Table of Contents

Table of Contents

Table of Contents

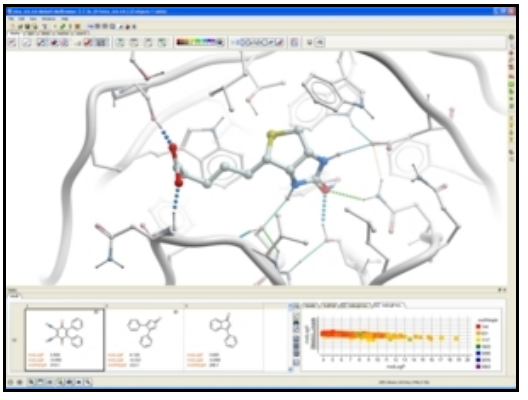
Table of Contents

Table of Contents

Table of Contents

ICM-Browser-Pro User Guide v.3.8

by Ruben Abagyan, Andrew Orry, Eugene Raush, and Maxim Totrov



Oct 28 2016

Feedback.

1 Introduction

ICM-Browser-Pro is a high quality visualizer and annotator for three dimensional molecular structures, sequences, alignments, chemical spreadsheets and biological data. It allows you to read data from multiple file formats, annotate the data, and write multi-slide documents in a single small cross-platform file. ICM Browser Pro is well suited for creating, storing and sharing structural, biological and chemical information. The files can then be opened and viewed with the free ICM Browser.

Features

Please visit our product web pages for a full description of all the features in `ICM-Browser-Pro`.

Download

You can download ICM-Browser-Pro from `here`.

2 Reference Guides and Videos

Chapter Contents:

ICM-Browser Reference Guide

ICM-Browser-Pro Reference Guide

ActiveICM Reference Guide - Create 3D Molecular Documents for the Web and PowerPoint

ICM-Chemist Reference Guide

ICM-Chemist-Pro Reference Guide

Menu and Tab Reference Guide:

Menu Option Guide

Tab Guide

2.1 ICM-Browser Reference 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
- Creating Fully Interactive Slides for PowerPoint and the Web Tutorial

2.1.1 Download and Install ICM-Browser

Getting Started: Download and Install ICM-Browser and ActiveICM.		
Download ICM-Browser Distribution.	Download	video
Install ICM-Browser Instructions.	Windows Linux Mac	
Download ActiveICM Distribution.	Download	video
Install ActiveICM.	Windows Linux Mac	

2.1.2 How to use the Graphical Display

'; winRef.document.write(str); }

How to use the Graphical Display		
How to search the PDB.	HTML GUI Manual	video

How to Move a Structure in the Graphical Display.	HTML GUI Manual	video
How to use the Graphics window controls.	HTML GUI Manual	
How to use the ICM Workspace Panel	HTML GUI Manual	video
How to Display a Molecule.	HTML GUI Manual	video
How to Change Protein Representation.	HTML GUI Manual	video
How to Change Ribbon Representation.	HTML GUI Manual	video
How to color wire or xstick carbon atoms.	HTML GUI Manual	video
How to Display the Residues Surrounding the Ligand Binding Pocket.	HTML GUI Manual	video
How to remove chain breaks (dotted lines).	HTML GUI Manual	video
How to Color.	HTML GUI Manual	video
How to Change the Color of Molecule Representations.	HTML GUI Manual	video
How to Change the Background Color.	HTML GUI Manual	video
How to Display a Binding Pocket Surface	HTML GUI Manual	video
How to (Un)Display Hydrogens.	HTML GUI Manual	video
How to Save an ICM Object.	HTML GUI Manual	video
How to Save an ICM Project File.	HTML GUI Manual	video
How to Drag and Drop.	HTML GUI Manual	
How to: Right Click Options.	HTML GUI Manual	
How to Move Windows.	HTML GUI Manual	video
How to Arrange Windows	HTML GUI Manual	video

2.1.3 How to make Graphical Selections

How to Make Selections.	HTML GUI Manual	
How to Select an Object	HTML GUI Manual	video
How to Select a Molecule	HTML GUI Manual	video
How to Select Residues	HTML GUI Manual	video
How to Select Atoms	HTML GUI Manual	video
How to Make a Spherical Selection.	HTML GUI Manual	video

How to Invert a Selection.	HTML GUI Manual	video
How to Remove a Selection.	HTML GUI Manual	video
How to Change the Selection Level and Mode.	HTML GUI Manual	video
How to Check What is Selected.	HTML GUI Manual	

2.1.4 How to Convert Proteins, Display Hydrogens and Ligand Binding Pocket.

Convert Protein, Display Hydrogens and Ligand Binding Pocket.		
How to Convert a PDB Structure into an ICM Object.	HTML GUI Manual	video
How to Display Ligand Binding Pocket.	HTML GUI Manual	video
How to Display Hydrogen Bonds.	HTML GUI Manual	video

2.1.5 How to change Graphics Effects

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

2.1.6 How to add Labels and Annotations

How to add Labels and Annotations		
How to Label Residues.	HTML GUI Manual	video
How to Label Atoms.	HTML GUI Manual	video
How to Label Variables.	HTML GUI Manual	video
How to Display and Undisplay Sites.	HTML GUI Manual	

How to Make and Display Sites (Annotations).	HTML GUI Manual	
How to Make and Display 2D and 3D Labels.	HTML GUI Manual	video

2.1.7 How to Make High Quality Publication Images

How to Make High Quality Publication Images		
How to Toggle High Quality Display	HTML GUI Manual	video
How to Toggle Antialiasing.	HTML GUI Manual	video
How to Copy Image to ClipBoard	HTML GUI Manual	video
How to Write an Image.	HTML GUI Manual	video
How to Use the Advanced Write Image Options.	HTML GUI Manual	video
How to Add an Image to the ICM Photo Album.	HTML GUI Manual	video

2.1.8 How to Superimpose Protein Structures.

How to Superimpose Protein Structures.		
How to Superimpose Two or More Protein Structures.	HTML GUI Manual	video

2.1.9 How to Measure Distances and Angles.

How to Measure Distances and Angles.		
How to Measure Distances Between Two Atoms.	HTML GUI Manual	video
How to Measure Distances From One Atom to Many.	HTML GUI Manual	video
How to Show Corresponding Distances in Two Objects.	HTML GUI Manual	video
How to Display the Ruler Bar.	HTML GUI Manual	video

2.2 ICM-Browser-Pro Reference Guide

NOTE: ICM-Browser-Pro contains all the features in ICM-Browser. Click here for the ICM-Browser Reference Guide.

2.2.1 Download and Install ICM-Browser-Pro

Getting Started: Download and Install ICM-Browser-Pro	
Download ICM-Browser-Pro Distribution.	Download
Install ICM-Browser-Pro.	Windows Linux Mac

2.2.2 Graphics

Graphics and Movie Making	
How to generate the shadow effect.	HTML GUI Manual
How to make a screenshot movie.	HTML GUI Manual
How to make a movie from a set of slides.	HTML GUI Manual
How to move a molecule independently of the other display objects (Connect).	HTML GUI Manual

2.2.3 Protein Structure Analysis

Protein Structure Analysis	
How to calculate contact areas between molecules.	HTML GUI Manual
How to identify closed cavities.	HTML GUI Manual
How to calculate surface area.	HTML GUI Manual
How to generate interactive Ramachandran plots.	HTML GUI Manual

2.2.4 Surfaces

Surfaces	
How to generate electrostatic and binding property surfaces.	HTML GUI Manual
How to connect and rotate/translate surface (mesh).	HTML GUI Manual
How to crop a mesh/surface.	HTML GUI Manual
How to save a mesh/surface.	HTML GUI Manual

2.2.5 Superimpose Proteins

Superimpose Proteins	
How to superimpose proteins based on 3D by visible atoms, C-alpha, backbone or heavy atoms.	HTML GUI Manual
How to superimpose multiple proteins based on aligned residues..	HTML GUI Manual

2.2.6 Crystallographic Tools

Crystallographic Tools	
How to contour electron density.	HTML GUI Manual

How to display crystallographic cell.	HTML GUI Manual
How to display crystallographic symmetry.	HTML GUI Manual
How to convert x-ray density to a grid.	HTML GUI Manual

2.2.7 Sequence Analysis

Sequence Analysis	
How to annotate an alignment - box and shade.	HTML GUI Manual
How to annotate an alignment with text.	HTML GUI Manual
How to display secondary structure in an alignment.	HTML GUI Manual
How to extract sequences from pdb files.	HTML GUI Manual
How to assign secondary structure.	HTML GUI Manual
How to link sequence, alignments, and structures.	HTML GUI Manual
How to save as image, print, and delete sequences and alignments.	HTML GUI Manual

2.2.8 Plotting Tools

Plotting Tools	
Make fully interactive colorful X-Y plots and histograms with up to 4 dimensions.	HTML GUI Manual
Save plot and histogram as image.	HTML GUI Manual

2.3 ActiveICM Reference 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

Creating fully interactive 3D documents for PowerPoint, the web, and standalone browser is straightforward.

