
--><a name="script2" href="#_">script2</a>
```

### **6.6.5 Insert a Dialog Box**

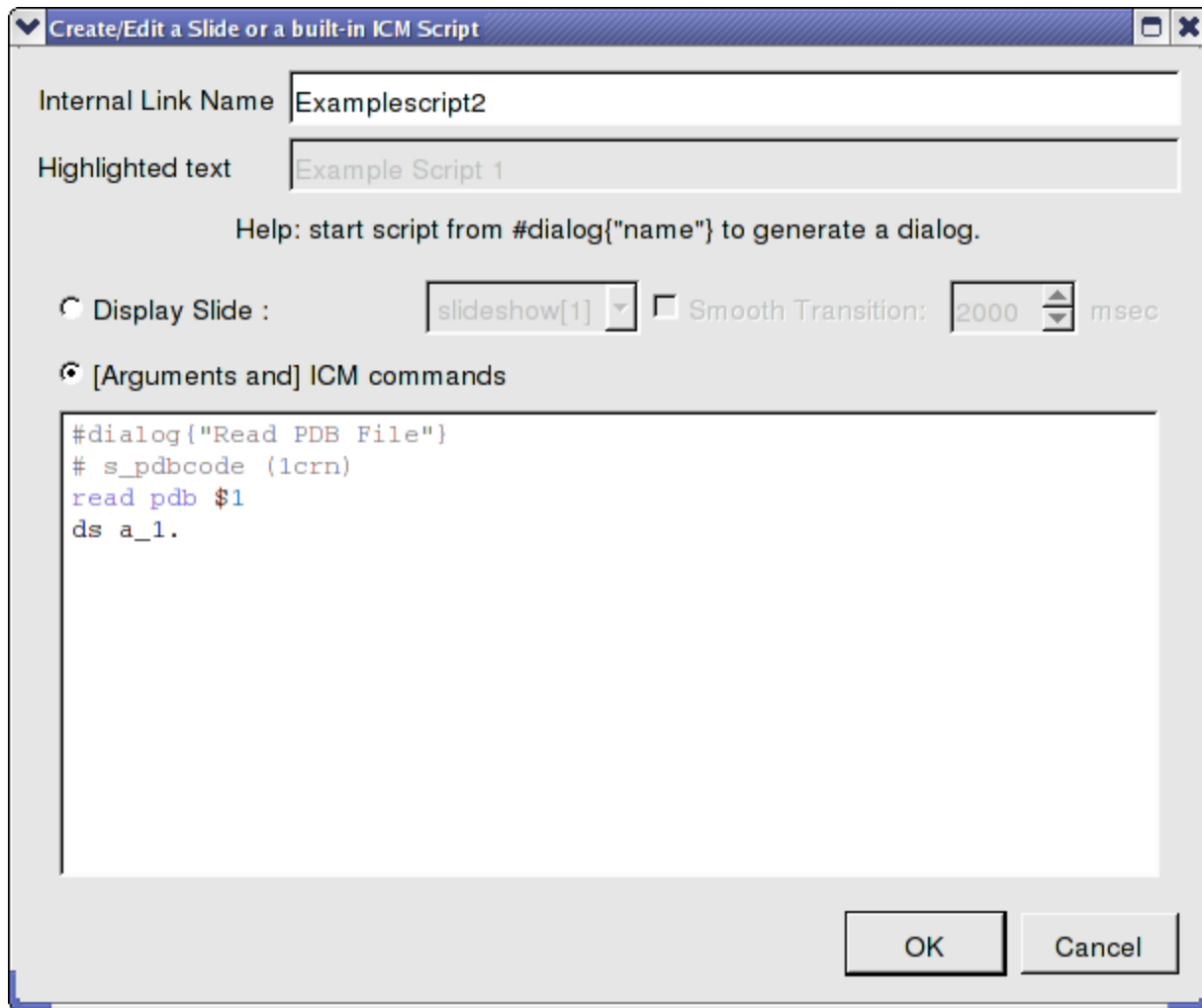
Dialog boxes are provided to enable a viewer to interact with a presentation or document file. The dialog box will be a gui data entry box. For an example here is a script to prompt the user of the file to enter a pdb code:

```
read pdb $1  
ds a_1.
```



The code above can be saved as a script or inside the html text. To do this:

1. Right click on the HTML text display and select "Edit Source".
2. Highlight the text you wish to link to a dialog box and then select the right click and select 'Insert Slide or Action' or select the button in the HTML Source Editor and a window as shown below will be displayed.



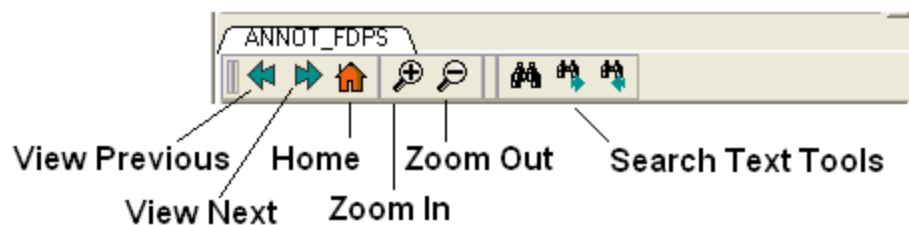
OR.

1. Right click on the HTML text display and select "Edit Source".
2. Add a link to a script as shown below.