1. Download ICM-Browser and the ActiveICM plugin. They are completely free! [video]
2. Open the ICM-Browser and make a series of animated fully-interactive slides showing different colored and rendered views of your molecules. [video]
3. Add hyperlinked HTML text to annotate and link to your slides. [video]
4. Save your file in ICM-Browser and then insert into PowerPoint or the web using the ActiveICM plugin. You can also share your documents in the standalone ICM-Browser. [video – powerpoint] [video –web browser]

'; winRef.document.write(str); }

2.3.1 Getting Started

Getting Started: Download and Install ICM-Browser and ActiveICM.		
Download ICM-Browser Distribution.	Download	video
Install ICM-Browser Instructions.	Windows Linux Mac	
Download ActiveICM Distribution.	Download	video
Install ActiveICM.	Windows Linux Mac	

2.3.2 How to Create a Series of Fully-Interactive 3D Slides.

Creating Slides How to Create a Series of Fully-Interactive 3D Slides.	video
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

2.3.3 How to Create Molecular Documents

How to Create Molecular Documents: Linking Slides to HTML Text.	video
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

2.3.4 How to Display Molecular Documents in PowerPoint

How to Display Molecular Documents in PowerPoint	video
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

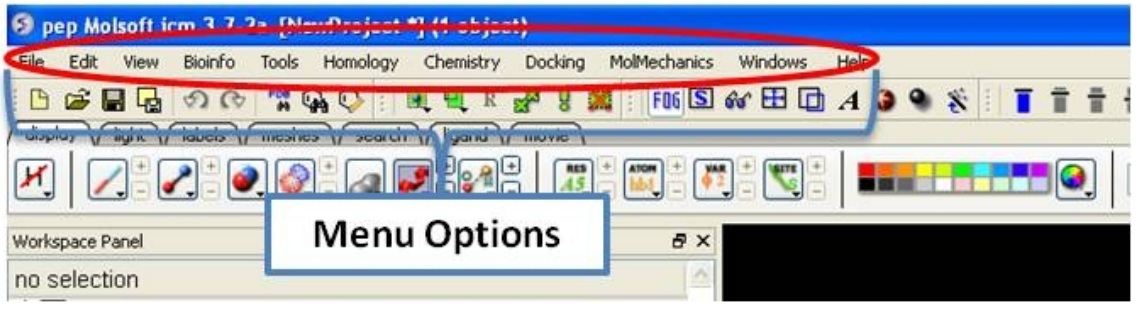
2.3.5 How to Display Molecular Documents on the Web

How to Display Molecular Documents in Web Browsers	`video`
How to Display Molecular Documents in Web Browsers	`HTML GUI Manual`

2.4 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.



2.4.1 File Menu

2.4.1.1 New

This option allows you to create new peptides, dna, sequences etc... and is described in the `Create New Objects` chapter.

2.4.1.2 Open

This option is described in the `Open and Read` chapter.

2.4.1.3 Open with Password

This option is described in the `Open and Read` chapter.

2.4.1.4 Extract from ICB

This option is described in the `Open and Read` chapter.

2.4.1.5 Convert to Local Database

Please see the Local Databases chapter for more information about this option.

2.4.1.6 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.

2.4.1.7 Save Project

This is described in the `Save File` chapter.

2.4.1.8 Save Project As

This is described in the `Save File` chapter.

2.4.1.9 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

2.4.1.10 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** .

2.4.1.11 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..

2.4.1.12 Close Project

To close a project:

File/Close Project

2.4.1.13 Quick Image

See the `High Quality Publication Image` chapter.

2.4.1.14 Write Image

See the `High Quality Publication Image` chapter.

2.4.1.15 Preferences

Preferences are described in the `Preferences` chapter.

2.4.1.16 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.

2.4.1.17 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.

2.4.1.18 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 quiting.

2.4.2 Edit Menu

2.4.2.1 Delete

This option will delete anything that is `selected`.

2.4.2.2 Delete All

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

2.4.2.3 Select All

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

2.4.2.4 Search in Workspace

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

2.4.2.5 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.

2.4.2.6 Invert Selection

This option will select everything that is not currently selected.

2.4.2.7 Clear Selection

This option will remove all selections. For more information on selections see the `Making Selections Chapter`.

2.4.2.8 Neighbor Selection

This option will allow you to select neighboring atoms. For more information see the `Select Neighbors` section in the Selections Chapter.

2.4.2.9 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.

2.4.2.10 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.

2.4.2.11 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

2.4.2.12 PDB Search

See `PDB Search Tab`

2.4.2.13 PDB Search by Field

See `PDB Search Tab`

2.4.2.14 PDB Search by Identity

See `PDB Search Tab`

2.4.2.15 PDB Search by Homology

See `PDB Search Tab`

2.4.2.16 PDB Search with External Seqeuence

See `PDB Search Tab`

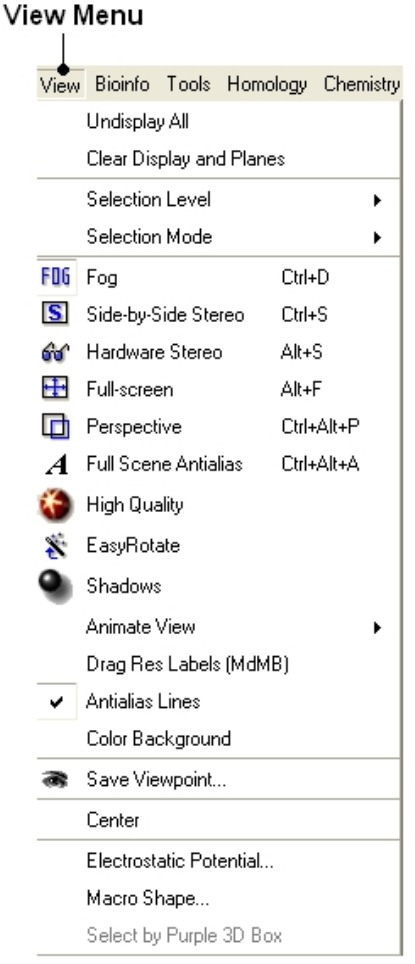
2.4.2.17 Ligand Tools

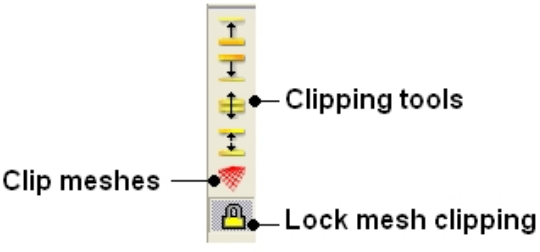
See the ligand editor section of the manual.

2.4.2.18 Ligand Editor Preferences

See the ligand editor section of the manual.

2.4.3 View Menu





2.4.3.1 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.

2.4.3.2 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`.

2.4.3.3 Selection Level

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

2.4.3.4 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.

2.4.3.5 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

2.4.3.6 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

2.4.3.7 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

2.4.3.8 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

2.4.3.9 Perspective

Toggle perspective Ctrl_P this will add perspective to your structure, enhancing depth in the graphical display.

- View/Perspective

2.4.3.10 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

2.4.3.11 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

2.4.3.12 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

2.4.3.13 Shadows

- View/Shadows

See `Graphics Effects` chapter.

2.4.3.14 Sketch Accents

To make images as shown below use:

- View/Sketch Accents

See `Graphics Effects` chapter.

2.4.3.15 Animate View

This tool is described in more detail in the `Molecular Animations and Transitions` section.

2.4.3.16 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.

- 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**

2.4.3.17 Antialias Lines

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

- View/Antialias Lines

2.4.3.18 Color Background

To change the background color

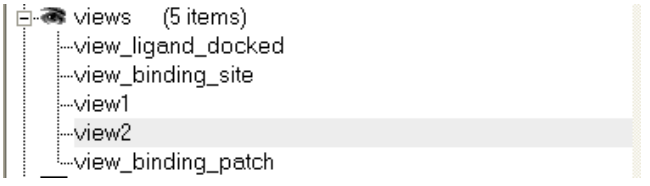
- View/Color Background
- Select a color from the panel and press OK.

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

2.4.3.19 Save Viewpoint

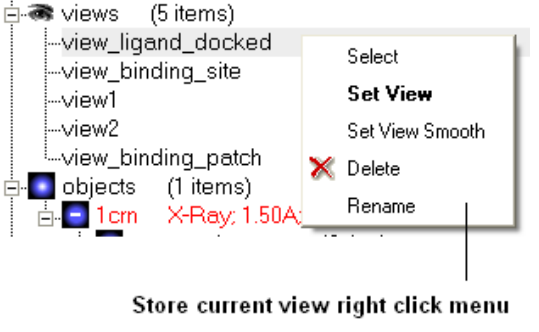
It is possible to store a current view using the button shown below.

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.



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.

2.4.3.20 Center

To center on an object displayed in the graphical display

- Make a selection on the region on which you wish to center on.

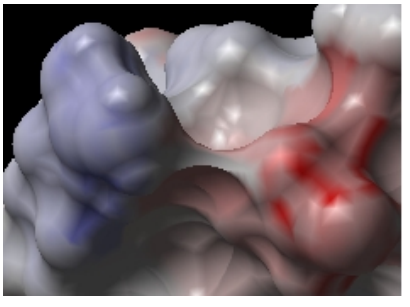
- Tools/Center (or use the `center` button on the right hand-side of the graphical display).