```
<a href="#icm/script/script1">Example Script 2</a>
```

### 6.6.6 Document Navigation

The following buttons shown below aid document navigation. Also remember that more than one document can be stored and the header of each document file will be displayed in multiple tabs in the text panel window.



### 6.6.7 Protect Shell Objects From Deletion

When making a molecular document you can protect objects from deletion by the person who reads your document by:

- Right click on the object in the ICM Workspace.
- Select the **Protect** option.

---

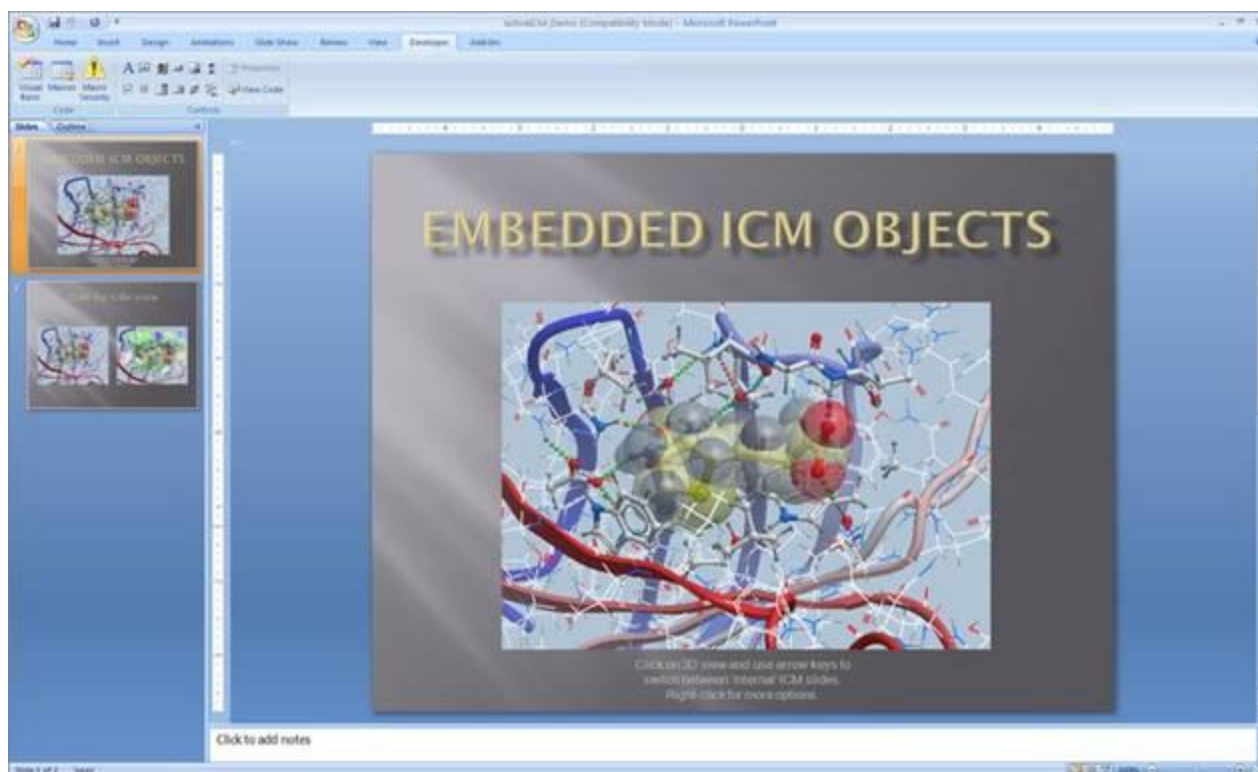
## 7 ActiveICM

ActiveICM enables you to view and display ICM graphical slides and animations interactively inside Microsoft PowerPoint and web browsers such as Internet Explorer and Mozilla Firefox.

### *System Requirements:*

- Windows 2000/XP/Vista
- Internet Explorer 7.0 (and above) or Mozilla Firefox 2.0 (and above)





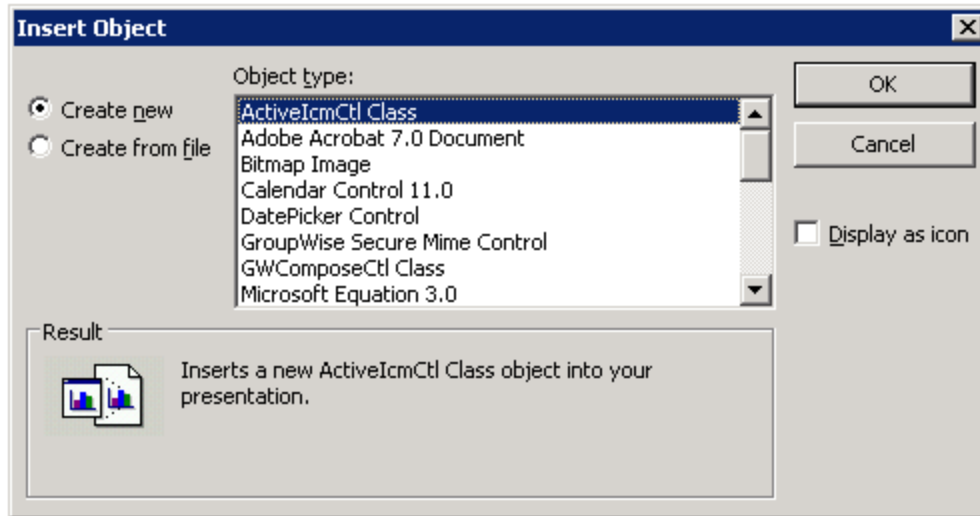
## 7.1 How to Embed in Microsoft PowerPoint 2003

### *Setup*

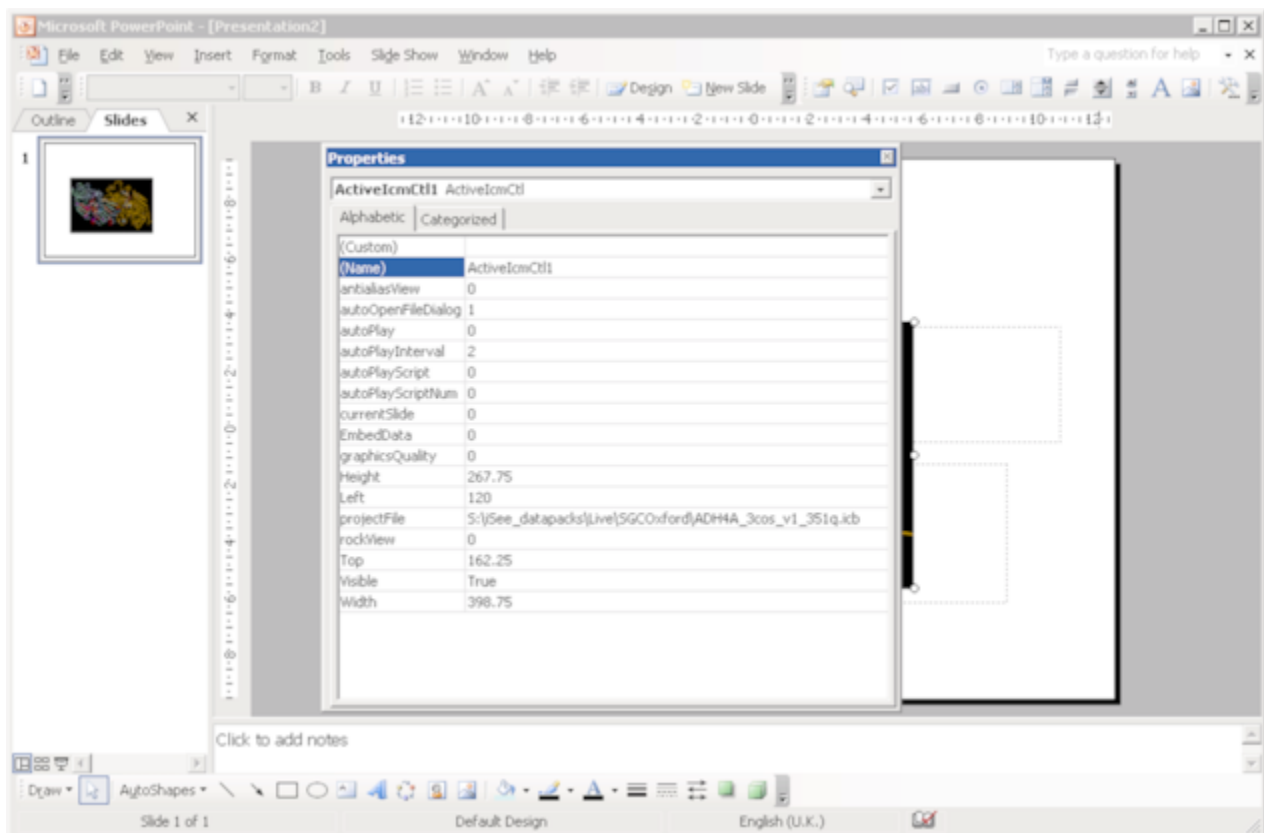
- Download ActiveICM from [www.molsoft.com/support](http://www.molsoft.com/support)
- Save an ICM file (.icb) containing slides. Click [here](#) to see how to make slides.

### *Embed icb file*

- Open the Insert menu from the top bar of PowerPoint and select **Object**
- This opens up the Object dialogue. Select **ActiveIcmCtlClass**:



- Click on OK. A file dialogue will then be opened. Open the ICB file you wish to use via this dialogue. **IMPORTANT:** To avoid later problems, make sure the ICB file is in the same folder as the PowerPoint file.
- A low-resolution snapshot of the first slide in the ICB file will be shown in the activeICM control you created. You can change the shape of the control by dragging the corners of the control with the mouse, once selected.
- Right-click on the activeICM control and select the Properties menu item



- Save the PowerPoint presentation

## 7.2 How to Embed in Microsoft PowerPoint 2007

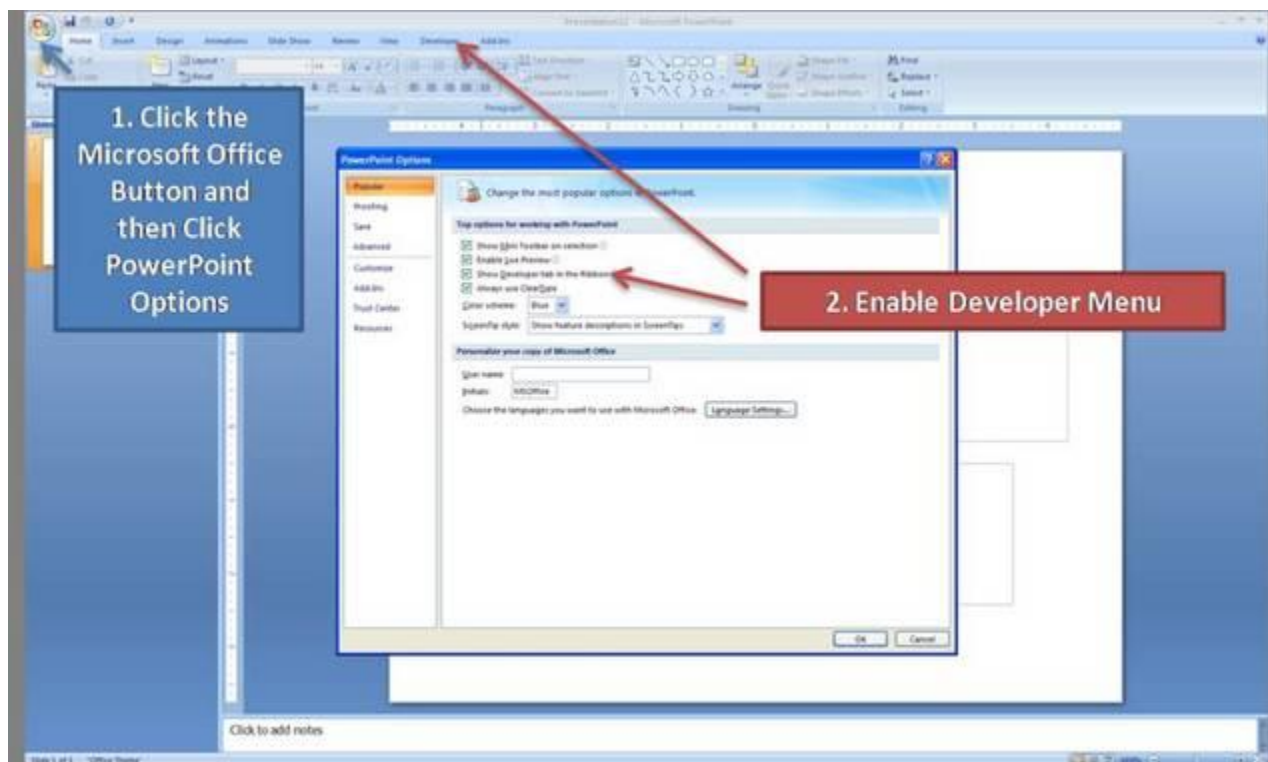
### Setup

- Download ActiveICM from [www.molsoft.com/support](http://www.molsoft.com/support)
- Save an ICM file (.icb) containing slides. Click [here](#) to see how to make slides.

**NOTE:** Here are the instructions for ActiveICM in Microsoft Office 2007, for older versions of PowerPoint see [here](#).

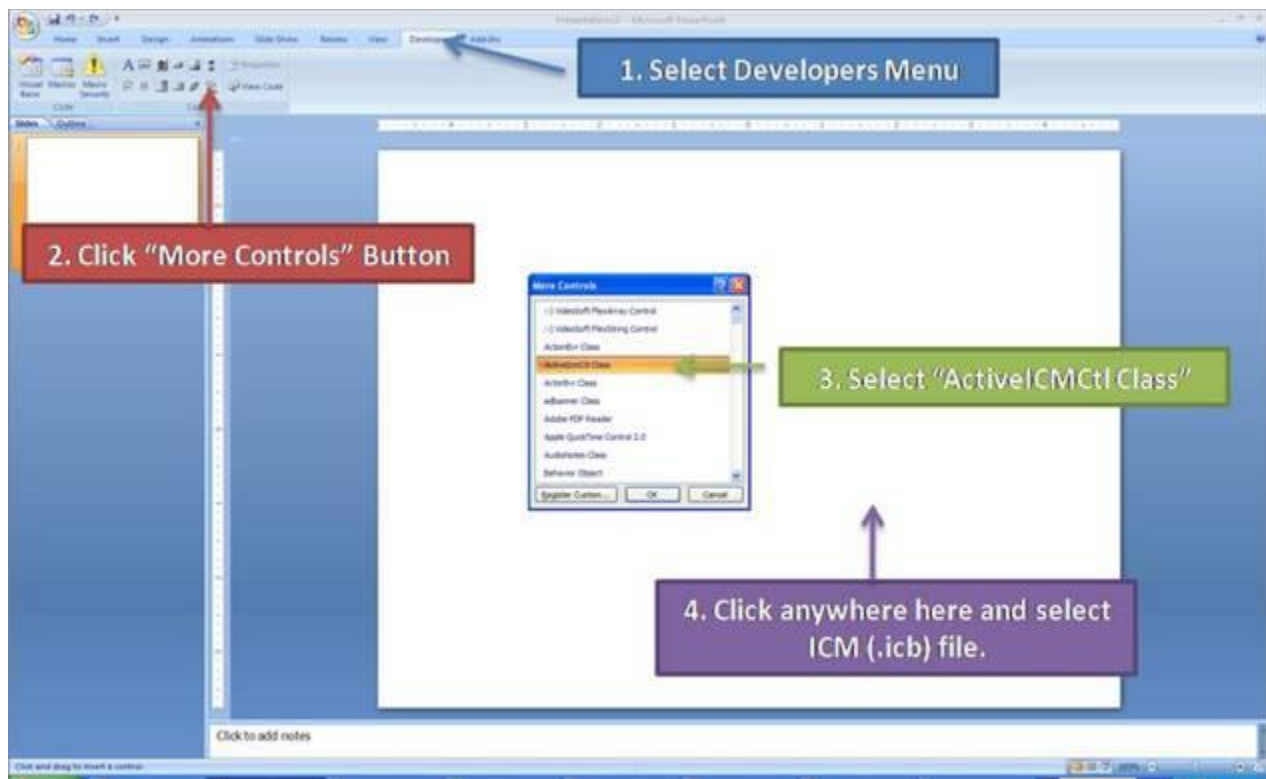
### Enable the Developer Menu:

- Click the **Microsoft Office Button** (button top left), and then click **PowerPoint Options**.
- In the **PowerPoint Options** dialog box, click Popular.
- Under **Top options for working with PowerPoint**, select the **Show Developer tab in the Ribbon** check box, and then click **OK**.



### Insert ActiveICM into PowerPoint:

- Select the **Developer** menu.
- Select the **More Controls** button in the **Controls** field.
- Select **ActiveICMctl Class** from the list of controls and click **OK**.
- Click the mouse anywhere in the white PowerPoint space and a dialog box will be displayed asking you to select your ICM (.icb) file.
- Click and drag at the corners of the image to resize the normal way you would resize an object in PowerPoint.



## 7.3 Embed in Web Browser

To embed in a web browser.

1. Download ActiveICM from here  
<http://www.molsoft.com/getbrowser.cgi?product=activeicm&act=list> (it is free!).
2. Create an HTML page in ICM (File/New/Html).
3. Add a series of slides.
4. File/Export As ActiveICM Html..

## 7.4 How to Use ActiveICM in PowerPoint

***\*\*IMPORTANT There are two ways to open a presentation:***

- Double click on the ppt file in windows folder. (in this case PowerPoint will set the current directory to the one which contains the file and there should be no problems with both relative and absolute paths)
- Open ppt through the "File-Open" or recent files. (in this case PowerPoint DOES NOT SET the current directory to the one which contains the file -> relative path might not work and user will be prompted to locate the ICB file unless file is found in absolute location)

***To view the slides you must be in Slide Show mode***

- Press the **F5** button to start the **Slide Show**. In edit mode (i.e. not presentation mode), the control is shown as a static image  $\frac{1}{2}$  it is not possible to interact with the ICB file. Therefore, to prepare the presentation so that the control shows the correct initial visualisations it is necessary to run the PowerPoint slide(s) in presentation mode

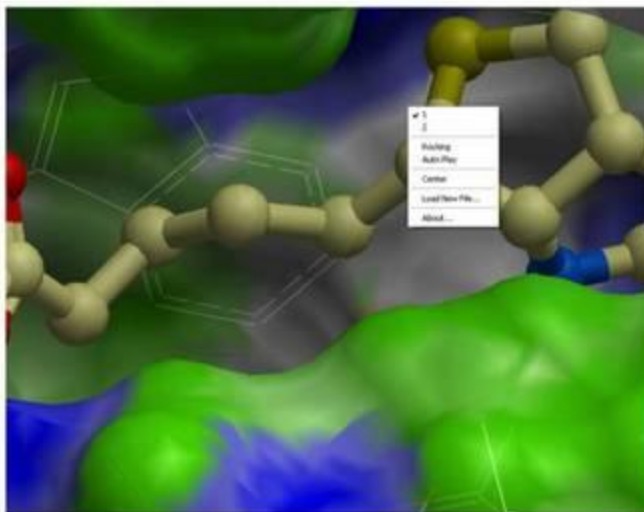
***Change Slides***

- Use the left and right cursor keys to change slides.

***A number of other options can be accessed by right clicking on the slide. These options include:***

- Select Slide
- Auto Play
- Set on/off rocking
- Center
- Load a new ICM File

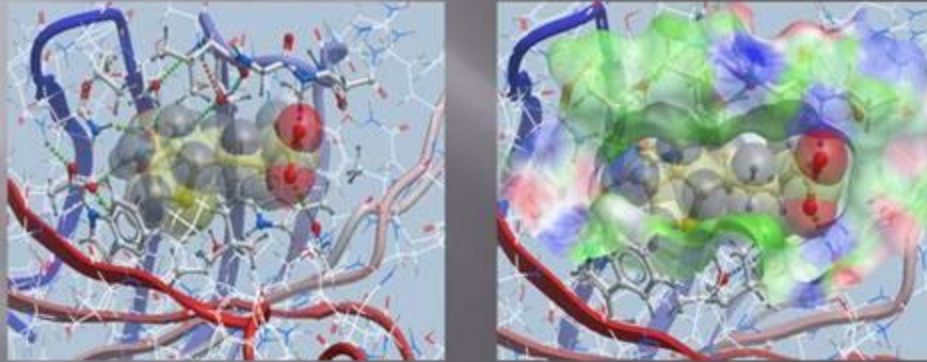
## ICM Embedded Into PowerPoint in Slide Show Mode (F5 button)



*You can also add multiple ActiveICM 3D displays in one slide:*

- To display multiple ActiveICM 3D displays in one slide just copy the original display or repeat the steps described above. All powerpoint slides should point to the same ICM file (.icb) but they can point to different slides.

## Side-by-side view



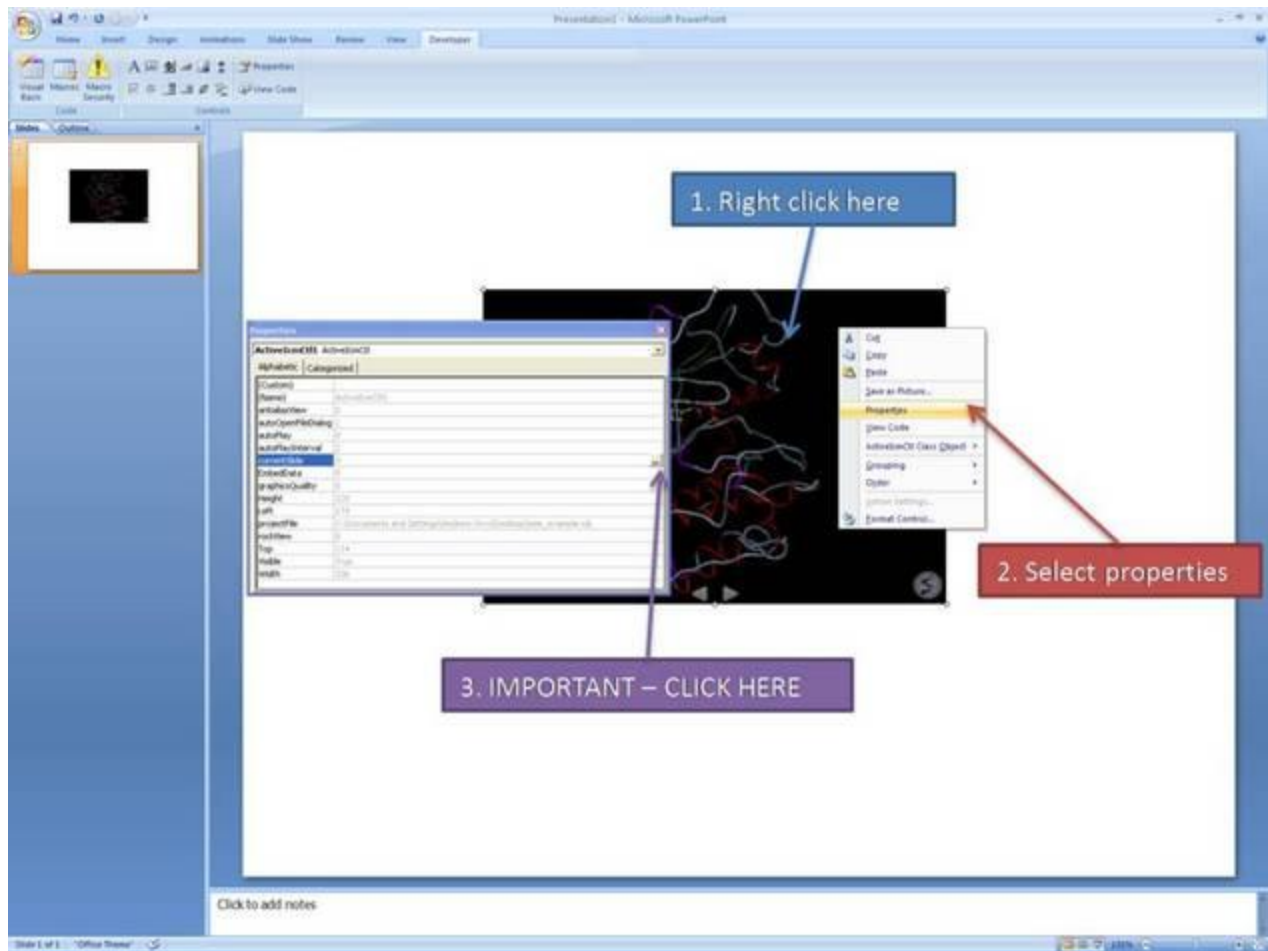
### 7.5 How to Change ActiveICM Component Properties

A number of properties of ActiveICM can be changed once embedded in powerpoint. The options include:

- Select the first slide to be displayed.
- Set slide auto play.
- Set auto play of a script.
- Embed the powerpoint file and the icb file all into one file.

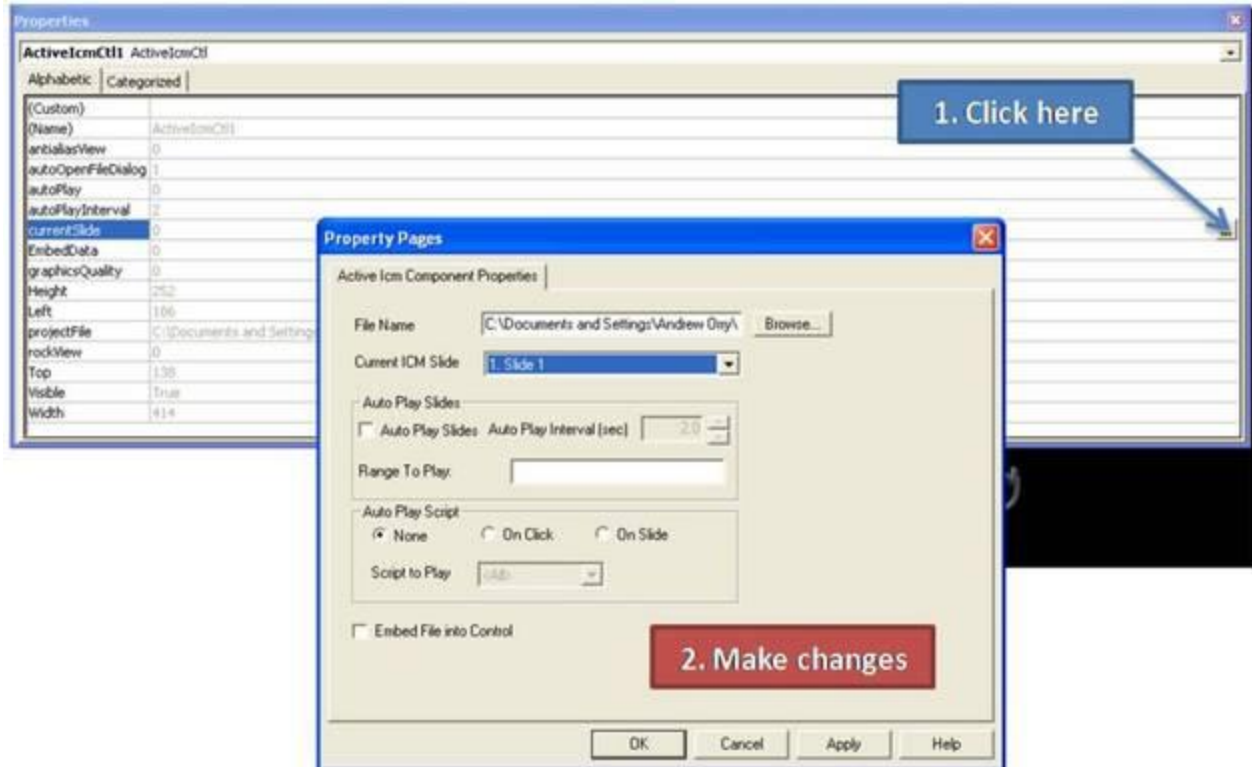
To change these options:

- Right click on your embedded activeICM in Powerpoint.
- Select **Properties** and click on the button shown below.



- A **Property Pages** window will then be displayed as shown below.





**To change the file name of the icb file linked to activeICM:** Simply type in the path to the file or use the browse option.

**To change the current ICM slide:** Use the drop down button next to **Current ICM Slide** to select the slide you wish to display first in your presentation.

**To auto play slides:** Check the **Auto Play Slides** box and select the interval between slides option. A range of slides can be played by entering the number of the slides separated by a comma.

**To auto play a script:** Select whether you want the script to run **On Click** or **On Slide** then select the script from the **script to play** drop down button. You should first save your script in the icb file.

**To embed the icb file in the ppt file** Click the **Embed File into Control** option. **Important** - Please save your PowerPoint file in the t 1997-2003 ppt format not pptx.

## 7.6 Advanced use of activeICM: Macros to direct visualisation changes

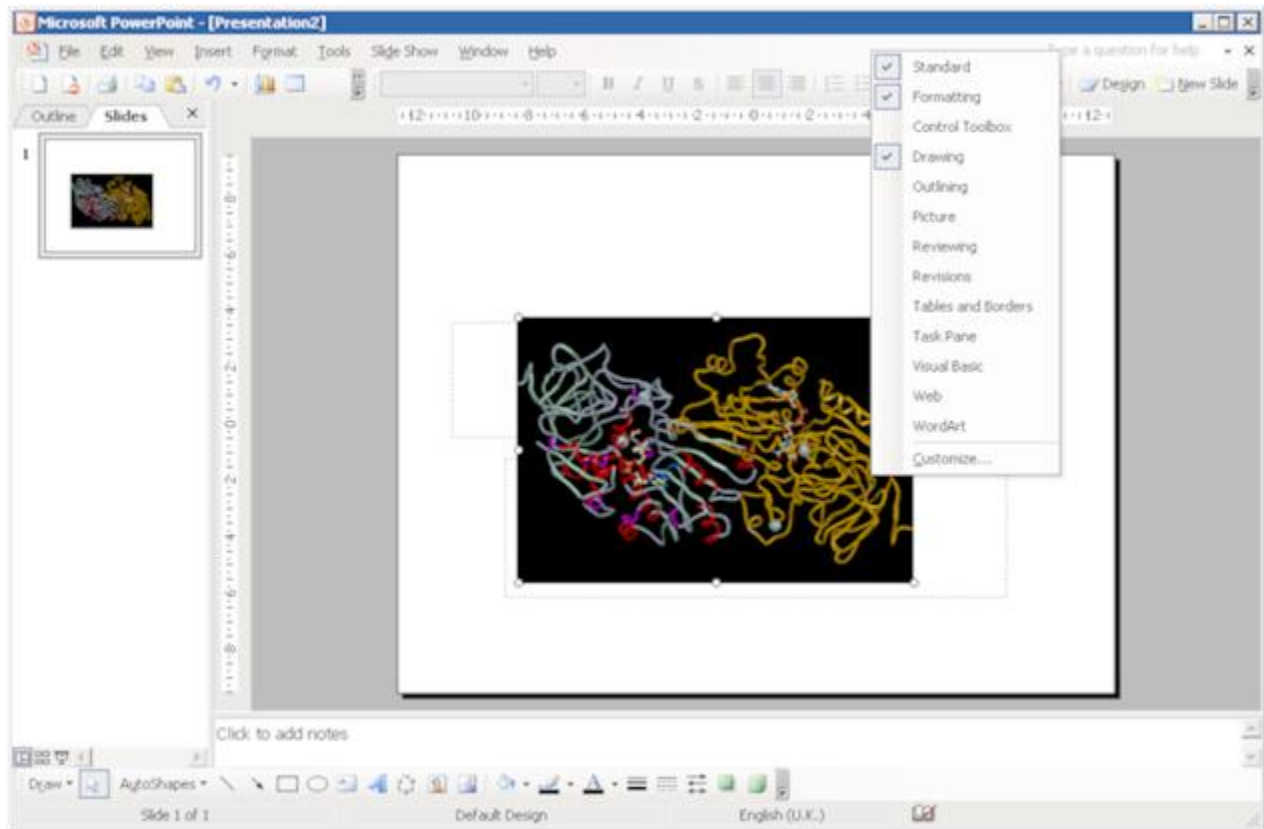
Documentation kindly provided by Dr. Brian Marsden (SGC Oxford  
<http://www.sgc.ox.ac.uk/people/brian/> )

It is possible to write simple VisualBasic scripts to avoid having to use the right-click menu approach to changing activeICM control slides within the control itself. This allows one to place buttons outside of the activeICM control, but in the same PowerPoint slide, which controls the control's behaviour. Below are a couple of useful examples of this approach.

### *Creating a button to set the control's active slide:*

#### *Insert a button Office 2003*

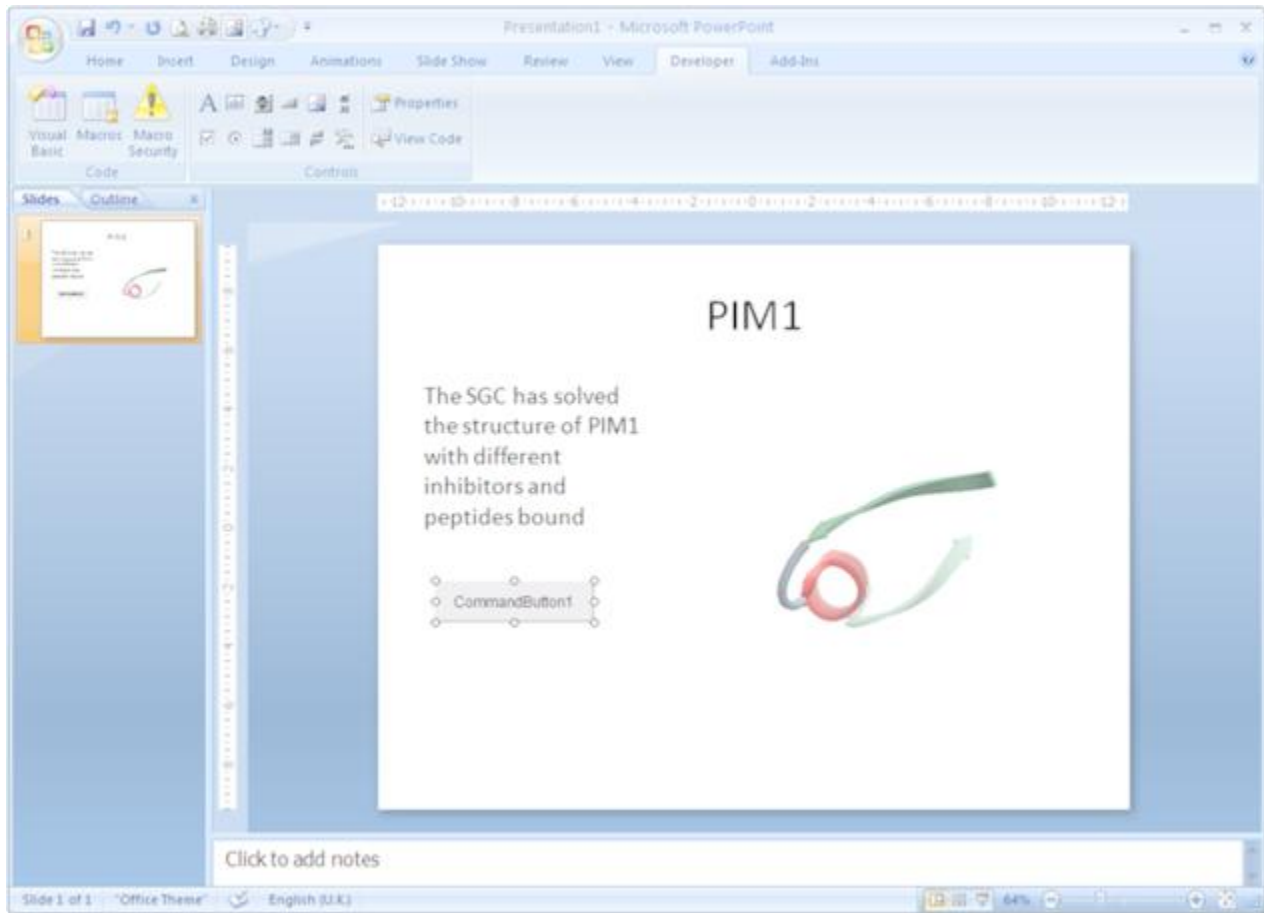
- In edit mode, make sure the control toolbox toolbar is shown by right-clicking the blank area at the top of the top bar and ensuring **Control Toolbox** is ticked.



- Click on an icon in the Control Toolbox which corresponds to the sort of button you wish to use. Then click and drag in the PowerPoint slide to generate the button.

#### *Insert a button Office 2007:*

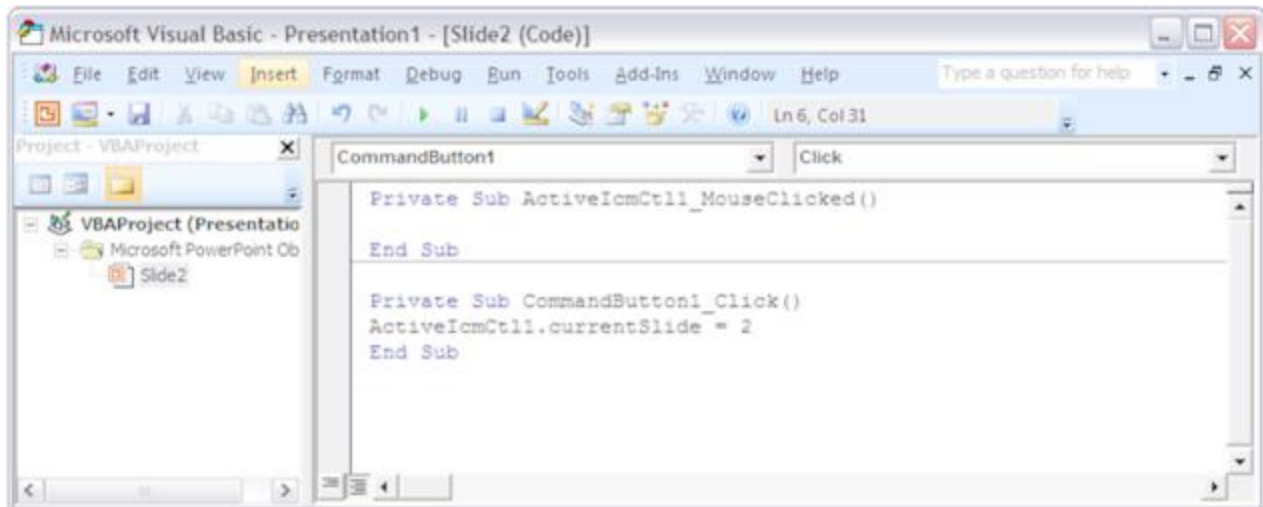
- In edit mode, click on an icon in the Developer menu or ribbon which corresponds to the sort of button you wish to use. Then click and drag in the PowerPoint slide to generate the button.



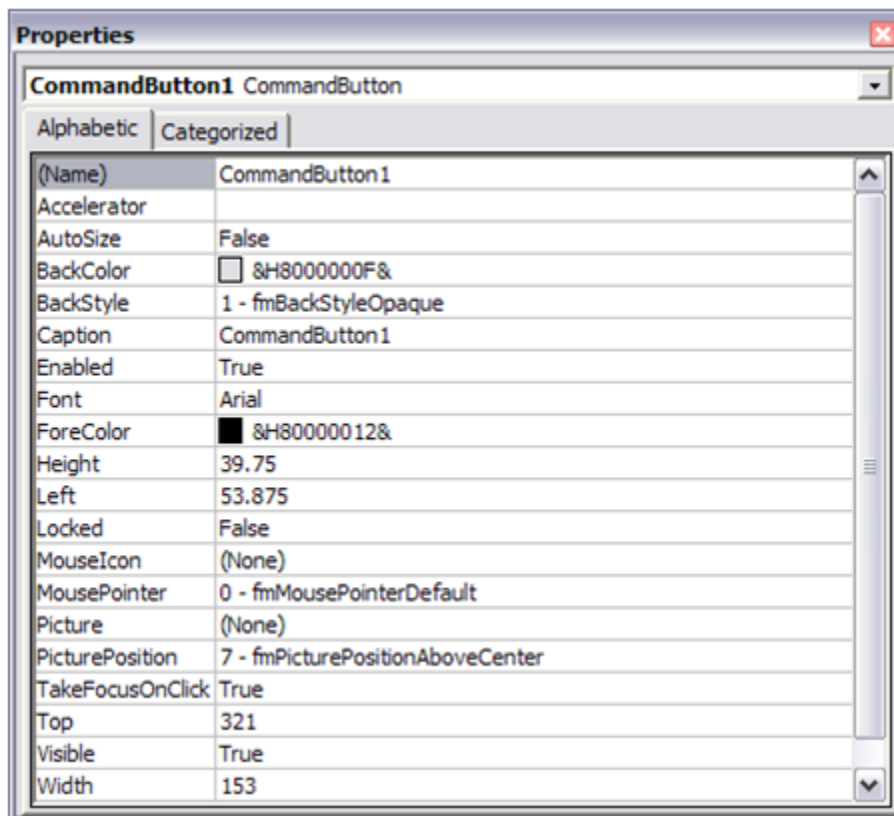
- Double-click on the new button to open the VisualBasic editor with two empty functions pre-defined. The first one pertains to the control itself and can be ignored in this context \*For the second function (which is for the newly-created button), copy the following into the editor, between the two lines of function code:

```
ActiveIcmCtl1.currentSlide = 2
```

- This sets the current activeICM control's slide to be number 3 **note** that the value placed in this code needs to be 1 less than the actual slide number (confusing, no?). Obviously, use a value here that makes sense in the context of your ICB file.
- This should leave the editor looking like this:



- Close the Visual Basic editor
- To change the physical properties of the button e.g. text, colour e.t.c.right-click on the button and select the Properties menu option. This opens up a dialogue as below, where many properties of the button can be changed:



- Using this dialogue, it should be possible to disguise the button to look like normal text (for example) which can be clicked on during the presentation to change the visualisation

of the control, apparently magically. Note that the button will only work in presentation mode.

- **IMPORTANT:** In Office 2007, remember to save the PowerPoint presentation now as a pptm file that is, a macro-enabled PowerPoint file otherwise the macros will not work next time you load the presentation.

**Other code examples:** Just copy and paste the example of interest inside the function for the button in the Visual Basic editor. Code that enables a button to cycle through the ICB files slides in order (including wrap-around)

```
currentSlide = ActiveIcmCtl1.currentSlide
numSlides = ActiveIcmCtl1.nofSlides
If currentSlide = numSlides - 1 Then
ActiveIcmCtl1.currentSlide = 0
Else
ActiveIcmCtl1.currentSlide = currentSlide + 1
End If
```

### 7.6.1 PowerPoint Cache Errors

PowerPoint caches some information about active controls. Sometimes after an ActiveICM upgrade you may get an error when trying to access some property or method: "Wrong number of arguments or invalid property assignment" or something similar.

In this case you need to close PowerPoint and remove all files from the location below:

C:\Documents and Settings\seva\Local Settings\Temp\PPT11.0

---

## 8 Protein Superposition

**Note:** Click **Next** (top right hand corner) to navigate through this chapter or click on the links below. Headings are listed on the left hand side (web version) or by clicking the **Contents** button on the left-hand-side of the help window in the graphical user interface.

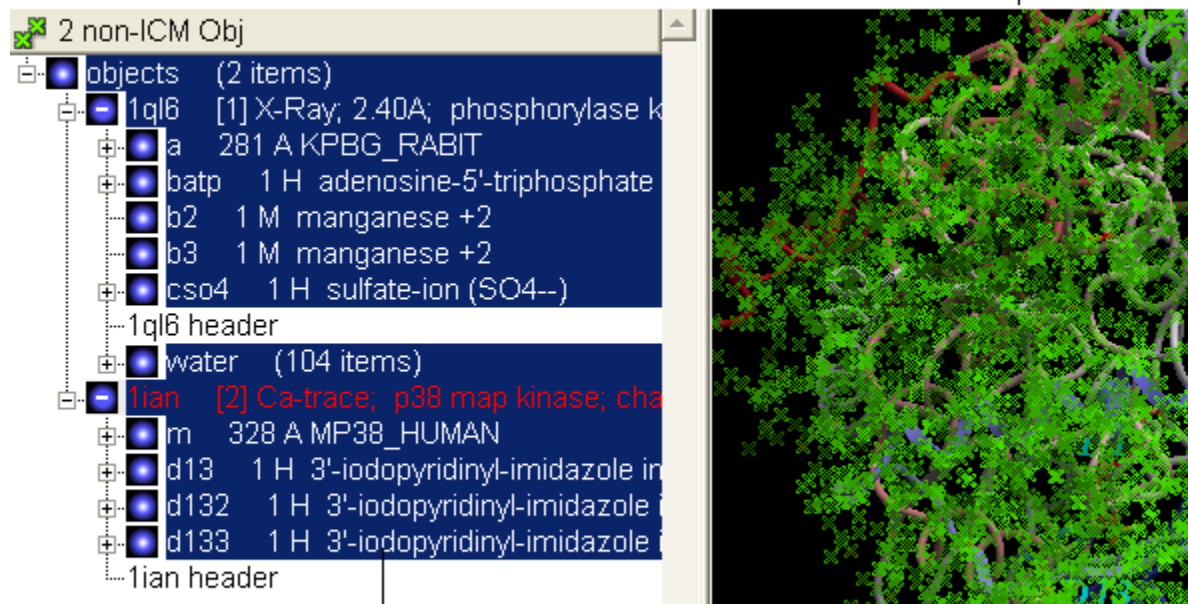
### 8.1 Protein Superposition

Before any superposition operation can be undertaken you need to select the protein structures you wish to superimpose.

One way to do this is by selecting in the ICM workspace. For other selection tools please see the **Making Selections** section of the manual.

- Select both receptors by double clicking on the name of the receptor in the ICM Workspace. To select two receptors use the Ctrl button or use the shift button to select a range of objects in the ICM Workspace. A receptor which is selected will be highlighted in blue in the ICM Workspace and with green crosses in the graphical display.

**Green crosses indicates that the object is selected in the graphical display**



**Highlighted blue means that the object is selected in ICM Workspace**

## 8.2 Superimpose Button

In order to calculate the root mean square deviation (RMSD) between two structures it is necessary to superimpose them. By using the superimpose button in the **display** tab, ICM will calculate the Ca-atom, backbone atom and heavy atom differences between the two structures. More advanced superimpose options can be found in the **Tools/Superimpose** menu.

To superimpose two structures which have the same number of residues and atoms:

- First load the two structures into ICM.
- Select which parts or all of the two structure you wish to superimpose (see *selection toolbar*).
- Select the **display** tab (previously called Advanced tab) at the top of the GUI.
- Select the superimpose button.



Superimpose  
Button

The rmsd will be displayed in the terminal window as shown below:

```
Info> 64 atoms superimposed, rmsd=1.381643  
icm/ly6> superimpose ( Res( as_graph ) & a_./ca,c,n,o ) & Obj( as_graph )[1]  
Warning> [110] skipped 4 atom pairs with zero occupancies  
Info> 64 atoms superimposed, rmsd=1.381643  
icm/ly6>
```

RMSD displayed here

---

## 9 Tutorials

**Note:** Click **Next** (top right hand corner) to navigate through this chapter. Headings are listed on the left hand side (web version) or by clicking the **Contents** button on the left-hand-side of the help window in the graphical user interface.

### 9.1 Graphical Display Tutorial: Molecule Representation, Coloring, Labeling and Annotation

#### 9.1.1 Change Molecule Representation and Color

**1. Click on the "Search" tab**

**2. Enter search string "2vz6"**

**3. Click on the search button and a table of hits will be displayed**

**4. PDB structure is automatically listed in the ICM Workspace and displayed**

Load a kinase structure from the PDB.

```

... ICM startup file executed...
icm> generalSearchFromDB "PDB Search" "2vz6"
Info: PDB index loaded from C:\Program Files\Biosoft\ICM\ICM_Pdb_17\data\icm\pdb.tbl
Message: [177] 17 mapping SEQRES residues (met ...) before lev [x -5 ]
Message: [177] 8 mapping SEQRES residues (glp ...) before pbc [x 24 ]
Message: [177] 17 mapping SEQRES residues (met ...) before lev [x -5 ]
Message: [202] Structure: a_2vz6.d\*d1\lev_a_2vz6.d\F24.cx | * 0.01, too large
icm>2vz6>
  
```

7/16/1/06



2018-08-01 10:37:34 (NewProject) [1] vj[m]

File Edit View Search Tools Home Help Chemistry Docking Molecular Dynamics Windows Help

Change the background color.

1. Right click here

The screenshot shows the PyMOL interface with a protein structure rendered in a multi-colored ribbon representation. A callout box with the text "1. Right click here" points to the top toolbar, specifically to the color selection icons. The left sidebar contains a "Workspace Panel" with a list of objects including "2vrs", "291A", "294A", "ahf", "ago", "ago2", "ahf", "ago", and "W". The bottom status bar shows the command "set background rgb=155,155,155" and the text "Welcome to PyMOL".

Workspace Panel

- no selection
- objects (1 items)
- 2vrs [1] XPC\_23A
- a 291A 1 site FICCD2A\_HUMAN
- b 294A 1 site FICCD2A\_HUMAN
- ahf H (2z,3e)-2,7-bisindole-7,3(1h,1y)-diol
- ago H 6-1,2-propanediol
- ago2 H 6-1,2-propanediol
- ahf H (2z,3e)-2,7-bisindole-7,3(1h,1y)-diol
- ago H 6-1,2-propanediol
- calcium-calmodulin dependent protein kinase t
- W [311] water molecules

```
set background rgb=155,155,155
```

Welcome to PyMOL

2018 Microsoft Word 3.7.2x (NewProject) [1] (obj[1])

File Edit View Insert Tools Homepage Chemistry Docking 3DReference Windows Help

Display the "a" subunit and ligand.,

1. Click in the boxes to display and undisplay

2. Use these buttons to rotate molecule

The screenshot shows the PyMOL molecular visualization software interface. The main window displays a ribbon representation of a protein structure with multiple subunits colored in a rainbow gradient (red, orange, yellow, green, blue, purple). A 'Workspace Panel' on the left lists objects: 'a' (291 A 1 site FICCD2A\_HUMAN), 'b' (294 A 1 site FICCD2A\_HUMAN), and 'H' (2z,3e]-2,7]-indole-7,3]-th,11]-don). A callout box labeled '1. Click in the boxes to display and undisplay' points to the checkboxes next to these objects. On the right side of the interface, a vertical toolbar contains various controls, with a callout box labeled '2. Use these buttons to rotate molecule' pointing to the rotation icons. The bottom status bar shows the command history and the text 'Welcome to PyMOL'.