2.4.3.21 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

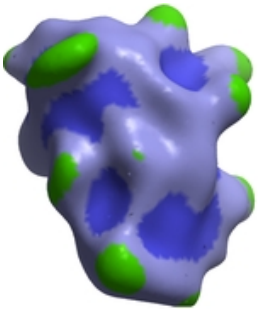
In order to color the skin of your molecule by electrostatic potential:

- 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.



2.4.3.22 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 controled by changing the number of harmonics, gridStep, and, contour level.



- View/Macro Shape

2.4.3.23 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.

2.4.4 Bioinfo Menu

The tools in this menu are described in the Bioinfo Menu chapter.

2.4.5 Tools Menu - Xray

The options in the menu are described in the `Crystallographic Analysis` chapter.

2.4.6 Tools Menu - 3D Predict

The options in this menu are described in the 3D Predict chapter.

2.4.7 Tools Menu - Analysis

The options in this menu are described in the `Protein Structure Analysis` chapter.

2.4.8 Tools Menu - Superimpose

The options in this menu are described in the `Protein Superposition` chapter.

2.4.9 Tools Menu - Extras

2.4.9.1 Plot Function

To plot a function:

- Tools/Extras/Plot Function
- Enter the Function(x) eg Sin(x)
- Enter the starting value of x (From).
- Enter the end point of x (To).
- Enter the number of points (N points).
- Click OK and your plot will be displayed next to a table of values for your function.

2.4.10 Tools Menu - Table

2.4.10.1 Build Prediction Model

Learn and Predict tools are described here.

2.4.10.2 Predict

Learn and Predict tools are described here.

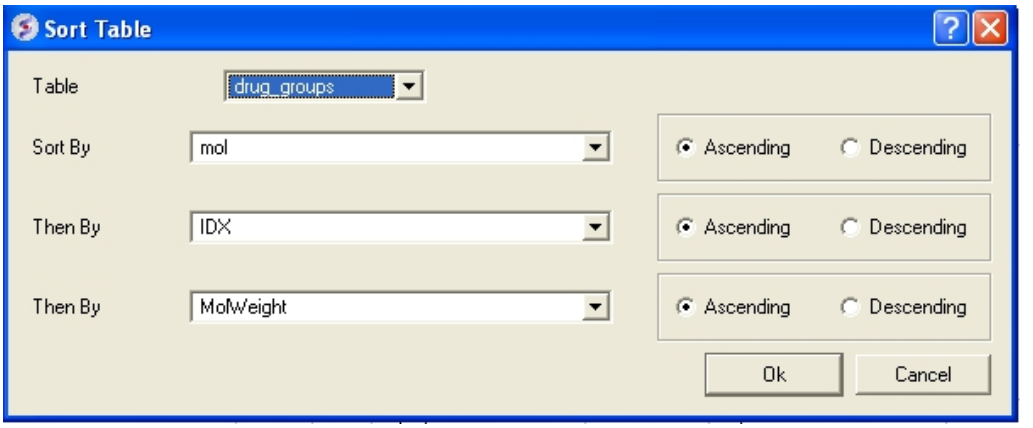
2.4.10.3 Cluster Set

This is described in the cluster section of the Working with Tables Chapter.

2.4.10.4 Sort Table

There are a couple of ways to sort a chemical table. You can right click on the a column header and select `sort` or you can use the option in the menu Chemistry/Sort Table.

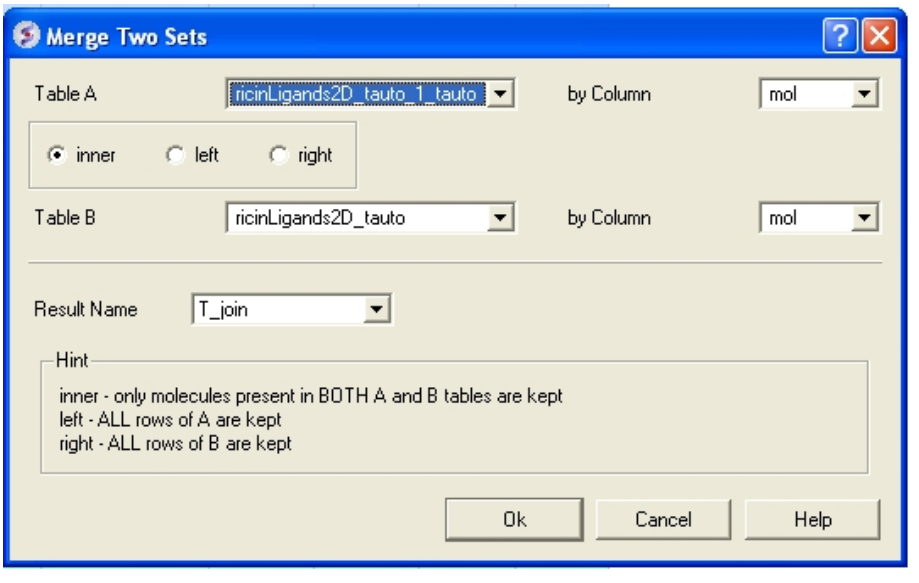
- Read a chemical table into ICM.
- Select the columns by which you wish to sort by as shown below.
- Select **Ascending** or **Descending** and for each **sort by** option and then click OK



2.4.10.5 Merge Two Sets

To merge two tables:

- Read the two tables into ICM.
- Tools/Table/Merge Two Sets
- Select the first table from the drop down list (Table A) and the column you wish to use to merge the table by.
- Select merge method 1. **inner** - only molecules present in BOTH A and B tables are kept; or 2. **left** ALL rows of A are kept ; or 3. **right** ALL rows of B are kept.
- Select the second table from the drop down list (Table B) and the column you wish to use to mergethe table by.
- Enter a name for the output table.
- Click OK and a new table will be displayed.



2.4.10.6 Add External Columns

To add external columns to a table:

- Read at least two tables into ICM - the table you want to add to and the table you want to add the column from.
- Tools/Table/Add External Columns
- Enter the target table name and the column you wish to match each table by.
- Enter the source of the new column (Other table and column name)
- Choose to add "all the columns" from the source or "overwrite matching columns" or select the columns you want to add by selecting the "choose column" option.

2.4.10.7 Append Rows

To append rows from one table to another one:

- Read at least two tables into ICM - the table you want to add to and the table you want to add the column from.
- Tools/Table/Append Rows
- Enter the name of the Target Table (where you will append).
- Enter the name of the Source Table (where you will append from).

2.4.11 Tools Menu - Chemical Search

Chemical searching is described in the Chemistry chapter here.

2.4.12 Tools Menu - Molecular Editor

The molecular editor is described in the Chemistry chapter here.

2.4.13 Homology Menu

The options in this menu are described in the Homology Modeling Chapter.

2.4.14 Chemistry Menu

The tools in the **Chemistry** menu are described here.

2.4.15 Docking Menu

The tools in the **Docking** menu are described in the Docking chapter.

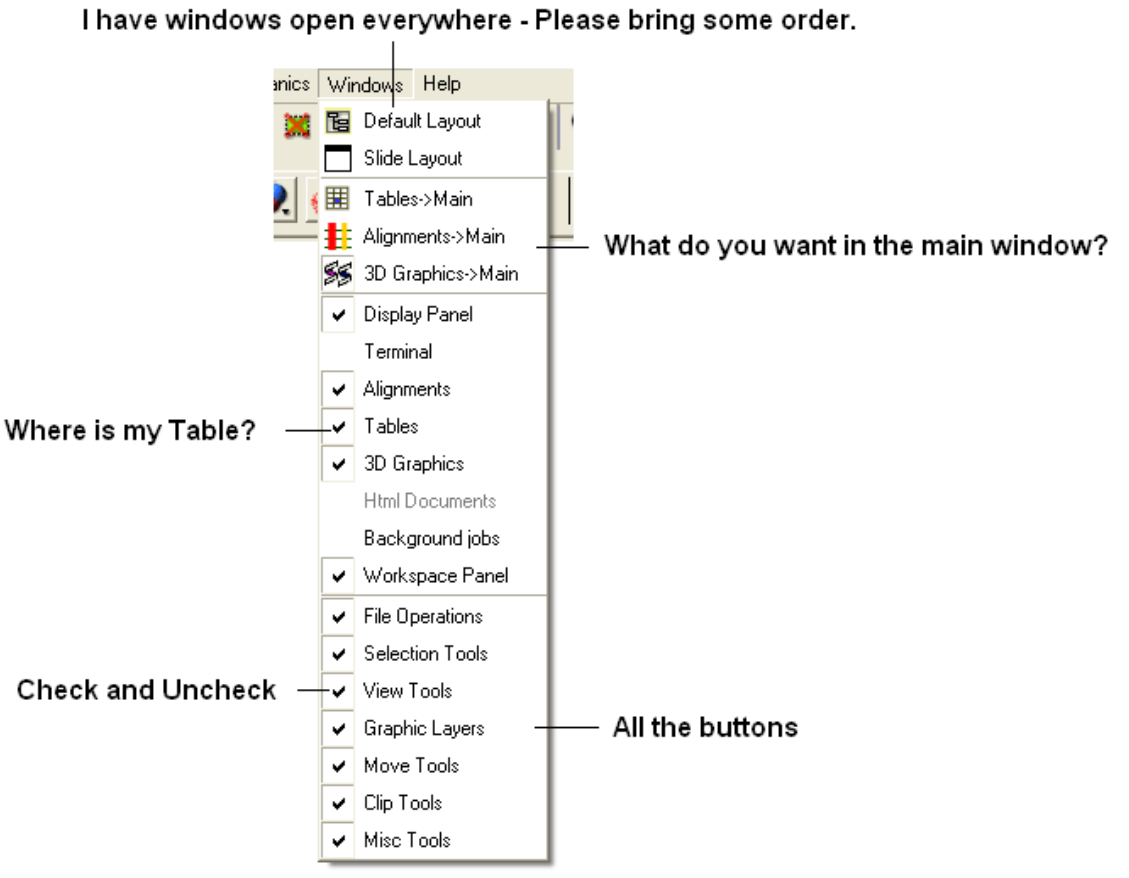
2.4.16 MolMechanics Menu

The options in this menu are described in the Molecular Mechanics chapter.