```
PyMOL> [102] 31840001 a_2vx6.a* 61126 a_2vx6.a* 914/26 1 0 8.31 500 large
PyMOL> color background rgb=(155,155,155)
PyMOL> undisplay atome a_2vx6.b
PyMOL> undisplay atome a_2vx6.bppp
PyMOL> undisplay atome a_2vx6.bttf
PyMOL> undisplay atome a_2vx6.bppp2
PyMOL> undisplay atome a_2vx6.bppp3
PyMOL>
```

Welcome to PyMOL

2/16/1/06

2vst Molsoft Inc 3.7.2a [NewProject #] (1 object)

File Edit View Search Tools Help/Help Chemistry Docking Mathematics Windows Help

1. Click and hold

Color ribbon by secondary structure segment.

Note: All representation buttons have similar coloring options

objects

- 2vst
- 1 KR\_2 3A
- 1 A 1 site KCC3A
- 1 A 1 site KCC3A
- H (2z\_3e) 2 2' 6e
- H s-1 2-proparg
- H s-1 2-proparg
- H (2z\_3e) 2 2' 6e
- H s-1 2-proparg
- n-calmodulin depo
- 11 water molecule

secondary structure

- residue
- residue
- object
- factor
- accuracy
- residue order
- accessibility
- hydrophobicity
- polarity
- hloc
- user field
- alignment

```
1)om/2vst> aa_graph * atom; Res; aa_graph | |
1)om/2vst> undisplay wire aa_graph
1)om/2vst> display wire aa_graph
1)om/2vst> undisplay wire Res(a_*///50)
1)om/2vst> color ribbon Res(a_*///50) ribbonColorStyle="Boc"
1)om/2vst> color ribbon Res(a_*///50) ribbonColorStyle="Boc"
1)om/2vst> color ribbon structure Res(a_*///50)
1)om/2vst>
```

Welcome to PyMOL 2.0.1.0

Color Beta 3 strand yellow.

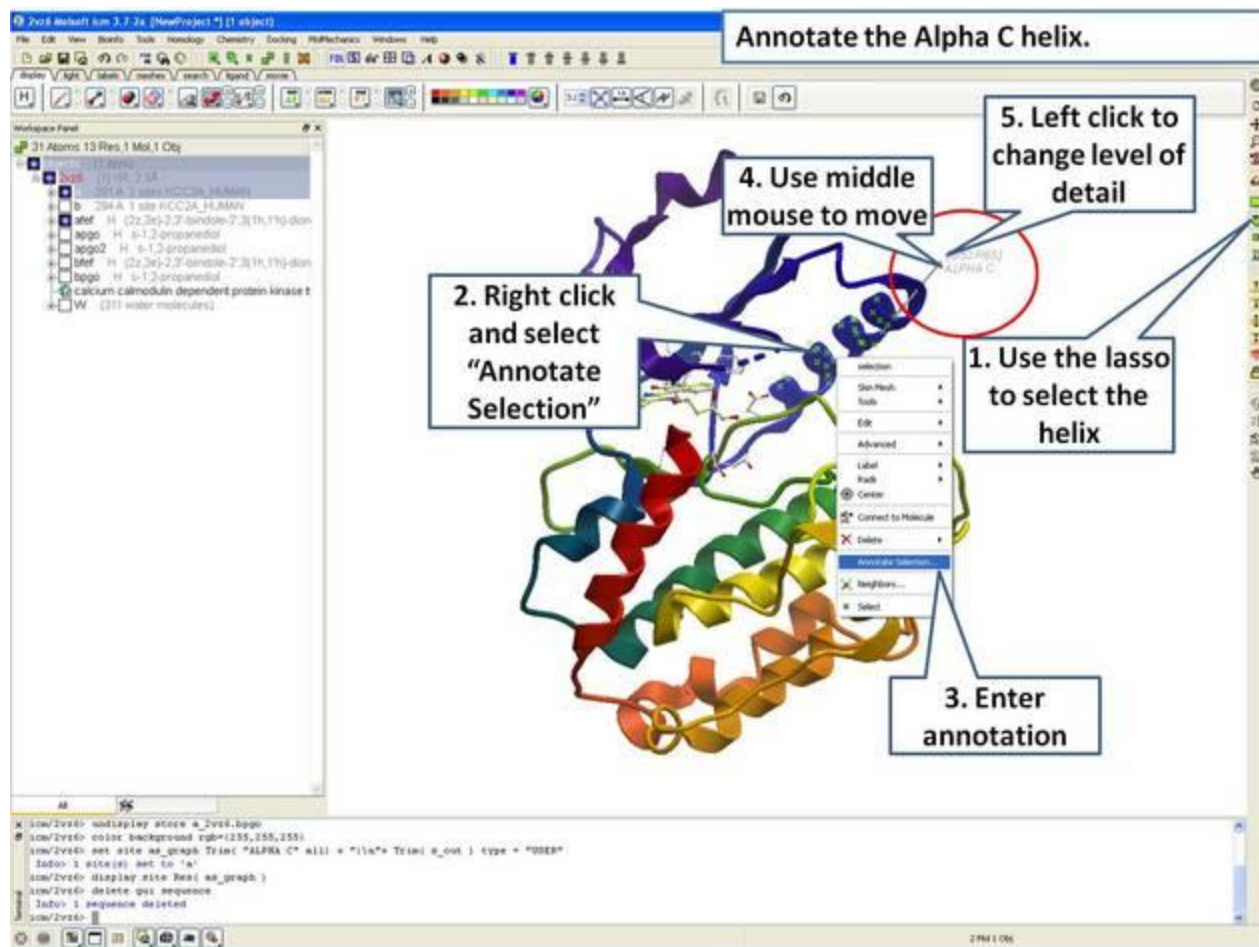
3. Click on yellow

2. Click and drag to select Beta 3 strand (residues 37 to 43)

1. Expand to see sequence here

The image shows a PyMOL 1.7.3.2 interface with a protein ribbon structure. The Beta 3 strand is highlighted in yellow and circled in red. The sequence viewer on the left shows the protein sequence: 1:STQQLFQLF EELQFDVVE, 2:KVVVLAQV DQVQITLTK, 3:LAAPDGLL DRAITLQV, 4:RSLVLSGLL ISEIQQTSL, 5:FLVYDGLL EELQFDVVE, 6:LAAPDGLL ILEAVLWQ, 7:KSLVLP ENLLADPL. The command console at the bottom shows the following commands: Info: 1 plot(0, 0, 0, 'a'), sm/2vs0 display site Res( aa\_graph ), sm/2vs0 delete qsi sequence, Info: 1 sequence deleted, sm/2vs0 aa\_graph = atom Res( aa\_graph ), sm/2vs0 color aa\_graph rgb=(155,155,0), sm/2vs0 color ribbon aa\_graph rgb=(155,155,0), sm/2vs0.

## 9.1.2 Annotation



### 9.1.3 Labels

# Display and Label Beta 3 to Alpha C Salt Bridge (1)

1. Click on "Filter Graphical Selection" button

2. Click "by type"

2. Check the charged residues (Asp, Glu, Arg, and Lys)

The image shows a PyMOL interface with a protein structure rendered in a multi-colored ribbon representation. A 'Selection properties' dialog box is open, showing the 'by type' section with checkboxes for various amino acid types. The 'asp' checkbox is checked. A callout box points to the 'Filter Graphical Selection' button in the top toolbar. Another callout box points to the 'by type' section of the dialog. A third callout box points to the checked 'asp' checkbox. The bottom of the window shows a command line with the following text:

```
Info: 1 site(s) set to 'A'  
sm/2vs0: display site Bse( aa_graph )  
sm/2vs0: delete qsi sequence  
Info: 1 sequence deleted  
sm/2vs0: aa_graph = Atom( Res( aa_graph ) )  
sm/2vs0: color aa_graph rgb=(155,155,0)  
sm/2vs0: color ribbon aa_graph rgb=(155,155,0)  
sm/2vs0:
```

2018 Molecules.com 3.7.2a [NewProject] (1 object)

File Edit View Reports Tools Home/Obj Chemistry Coding Help/Help... 201806\_2018

1. Click here to propagate selection to all atoms in residue

2. Click here to display all charged residues in wire

Display and Label Beta 3 to Alpha C Salt Bridge (2)

Workspace Panel

74 Res 1.0 Obj

2018

1-5 1.12  
29  
49  
69  
89  
109  
129  
149  
169  
189  
209  
229  
249  
269  
289

Site(s) (2 term(s))

- 204 A 1 site HCCGA\_HUMAN
- afef H (22\_3e)-2,3'-bisubtle-2,3'(1n,1f)-don
- apgo H s-1,2-gppanediol
- apgo2 H s-1,2-gppanediol
- bfef H (22\_3e)-2,3'-bisubtle-2,3'(1n,1f)-don
- bpgo H s-1,2-gppanediol
- calcium calmodulin dependent protein kinase t
- W (31) water molecules

```
sm/2vs0 delete gpi sequence  
Info: 1 sequence deleted  
sm/2vs0 as_graph + Atom Resi as_graph |  
sm/2vs0 color as_graph rgb=155,155,0  
sm/2vs0 color rslboon as_graph rgb=155,155,0  
sm/2vs0 as_graph + Atom Resi as_graph |  
sm/2vs0 display wire as_graph  
sm/2vs0
```

2018 06

### Display and Label Beta 3 to Alpha C Salt Bridge (3)

The image shows a PyMOL interface with a protein structure. The protein is shown as a ribbon with a color gradient from green to blue. Two residues, K42 and E60, are highlighted in red. The interface includes a toolbar at the top, a workspace panel on the left, and a command line at the bottom. Five numbered callouts provide instructions for displaying and labeling the salt bridge.

1. Undisplay all xstick representations for clarity
2. Use the zoom in button to locate alpha C to beta 3 salt bridge
3. Click on the residue label button
4. Click on each residue to label
5. Click and hold on the residue label coloring and style options

```
sm/2vs0 color ribbon as_graph rgb=(155,155,0)
sm/2vs0 color ribbon as_graph rgb=(155,155,0)
sm/2vs0 as_graph * Atom| Res| as_graph | |
sm/2vs0 display wire as_graph
sm/2vs0 color residue label Res[*_*//80] rgb=(0,0,0)
sm/2vs0 cancel sm/2vs0 as_graph
sm/2vs0 undisplay xstick Res[*_*//80]
sm/2vs0
```



1. Undisplay wire and other label annotations from previous examples

2. Right click on the "a" subunit ligand and choose "Select Neighbors"

3. Enter the parameters as shown

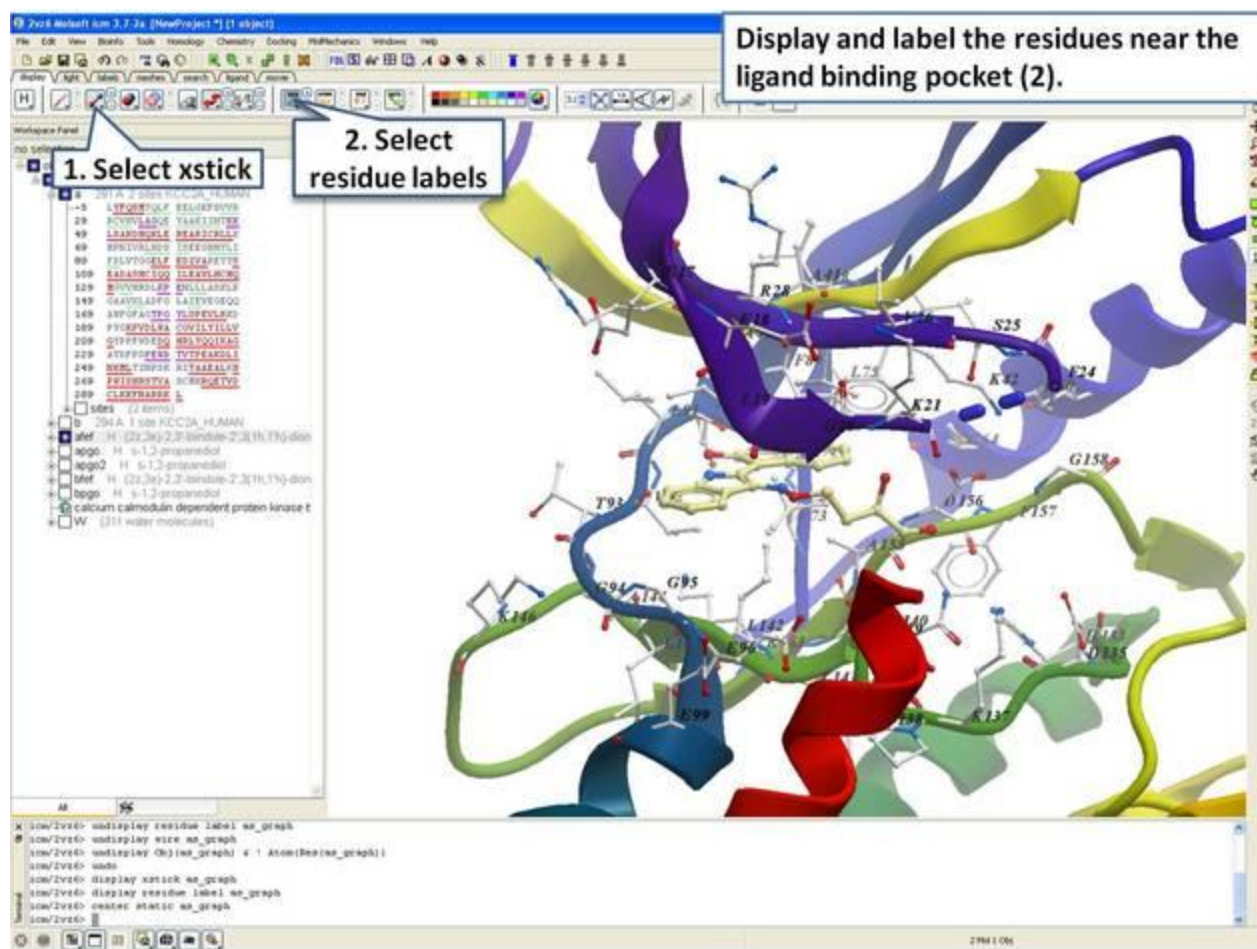
4. Propagate selection to all atoms

Display and label the residues near the ligand binding pocket (1).

```
1 sm/2vc6: no_graph = no_graph 4 a *.1R
2 sm/2vc6: GRASP5C0.selectionLevel = "atom"
3 sm/2vc6: no_graph = atom (Res( no_graph ) )
4 sm/2vc6: display wire no_graph
5 sm/2vc6: display residue label no_graph
6 sm/2vc6: undisplay residue label no_graph
7 sm/2vc6: undisplay wire no_graph
8 sm/2vc6:
```

Command line output:

```
49  ...  IDVARETYE
109  ...  ELKAVIKWQ
129  ...  ...
149  ...  LAITVEQGG
169  ...  ...
189  ...  ...
209  ...  ...
229  ...  ...
249  ...  ...
269  ...  ...
289  ...  ...
d 294 A 1 str HCC3A HUMAN
a 301 H 12.3e1-2.2f-bindole-2.3(1h,1h)-don
app0 s-1.2-proparedol
app2 s-1.2-proparedol
b 302 H 12.3e1-2.2f-bindole-2.3(1h,1h)-don
bpg0 s-1.2-proparedol
c 303 H 12.3e1-2.2f-bindole-2.3(1h,1h)-don
c 304 H 12.3e1-2.2f-bindole-2.3(1h,1h)-don
W
```



## 9.1.4 2D and 3D Labels

Create and display a 2D label.

1. Select the labels tab

2. Select the 2D label button

3. Add text and format

Calcium Calmodulin Dependent Protein Kinase



```
sm/2vs0: graphics.selectionLevel = "none"
sm/2vs0: aa_graph = atom [sel aa_graph ]
sm/2vs0: display xatom aa_graph
sm/2vs0: aa_graph = a_1//35
sm/2vs0: display xatom label aa_graph
sm/2vs0: display label "Calcium Calmodulin Dependent Protein Kinase" #size 36 #font "arial" bold rgb(255,0,0)
sm/2vs0: |
```

2018 Redshift 3.7.2a [NewProject] (1 obj[1])

File Edit View Panels Tools Hierarchy Chemistry Docking HMRFeatures Windows Help

2D 3D 3D

Right click here to edit or delete

How to edit, delete and move a 2D label.

Workspace Panel

no selection

objects (1 item)

- 2vc5 [1] XFC 2.3A, calcium-calmodulin dependent protein kinase type I
- a 291 A 1 site FICCGA\_HUMAN
- b 294 A 1 site FICCGA\_HUMAN
- ahf H [(2z,3e)-2,7]indole-2,3,4-tri-one-3-*o*-(3*o*)-3,4-dihydro
- agp0 H 5-1,2-propanediol
- agp2 H 5-1,2-propanediol
- ahf H [(2z,3e)-2,7]indole-2,3,4-tri-one-3-*o*-(3*o*)-3
- agp0 H 5-1,2-propanediol
- W [31] water molecules

Calcium Calmodulin Dependent Protein Kinase

label: Calc...

Edit

Delete

Click here with middle mouse button to move

Color

Font

Size

Style

OK Cancel