2.4.17 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 `Getting Started` 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 hasnt 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.



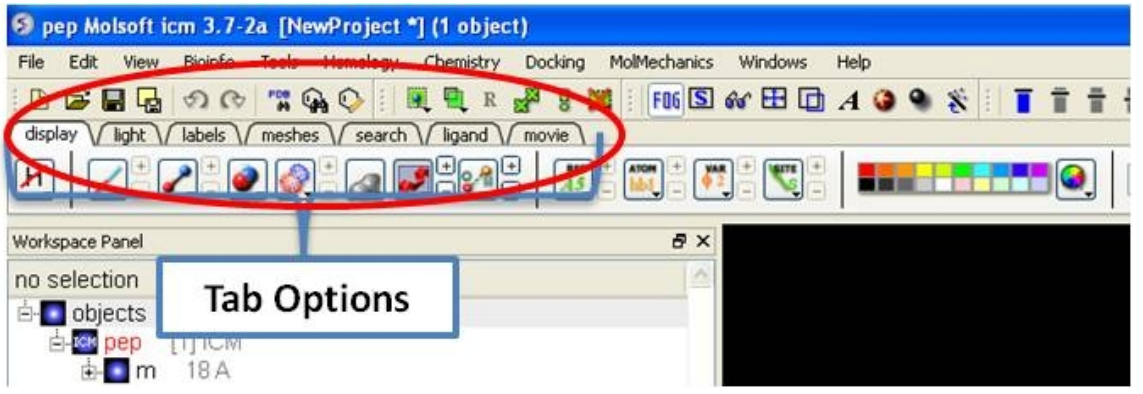
To return to the default display option select the 'Default layout' option in the windows menu.

OR

Click the default layout icon.

2.5 Tab Guide

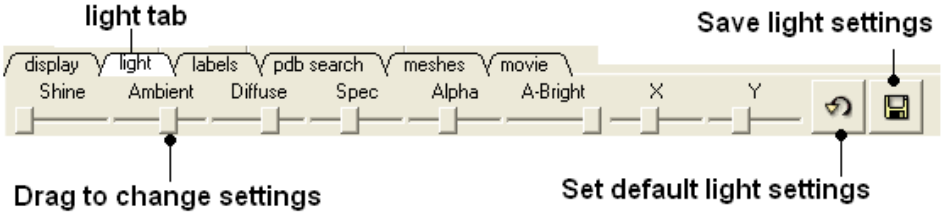
In this section we describe the contents of the tabs in the graphical user interface.



2.5.1 Display Tab

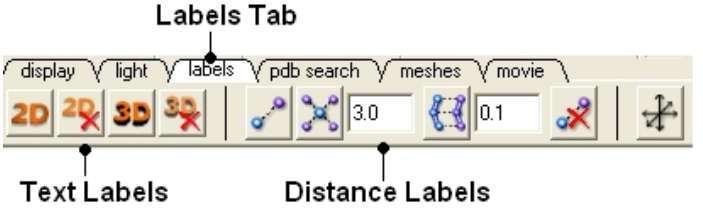
The display tab contains tools for a variety of functions including - structural `representations`, `coloring`, `labeling` and `superposition`. This tab is shown below.

2.5.2 Light Tab



The options in this tab are described in the `Lighting Section`.

2.5.3 Labels Tab



The options in this tab are described in the `labels` section of this manual.

2.5.4 PDB Search Tab

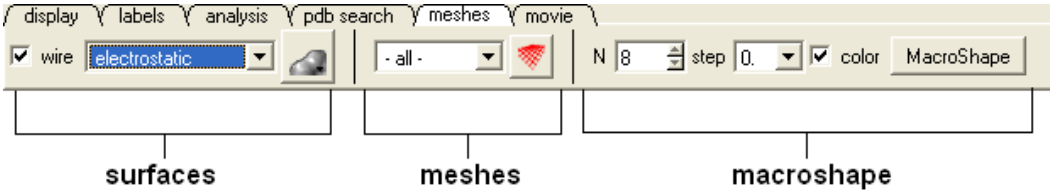
Instructions on how to use this tab can be found in the `Search PDB section`.

2.5.5 Ligedit Tab

Instructions on how to use the options in this tab can be found in the How to use the 3D Interactive Ligand Editor section.

2.5.6 Meshes Tab

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 the `section`.

3 Getting Started

Chapter Contents:

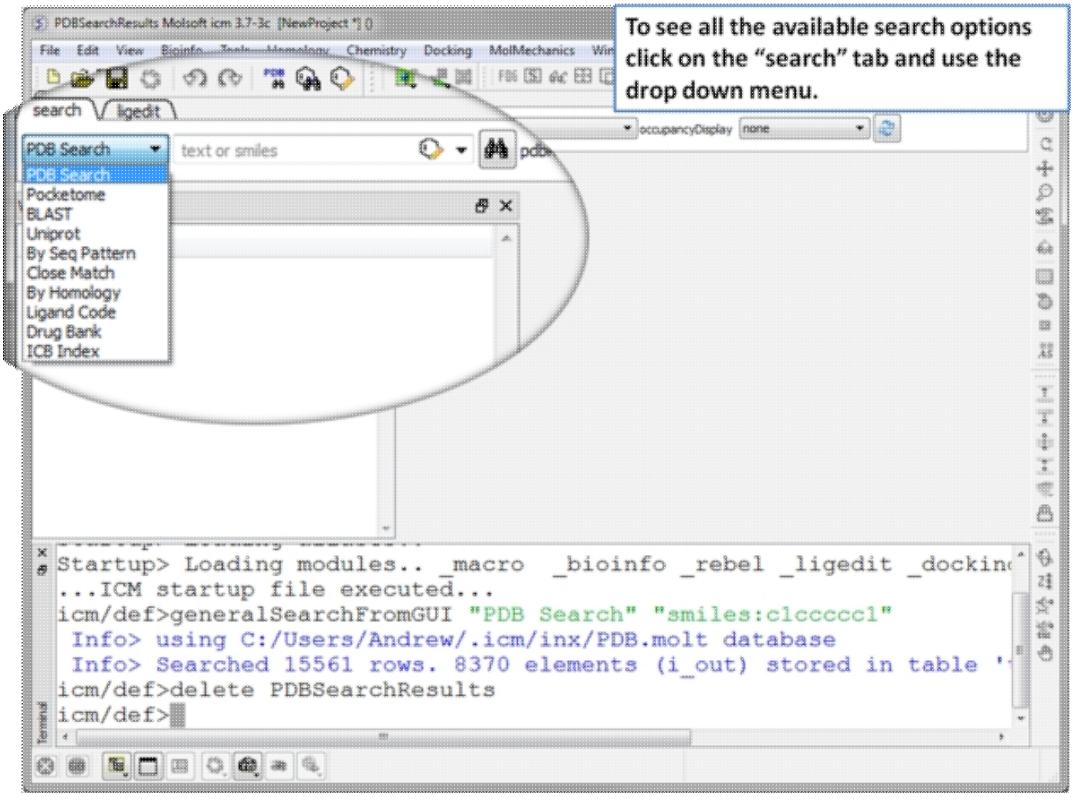
- How to search and Download Protein Structure, Sequences, and Chemicals
- How to create new Objects
- How to open files
- How to save files
- How to use the Graphical Display
- How to Make Selections
- Changing Preferences

3.1 How to search and download Protein Structure, Sequences, and Chemicals

Available in the following product(s): ICM-Browser | ICM-Browser-Pro | ICM-Pro | ICM-Chemist

The **Search** tab allows you to search and download content from the following databases:

- The Protein Databank www.wwpdb.org - search for protein and chemical
- The Pocketome Database http://pocketome.org/
- BLAST search the NCBI sequence database
- The UniProt Sequence database http://www.uniprot.org/
- Search the PDB by ligand code.
- Search Drug Bank http://www.drugbank.ca/
- Search PubChem https://pubchem.ncbi.nlm.nih.gov/
- Search the Crystallography Open Database http://www.crystallography.net/



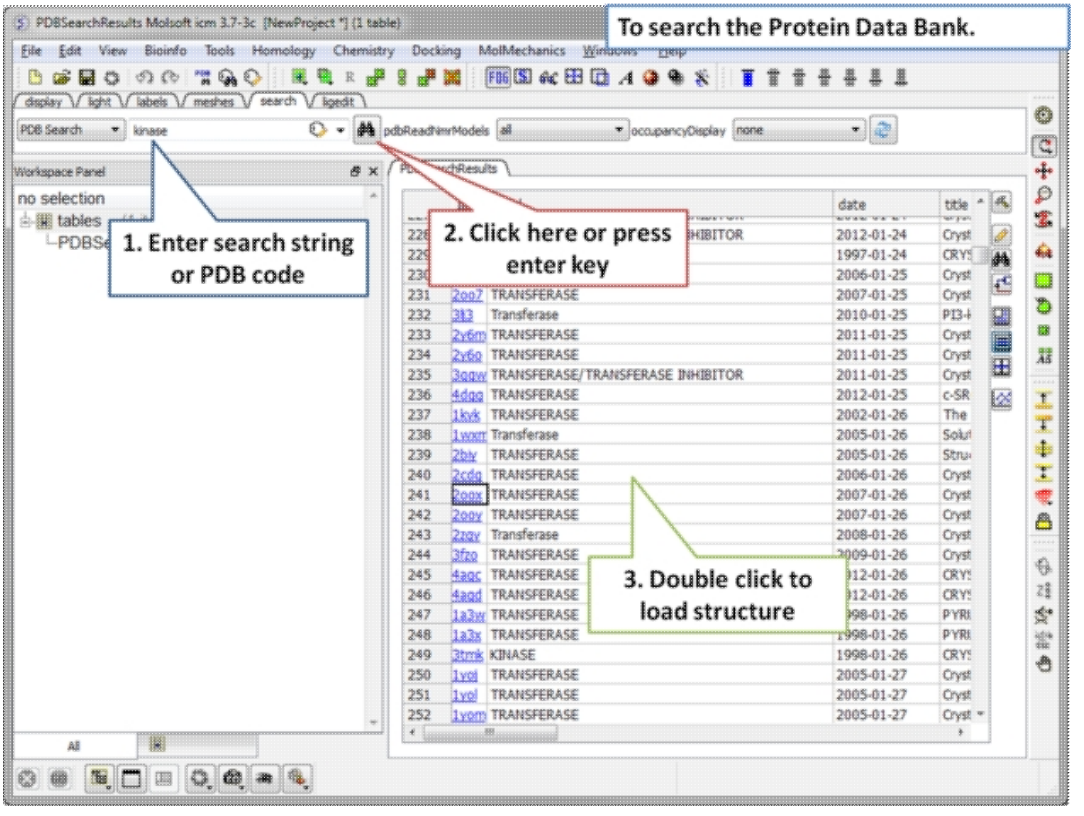
Click on the search tab and then use the drop down menu to identify the database you would like to search and download from.

3.1.1 Search the PDB

How to Search the Protein Databank and Download

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 entititled `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.

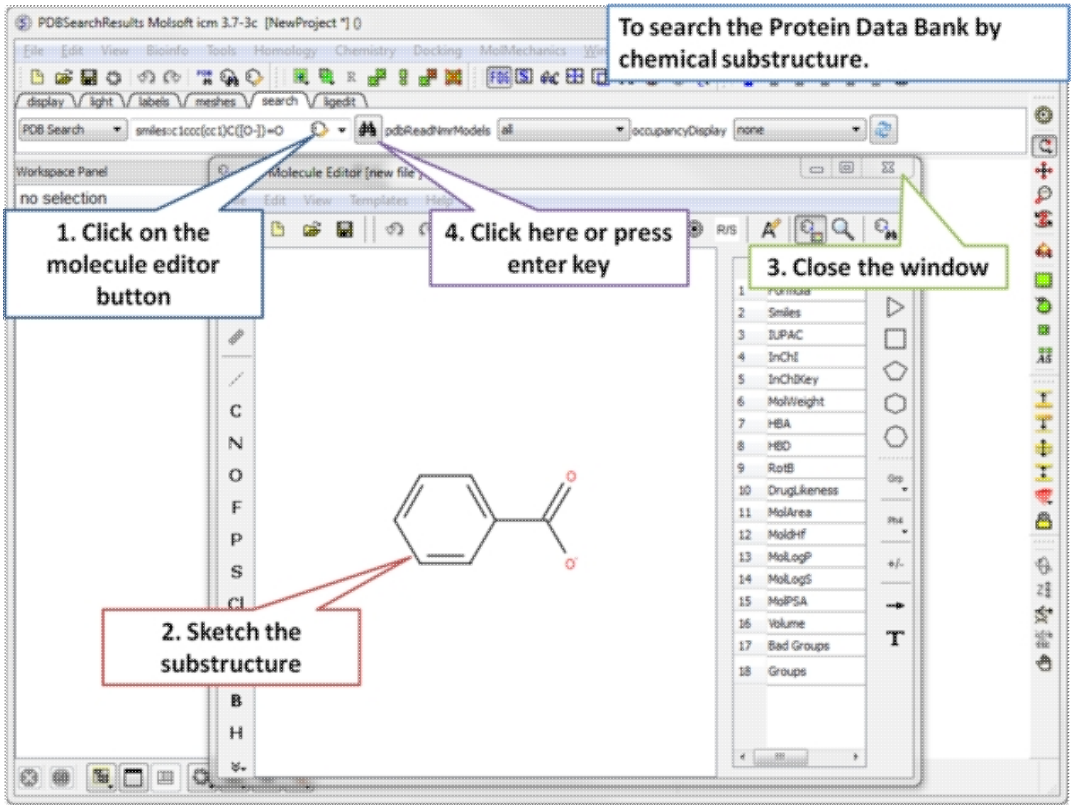


To Search the PDB and Download a Structure:

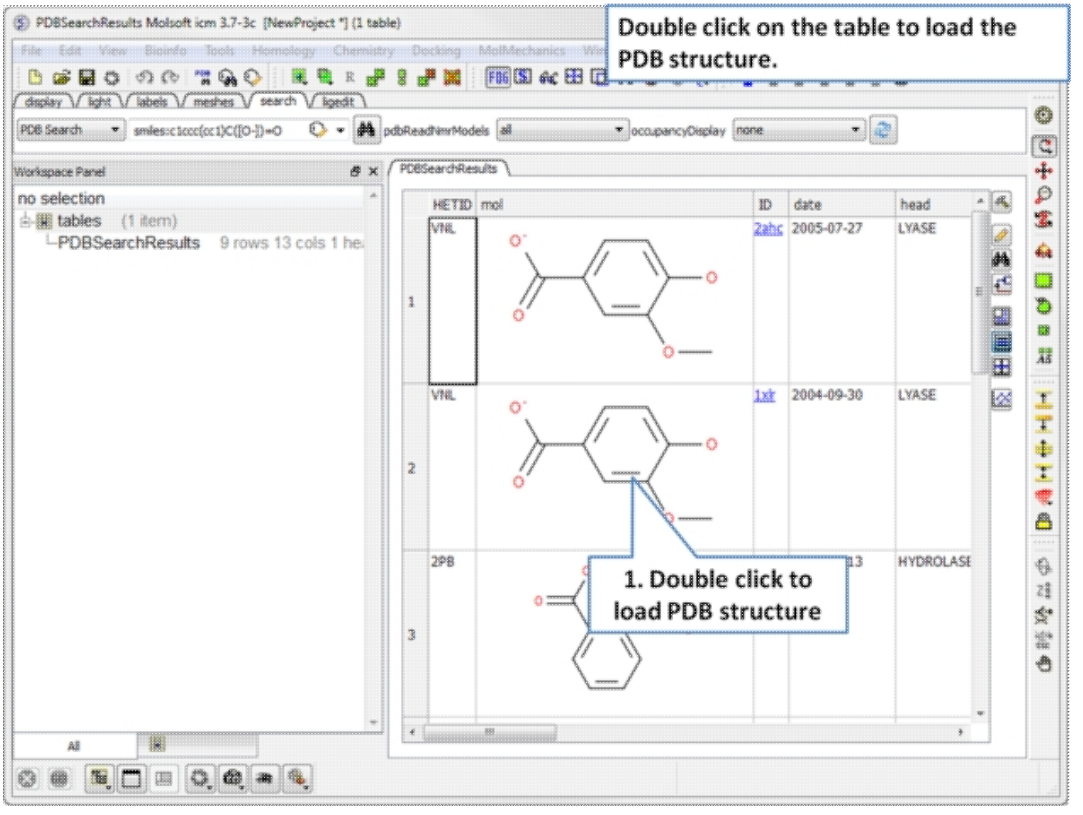
- Click on the search tab and enter a search string or PDB code.
- A table containing the results will be displayed.
- Double click on a row to load the PDB file. Read more about PDB search `here`.

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.

3.1.1.1 How to Search the Protein Databank by Chemical Substructure



Step 1: Click on the molecule editor button inside the search tab. Sketch the substructure you are interested in.



Step 2: A table containing the results will be displayed. Double click on a row to load the PDB file.

3.1.1.2 How to Query the PDB by Sequence

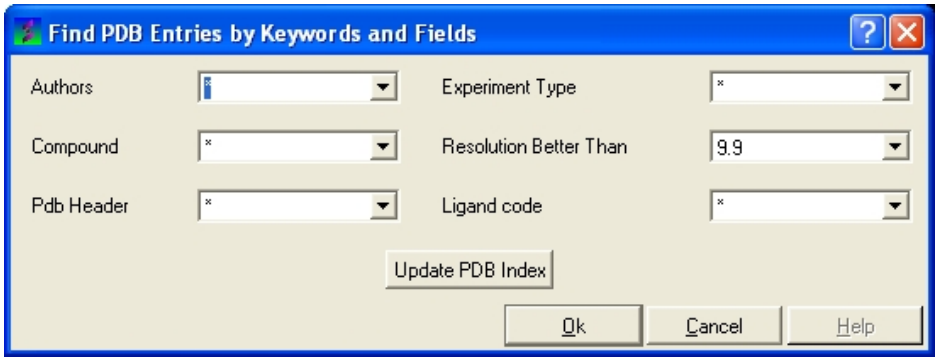
There are a number of ways to search the PDB by sequences.