```
sm/2vc5: OBJECTS.selectionLevel = "GROUP"
sm/2vc5: aa_graph = atom [aa] (aa_graph | )
sm/2vc5: display xstick aa_graph
sm/2vc5: aa_graph = a_1//3D
sm/2vc5: display xstick label aa_graph
sm/2vc5: display label "Calcium Calmodulin Dependent Protein Kinase" #size 20 #font "arial" bold cgb=(135,1,55)
sm/2vc5: |
```

2018 1.06

2018 Robert van 3.7.2a (BioProject "1") v3a(1)

1. Select the labels tab

2. Select the 3D label button

3. Add text and format

Create and display a 3D label. A 3D label will move with the object when rotated or translated.

Calcium Calmodulin Dependent Protein Kinase

PDB Code 2VZ6

New Label

PDB Code 2VZ6

Color: [Color palette]

Font: [Font dropdown]

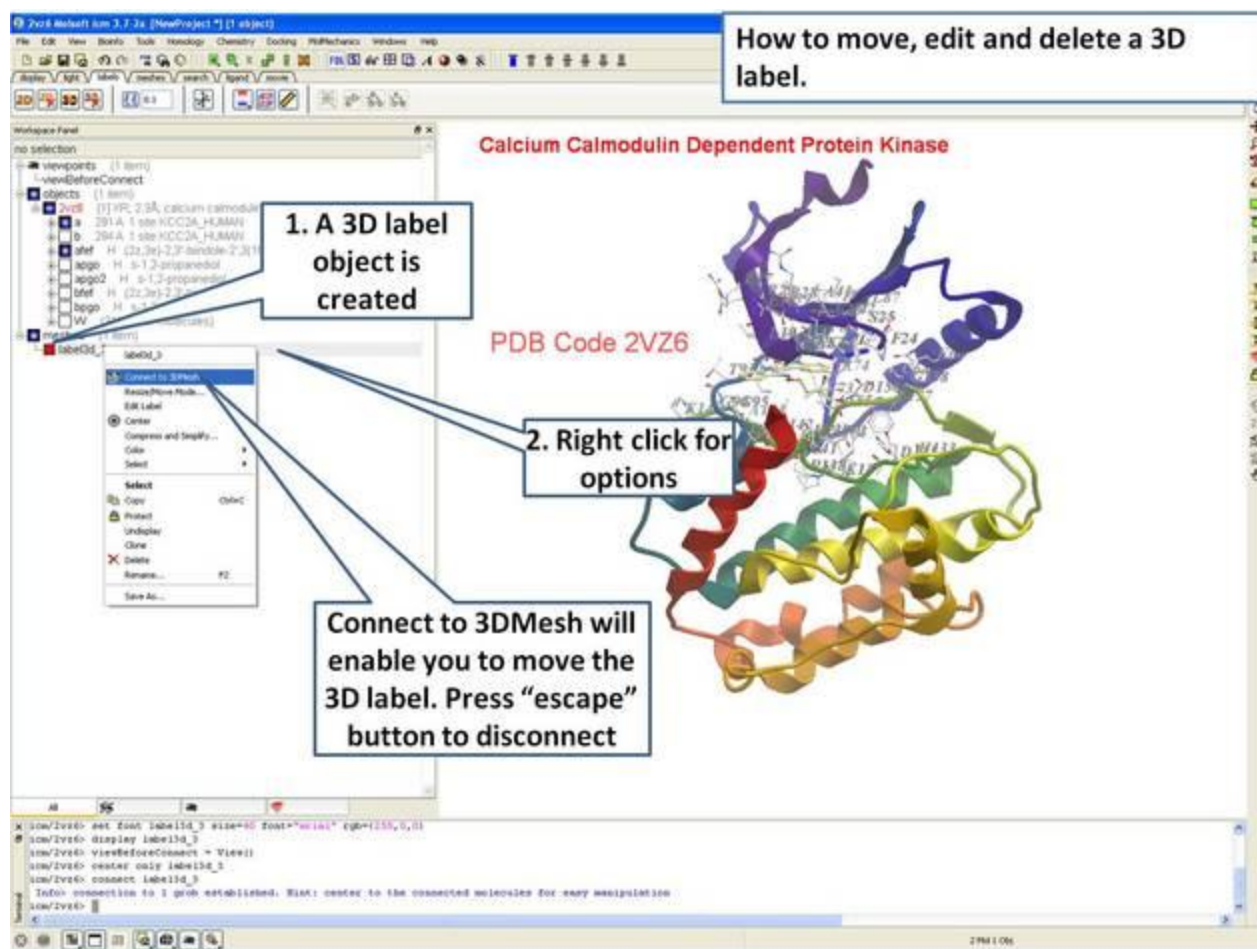
Size: [Size dropdown]

bold

Label will be placed at the graphically selected atom. Number it and press ESC.

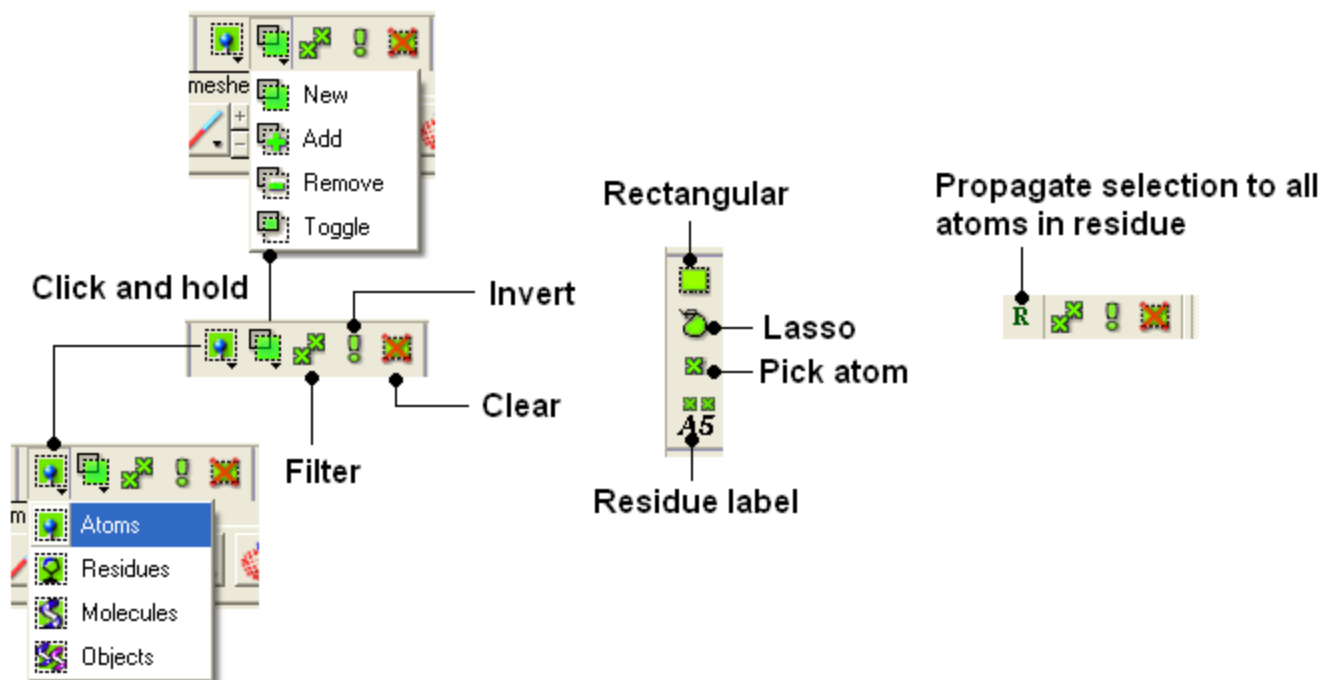
```
lsm/2vs6> set font label13_3 size=40 font="arial" rgb=(255,0,0)
lsm/2vs6> display label13_3
lsm/2vs6> viewBeforeConnect = View1
lsm/2vs6> center only label13_3
lsm/2vs6> connect label13_3
Info: connection to 1 grab established. Hint: center to the connected molecules for easy manipulation
lsm/2vs6>
```

2/16/1/06

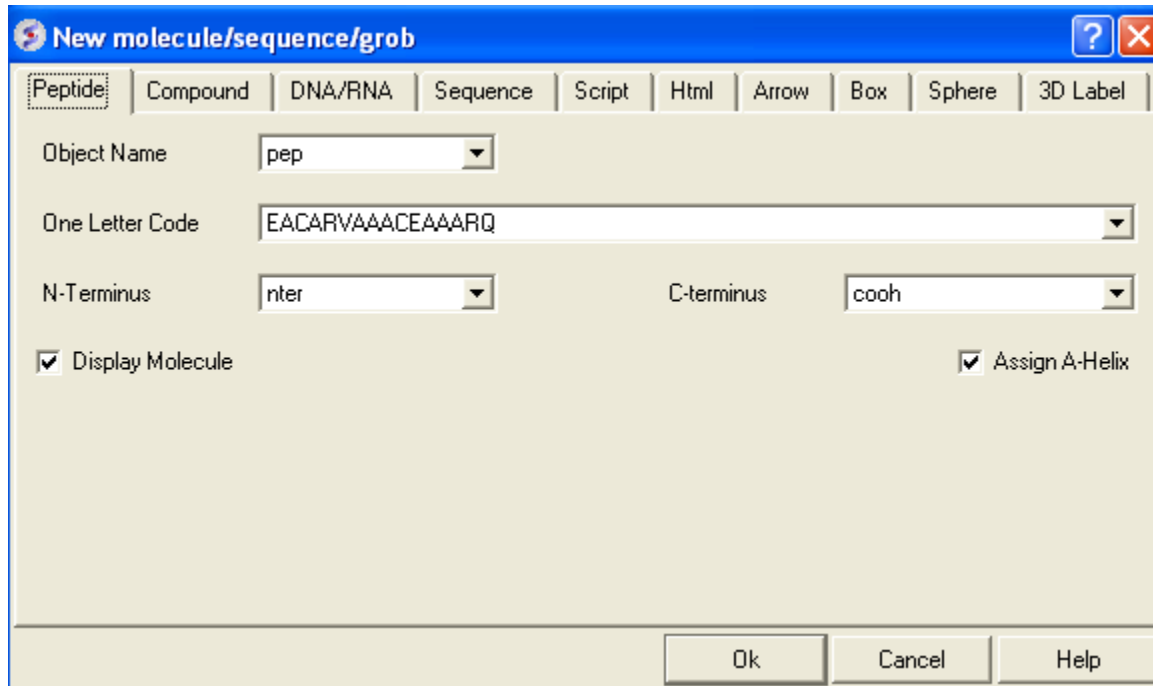


## 9.2 Graphical Selections Tutorial

All buttons relating to graphical selections are shaded green. These buttons are shown here and are located at the top of the graphical user interface and along the side.



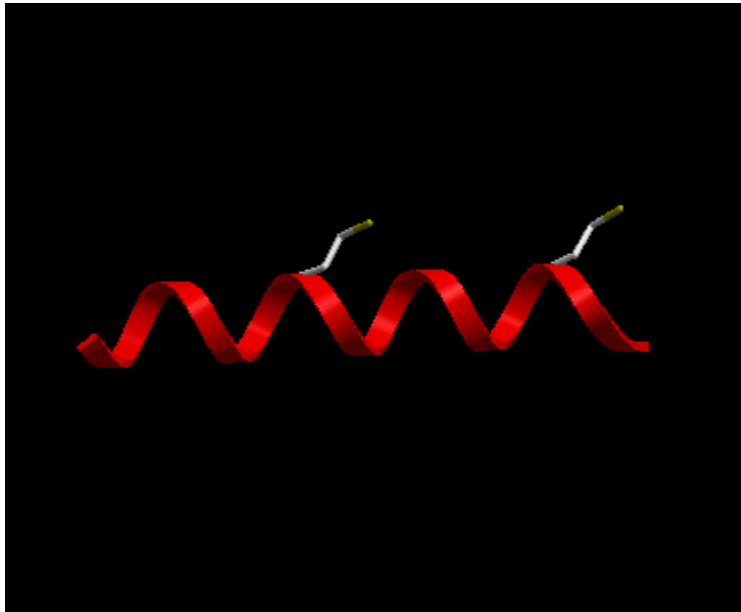
The **File/New window** is a great place to start learning how to use ICM as it provides a quick and easy way to generate new peptides, compounds, DNA/RNA, sequences and graphical objects.



The examples in this section will take you through the basics of making selections in the graphical user interface using objects generated from File/new.

## 9.2.1 Making Basic Selections

- File/New - Select Peptide Tab and use the default peptide entries and select OK. A peptide as shown below will be displayed in ribbon format and the cysteine side-chains in xstick.

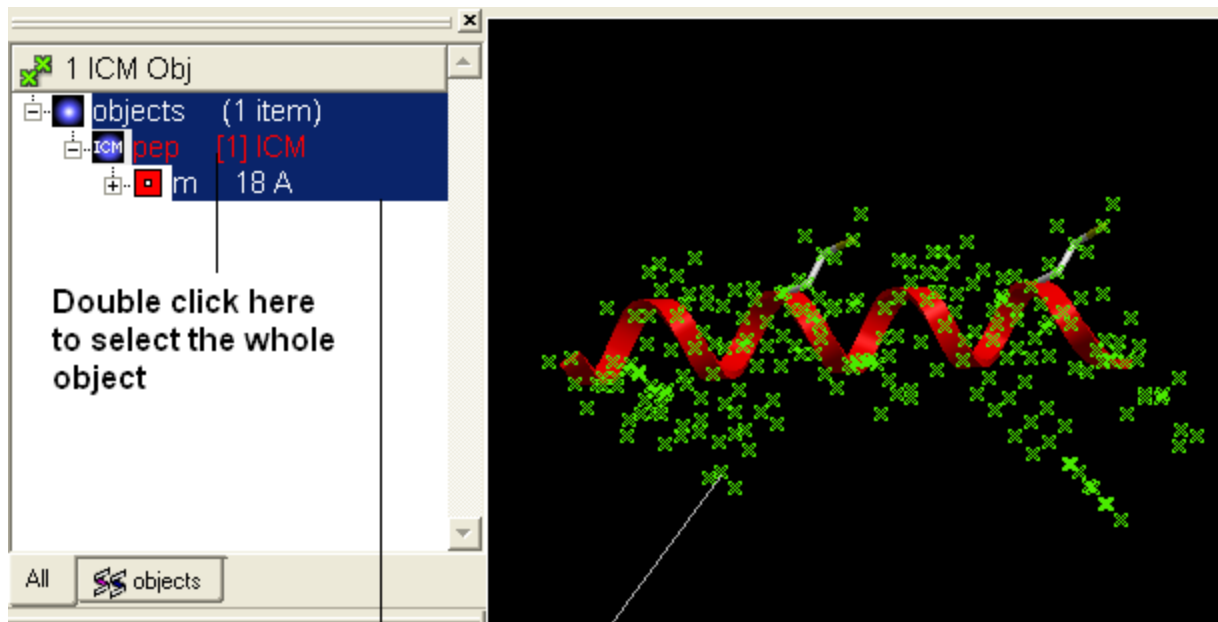


*Now let us display the peptide in wire format and remove the ribbon and xstick representation*

To do this:

- Select the whole object by double clicking on the name of the object "pep" in the ICM Workspace. When selected it will be highlighted in blue in the ICM Workspace and green crosses in the graphical display.





Selected regions will be highlighted blue in the ICM Workspace and as green crosses in the graphical display

- Select the "Display Tab" and select the wire button to display wire representation. Select the ribbon button and xstick button to undisplay ribbon and xstick.

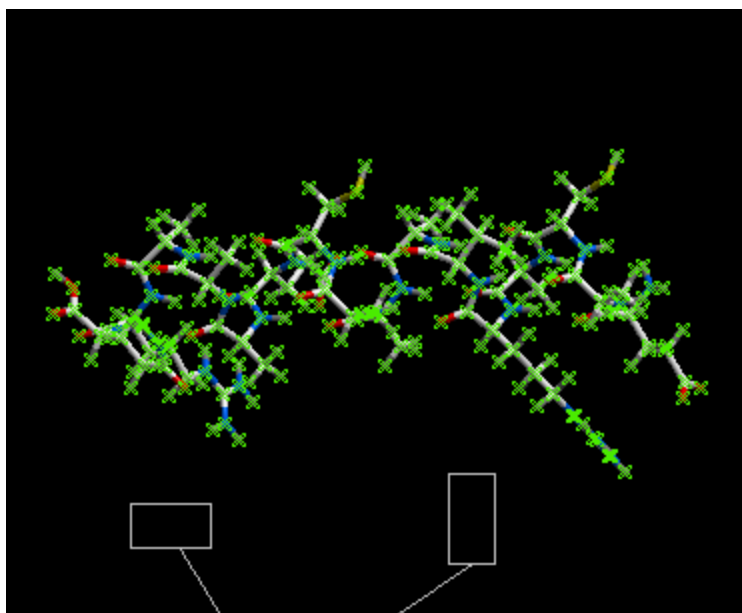


Click here to display wire

Click here to undisplay ribbon

Click here to undisplay xstick

- Your peptide will still be selected. See below on how to remove selections.



Right click and drag in any blank space to remove the selection (green crosses).

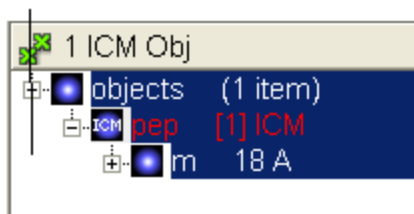
OR

Use the unselect button



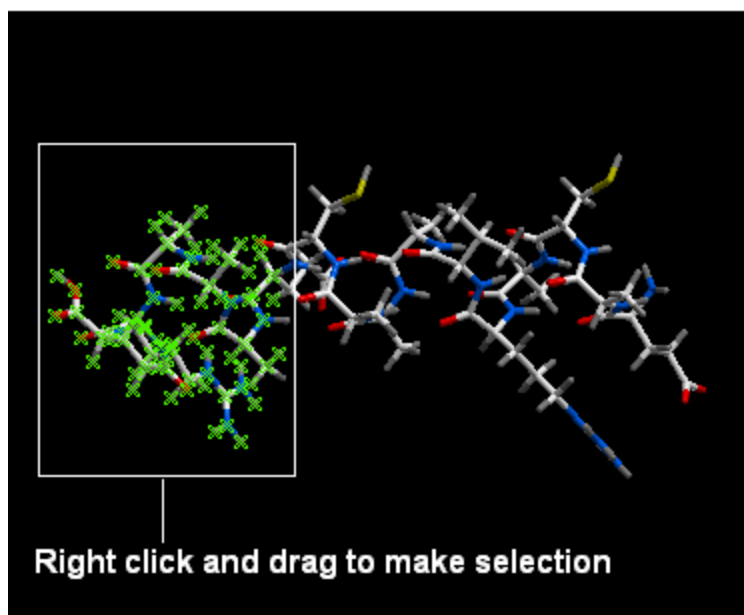
OR

Click in white space in the ICM Workspace

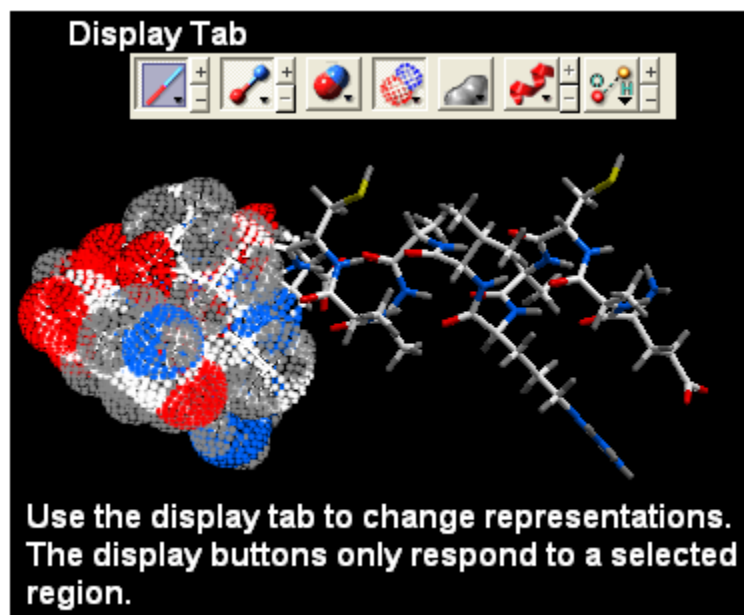


*Now we will display different parts of the peptide in different representations.*

- Right click and drag over a region of the peptide you would like to change.



- Use the display panel to select the representation you would like to display.



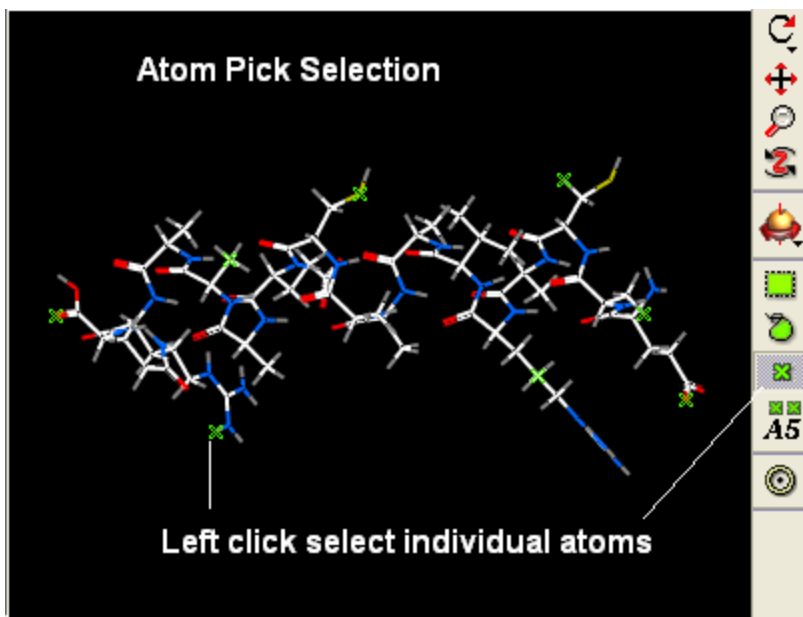
*Other ways of making selections.*

### Rectangular Selection

Select button and use left mouse button to make graphical selection

### Lasso Selection

Left click and drag



## 9.2.2 Making Sequence Selections in the ICM Workspace

- File/New - Select Peptide Tab and use the default peptide entries and select OK. A peptide as shown below will be displayed in ribbon format.

Selections can be made on the sequence of the peptide. This can be done by expanding the sequence display in the ICM Workspace and clicking and dragging on the sequence as shown below. Non-contiguous selections can be made by clicking/dragging over the sequence whilst holding down the Ctrl key.

Selection information highlighted here

Click here to expand sequence information

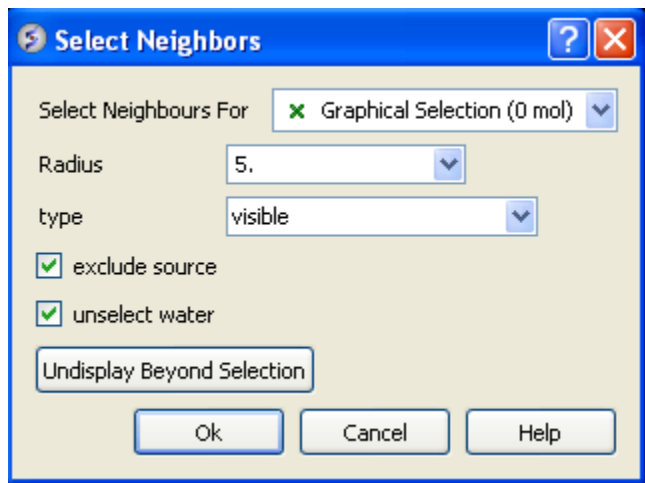
Click and drag to select sequence

Residues that have been selected are highlighted in blue

## 9.2.3 Making a Spherical Selection.

In this example we will select the residues surrounding a ligand.

- PDB Search tab (PDB code **1MVC**)
- Right click on the ligand **bm6** in the ICM Workspace.
- Select the **Neighbors** option

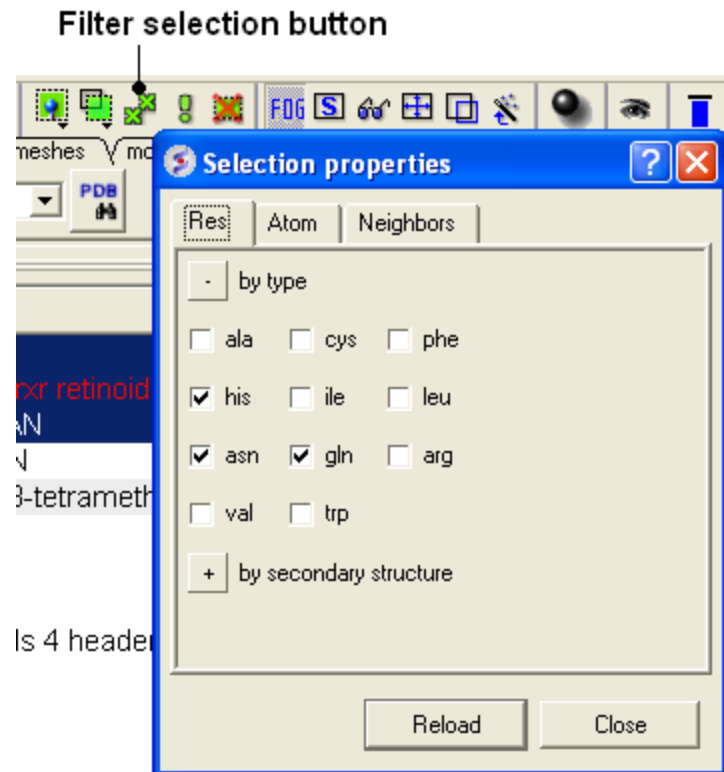


- In the "Select Neighbors For" box leave as Graphical Selection (1 mol)
- Enter Radius 5.
- Enter type **same\_object\_other\_chains**
- Choose **exclude source** and **unselect water**.
- You will see green crosses surrounding the ligand binding pocket.

#### 9.2.4 Filtering a Selection.

In this example we will filter the selection made in the previous example and select only His, Asn, Gln and Pro residues surrounding the ligand.

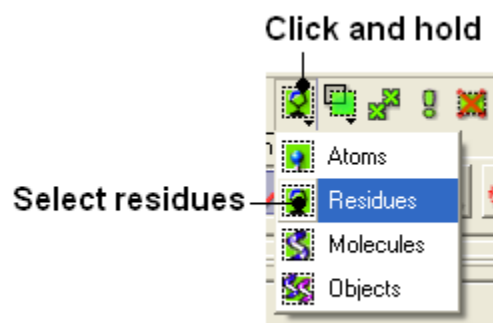
- Make a spherical selection surrounding the ligand in PDB structure \*1MVC (See earlier example).
- Click on the **Filter graphical selection button**.
- Click on the **Res** tab
- Select His, Asn, Gln and Pro residues.



**NOTE:** Only amino acid residues in the current selection will be available in the **Filter**.

Display the selected residues in wire format.

- Change the selection from **Atom** to **Residue**.



- Select the wire representation button in the **display** tab.

**9.2.5 Propogating a selection to all atoms in a residue.**

Sometimes it is useful to propagate a selection to all atoms in a residue. For example when selecting the residues surrounding a ligand within a certain angstrom radius the selection will only pick up certain atoms of a residue. The button shown below can be used to propagate the selection to all atoms in a residue.

Propagate selection to all atoms in residue



### 9.3 Generating Fully Interactive Slides for PowerPoint and the Web Tutorial

The screenshot shows the ICM software interface with the following steps and annotations:

- 1. Click on the "Search" tab**: The "Search" tab is selected in the top menu bar.
- 2. Enter search string "1xws"**: The search string "1xws" is entered into the search bar.
- 3. Click on the search button and a table of hits will be displayed**: The search button is clicked, resulting in a table of search hits.
- 4. PDB structure is automatically listed in the ICM Workspace and displayed**: The PDB structure is automatically listed in the ICM Workspace and displayed as a 3D ribbon model.

The command window at the bottom shows the following text:

```

x Backlog: Loading analysis... _save
...ICM startup file executed...
lcm/det> generalSearchFromPDB "PDB Search" "1xws"
Enter PDB index loaded from C:/Program Files/Molecular ICM/Source/ICM-Viewer-Pdb_0/Data/iso/PDB.tbl
Package (176) is waiting to get results from ... before you go [x]
lcm/lxws
  
```



Convert the structure from PDB format into an ICM object.

The screenshot displays the Jvarkit software interface. On the left, a tree view shows a list of objects, including '1. 273 A' and '1. 273 B'. A callout box points to the '1. 273 A' entry with the text: "1. Right click here and select 'Convert PDB'". The main window shows a 3D ribbon representation of a protein structure in various colors (blue, green, yellow, orange). A dialog box titled "Convert to ICM" is open, with two checked options: "delete water" and "replace the original". A callout box points to the "OK" button with the text: "2. Enter the options as shown and press OK." The bottom of the window shows a command prompt with the following text: "Startup: Loading modules... success", "...ICM startup file executed...", "Info: PDB index loaded from C:/Program Files/Boisont 1.0/Boisont 1.0-Resource-Pdb\_0/data/idx/PDB.tbl", "Warning: [175] 50 missing SEQRES residues (see ... and/or pss [w 11 ]", and "Jvarkit: [175]".

1. Right click here and select "Convert PDB"

2. Enter the options as shown and press OK.

Prepare the 1<sup>st</sup> slide: Orientate the structure in the graphical display.

1. Use these buttons to rotate and move the structure.

2. Undisplay the sulfate molecule by clicking here

3. Undisplay the default molecule labeling by clicking here

4. Undisplay the default molecule annotations by clicking here

The image shows a PyMOL software window with a protein structure rendered in a ribbon representation. The structure is primarily yellow and green, with some blue and red elements. The interface includes a menu bar at the top, a toolbar with various icons, and a console window at the bottom. Four callout boxes with white backgrounds and black text provide instructions on how to orientate and clean up the display. The first box points to rotation and movement buttons in the toolbar. The second box points to a button in the toolbar to hide the sulfate molecule. The third box points to a button in the toolbar to hide default molecule labeling. The fourth box points to a button in the toolbar to hide default molecule annotations. The console window at the bottom shows a series of messages related to the protein structure.

The image shows a screenshot of the ICM (Interchange) software interface. The main window displays a 3D ribbon model of a protein structure, colored in shades of purple, green, yellow, and orange. A callout box at the top right contains the text: "Make the 1<sup>st</sup> slide: A view of the first subunit with ligand displayed." A callout box on the left side of the workspace panel contains the text: "2. Note: Slide is listed in the ICM Workspace". A callout box at the bottom left points to a button in the interface with the text: "1. Click here to make a slide". The workspace panel on the left shows a tree view with "slides" and "objects" folders. The "slides" folder contains "Slide 1". The "objects" folder contains "ICM", "273 A", "273 B", "ligand", "site", and "proto-oncogene serine/threonine-protein kinase pim-1, chain". The bottom of the interface shows a command line with the following text: "lcm/lcm: create static on\_graph", "lcm/lcm: undisplay atom a\_lcm\_sen4", "lcm/lcm: undisplay residue label 100", "lcm/lcm: undisplay site Resid\_1", "lcm/lcm: add slide display", "lcm/lcm: "

1. Click here to expand display to sequence level.

2. Click and drag over glycine rich residues to select them.

3. Click on the center button.

4. Click on the color panel.

5. Click here to add rocking and or rotation.

6. Click here to make a slide

Make the 2<sup>nd</sup> slide: Center on the glycine rich loop and color.

The screenshot shows a software window titled "1.000 Molsoft MolViewer 3.7.2a [NewProject 7] (1 object)". On the left, a sequence viewer displays protein residues with some highlighted in red. The main area shows a 3D ribbon model of a protein structure in yellow and green against a dark background with small white dots. A toolbar at the top contains various icons, including a color palette and a center button. A terminal window at the bottom shows command-line instructions for the software.

Make the 3<sup>rd</sup> slide: Ligand binding pocket surface colored by property.

1. Display ligand.

2. Right click here and select center.

3. Right click here and select pocket/receptor pocket.

4. Click here to make a slide

```
low/low> set property q_ligand_m smooth no
low/low> display static q_ligand_m
low/low> undisplay q_ligand_m
low/low> set property q_ligand_m transparent smooth only
low/low> display static q_ligand_m
low/low>
```

Prepare HTML text for the molecular document.

1. File/New.

2. Click on the Html tab.

3. Enter name of document.

4. Click OK

```
lsm/lsmw create static aa_graph
lsm/lsmw undisplay aaucv graph
lsm/lsmw color Res1 Res1m_1//100 ; ribbon TriacB6wtoc; Res1 Res1m_1//100 ; 1,0,100.0//0.0//100.
lsm/lsmw display x1ide*elidesov,x1ides inda*1
lsm/lsmw display g_lsmw_m
lsm/lsmw
```

4x17 Atom (27) Res.1 PML.1 (36)

Add text to the Html document (1).

2. Right click in the white space select Edit.



The screenshot shows a software interface with a 3D molecular model on the right and a text editor on the left. The 3D model features a central protein structure with various atoms and bonds, surrounded by green and yellow leaf-like structures. The text editor on the left contains a list of residues and their corresponding amino acid names, such as 33 PLEUQ, 43 LLDGQ, 53 TRLIR, 63 PPALE, 73 RQIAR, 83 QYDVT, 93 LKVVQ, 103 VIFLL, 113 PPSPT, 123 PFPDQ, 133 PFGAG, 143 LKDTF, 153 KQVRS, 163 VLKRP, 173 TLISL, 183 KLIIF, 193 LQITV, 203 VTKYI, 213 LKTRP, 223 LKVVQ, 233 YSRVY, 243 PFIIT, 253 PFPDQ, 263 QGRLI, 273 LKFTD, 283 LKVVQ, 293 VLLFP, and 303 LKA. The text editor also shows a list of slides: 1 Slide 1, 2 Slide 2, and 3 Slide 3. The bottom of the interface displays a command line with various system messages and a status bar at the bottom right indicating the file path: 4427 Atom 273 Fac1.PML1 Obj.

**Add text to the Html document (2).**

**1. Type text here. Make sure you are in Edit mode (see below)**

**2. Use the formatting tools here.**

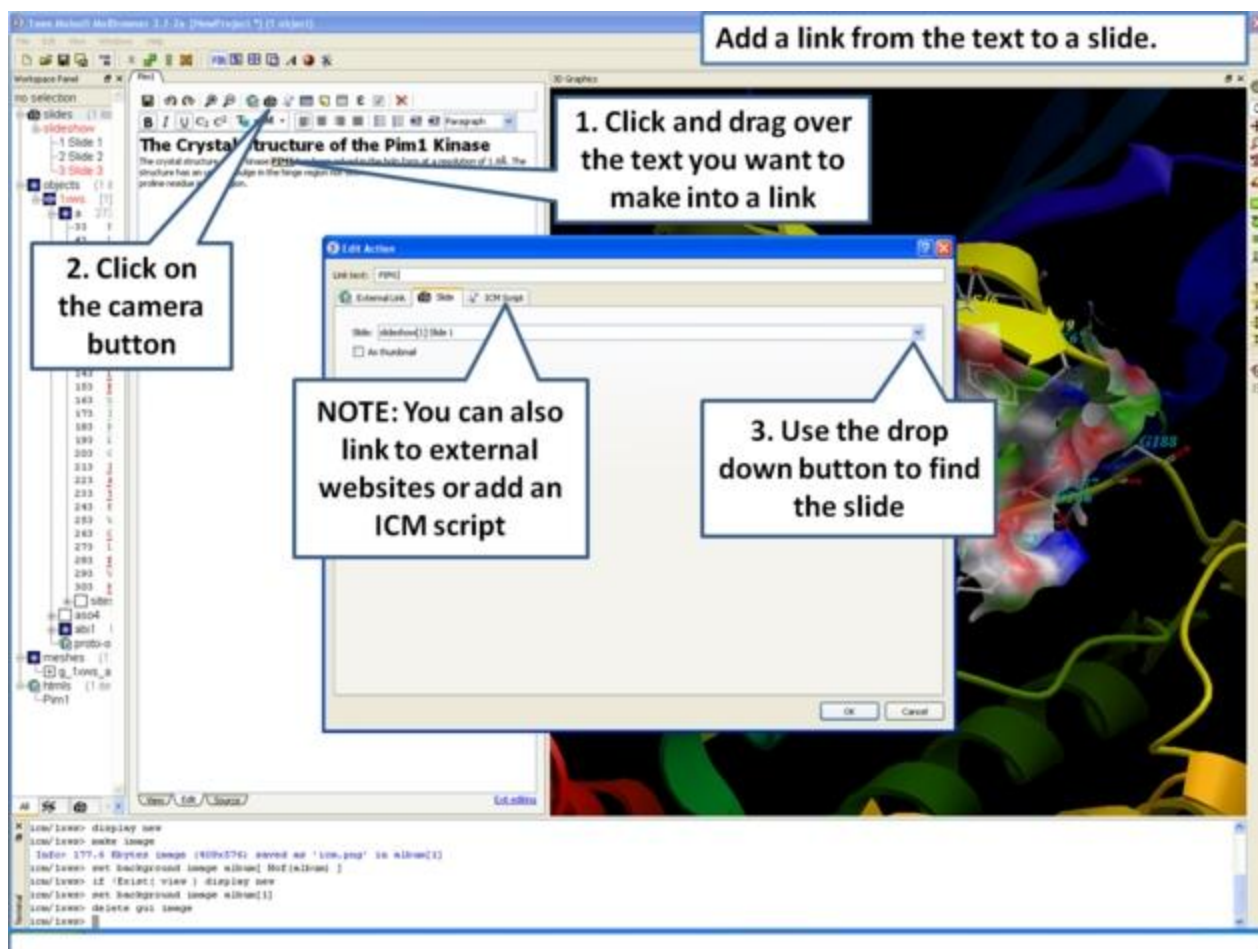
**3. Toggle between View, Edit and Source mode.**

**The Crystal Structure of the Pim1 Kinase**

The crystal structure of the kinase Pim1 has been solved in the holo form at a resolution of 1.65 Å. A surface has an unusual bulge in the hinge region not seen in other kinases. This bulge is due to a proline residue in this region.

4x17 Alone 273 Res, 3 PML, 1 Obj





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