1. BLAST search the NCBI datase using the option "Sequences from PDB".
2. Search by **Sequence Pattern** using the option in the Edit menu.
3. Search by **Identity** using the option in the Edit menu.
4. Search by **Homology** using the option in the Edit menu.

3.1.1.3 How to Query PDB by PDB Field

To query the PDB by field (Author, Compound, PDB Header, Experiment Type, Resolution or Ligand Code

- Select **Edit/PDB** search by field.
- Enter the search string or value
- Click **OK** and a list of related PDB entries based on your search will be displayed in the PDBSearchResults table of the graphical user interface.



3.1.1.4 Load and Display NMR Structures

Use the PDB Search tab to load NMR structures from the PDB. You can use the drop down button shown below to determine how you want to display your NMR structure. You can choose to display and download the first NMR model, all models in the PDB file or all models in the PDB in a stack. If you choose the stack option the the stack will be stored in the object as described here.

3.1.1.5 Occupancy Display

You can use the options in the PDB Search tab to control if and how the partial or zero atom occupancies are displayed. You can choose to circle or label the poor occupancy atoms.

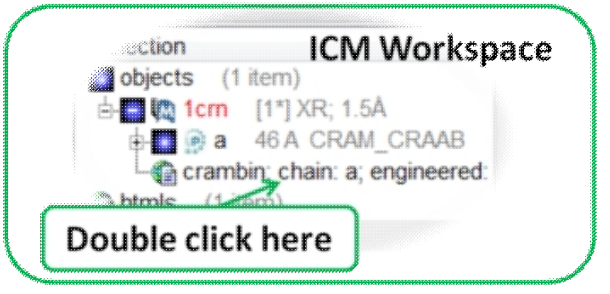
>>load-pdb-hyperlinks{pdb search hyperlinks} h4-- Hyperlinks to PDB Website and UniProt {Hyperlinks to Databases}

In the PDB Search Results Table you will see blue hyperlinks that will take you directly to the PDB website or Uniprot website.

3.1.1.6 Display PDB Header

To display the PDB Header for a PDB file.

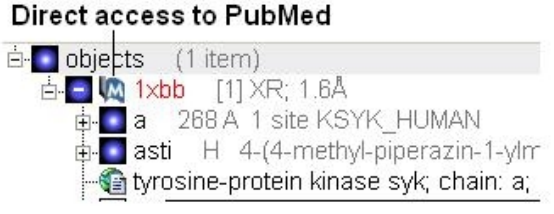
- First load a PDB file into ICM (see `Search PDB`)
- Double click on the word header in the ICM Workspace.



- The PDB Header information will be displayed.
- Click on the blue hyperlinked text to link to external web pages for additional information if needed.

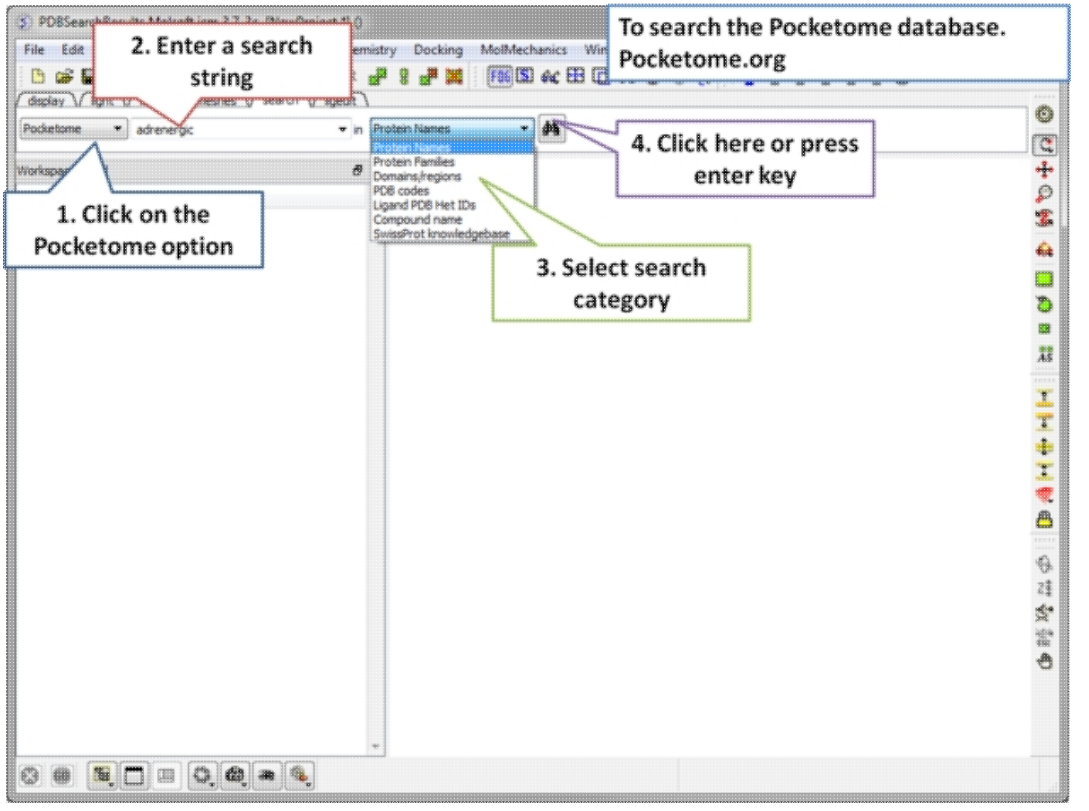
3.1.1.7 Direct link to PubMed

When you search for a PDB file and load it into ICM you will see an icon (shown below) next to your protein name in the ICM Workspace. Click the icon and you will be taken directly to the PubMed primary reference relating to the structure.

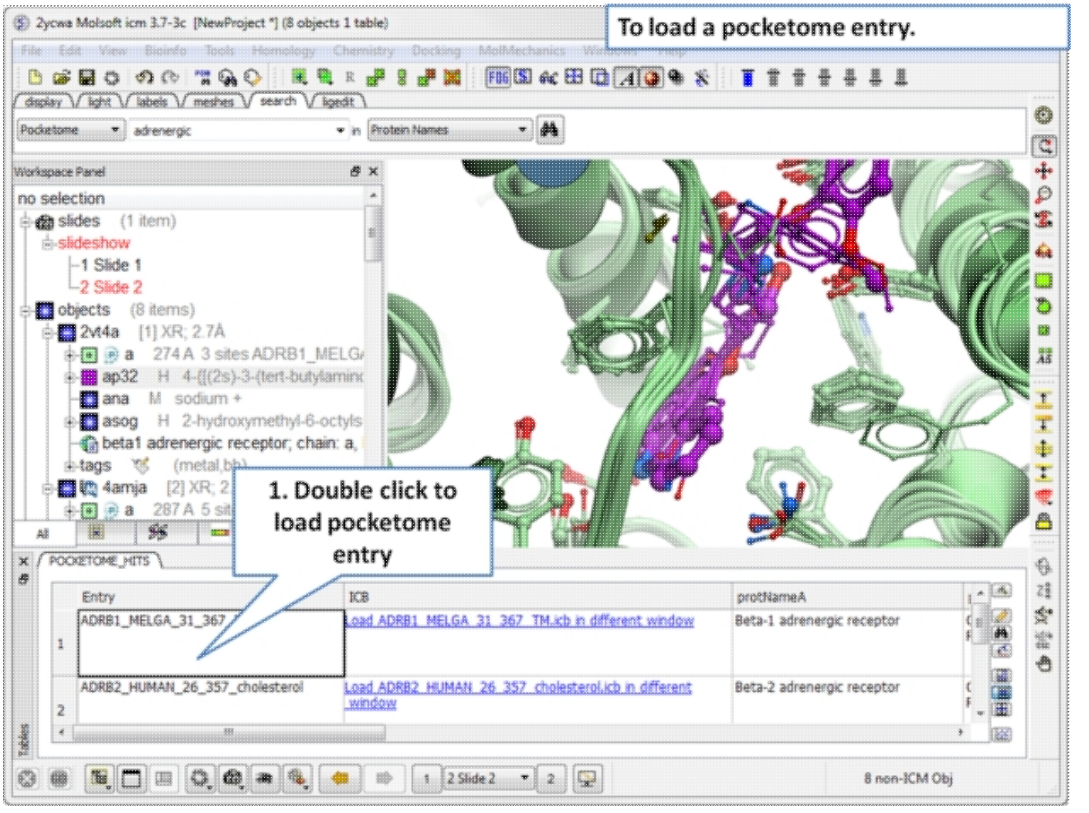


3.1.2 Search Pocketome

The Pocketome (www.pocketome.org) is an encyclopedia of conformational ensembles of all druggable binding sites that can be identified experimentally from co-crystal structures in the Protein Data Bank.



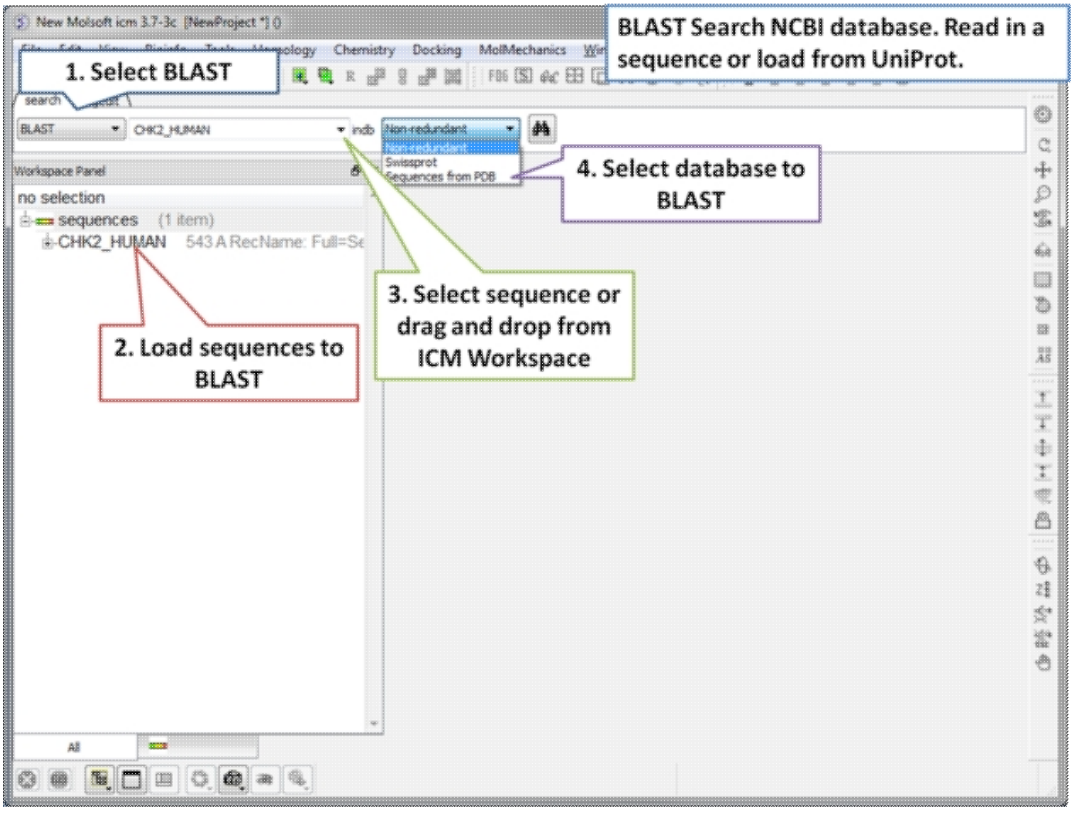
Step 1: Click on the search tab and choose the Pocketome option. Check a field you would like to search e.g. Protein Name, Family, domain...



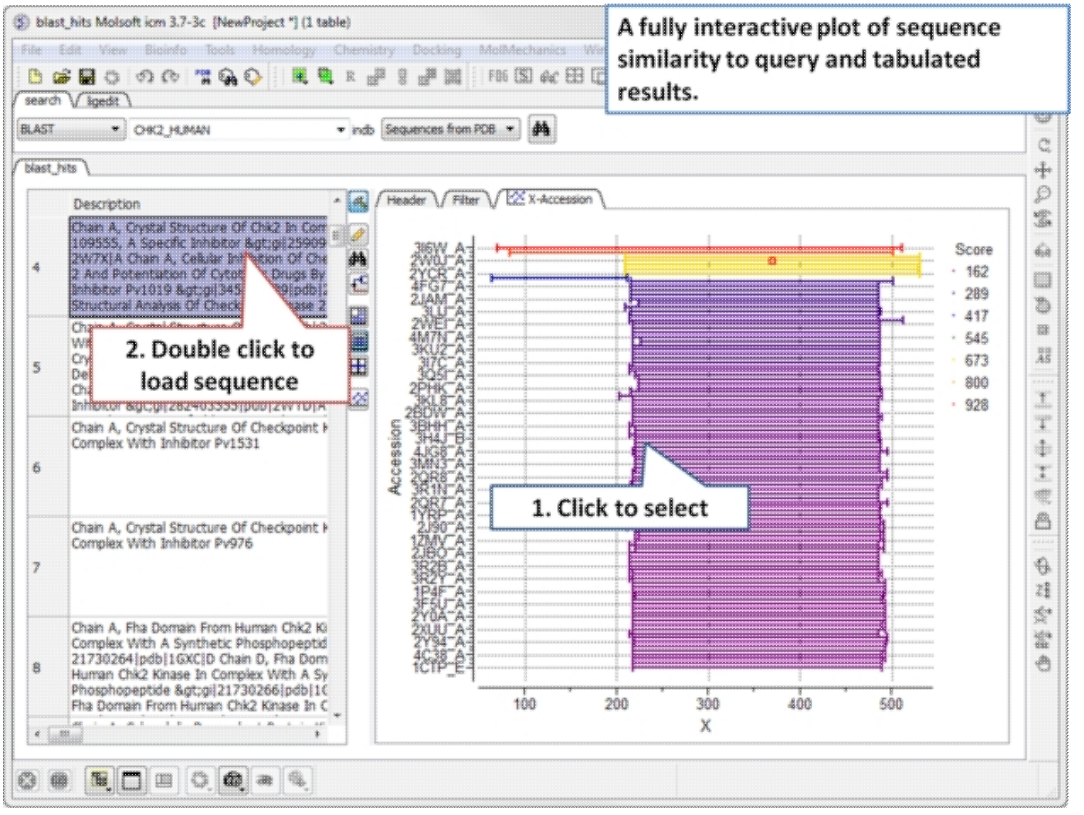
Step 2: A table of pocketome hits will be displayed. Browse the results and double click to load a pocketome entry.

3.1.3 BLAST Search

To BLAST search the NCBI sequence database:

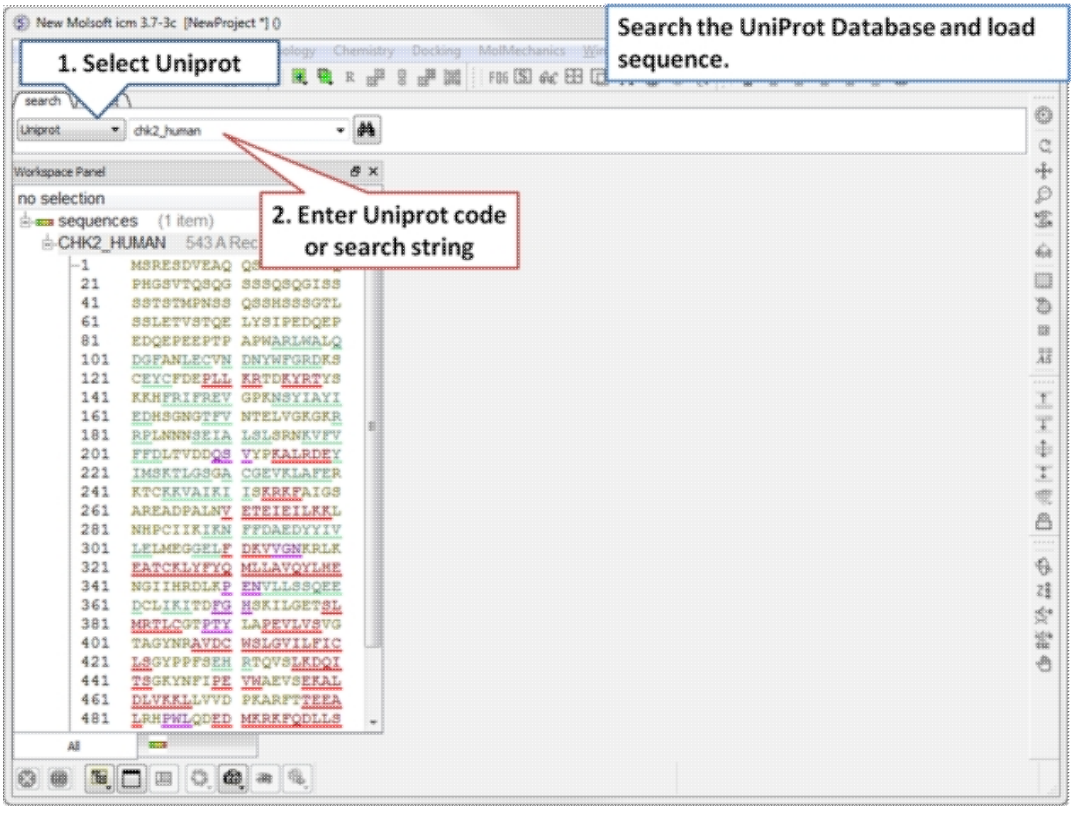


Step 1: Load a sequence into ICM. Select the Search tab and choose the BLAST option. Drag and drop the sequence into the search field, use the drop down menu or type the sequence name.



Step 2: A fully interactive table and plot of sequence conservation will be displayed. Double click to load a sequence.

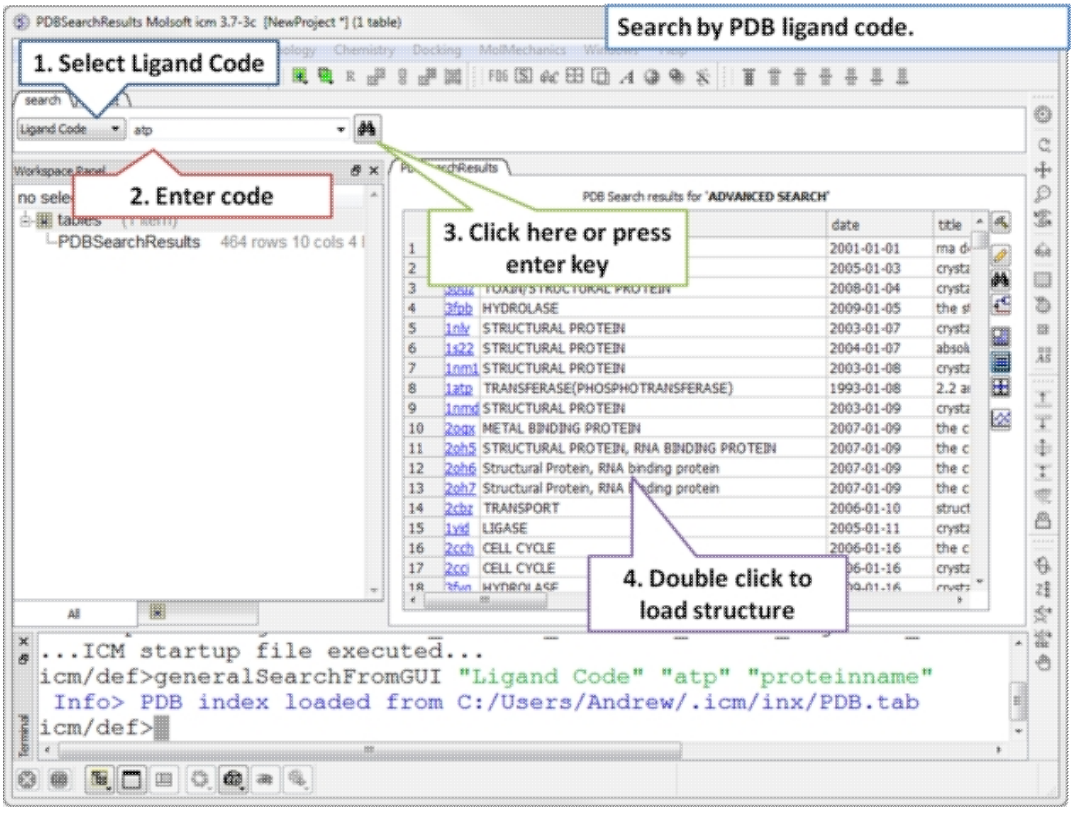
3.1.4 Search UniProt



Step 1: Click on the search tab and select **Uniprot** from the drop down menu. Enter the UniProt code. The sequence will be loaded directly into ICM and you will see it in the ICM workspace.

3.1.5 Search PDB by Ligand Code

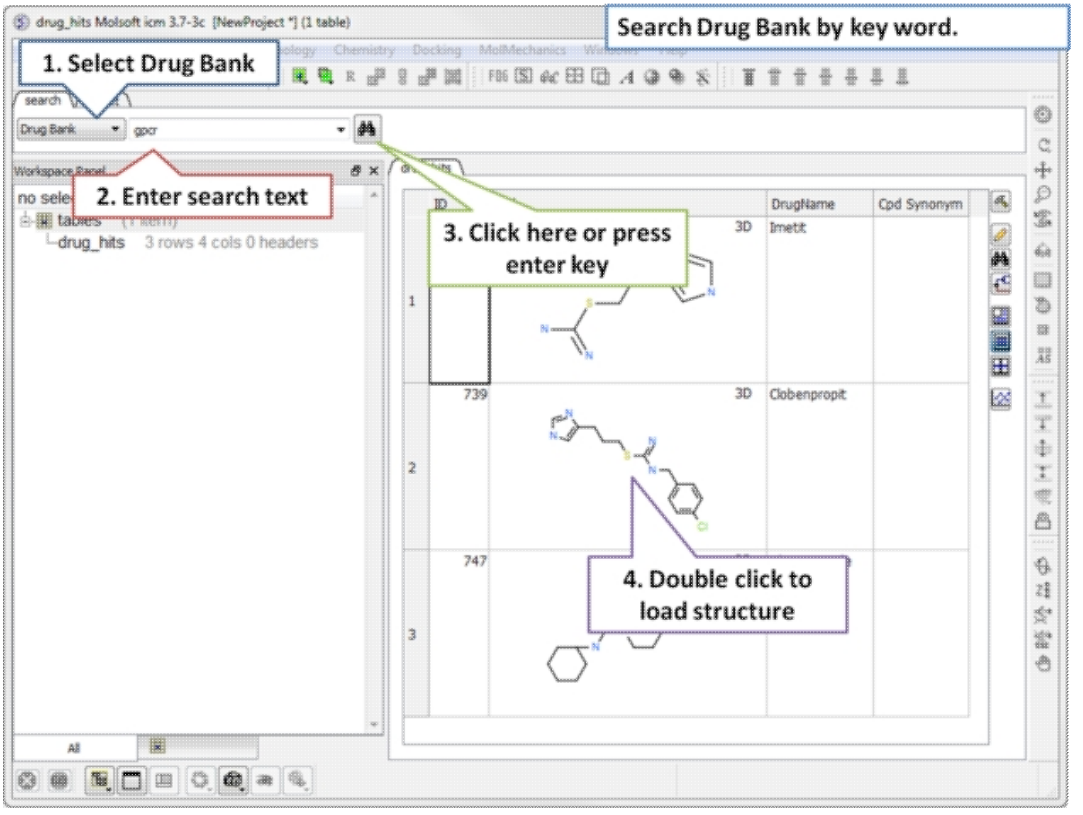
To find structures containing a particular ligand in the PDB.



Step 1: Click on the search tab and select **Ligand Code** from the drop down menu. Enter the Ligand code and a table of hits will be displayed.

3.1.6 Search Drug Bank

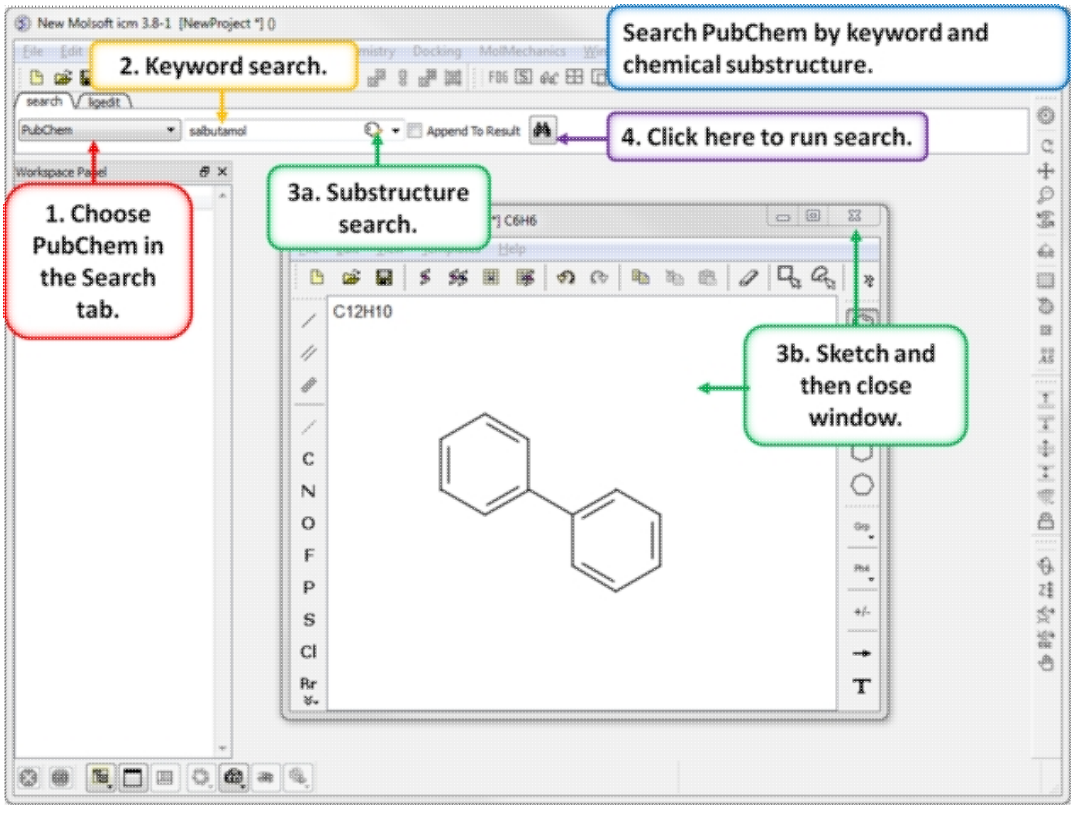
To search Drug Bank (`http://www.drugbank.ca/`)



Step 1: Click on the search tab and select **Drug Bank** from the drop down menu. Enter a search string and a table of results will be displayed.

3.1.7 Search PubChem

To search PubChem (https://pubchem.ncbi.nlm.nih.gov/):



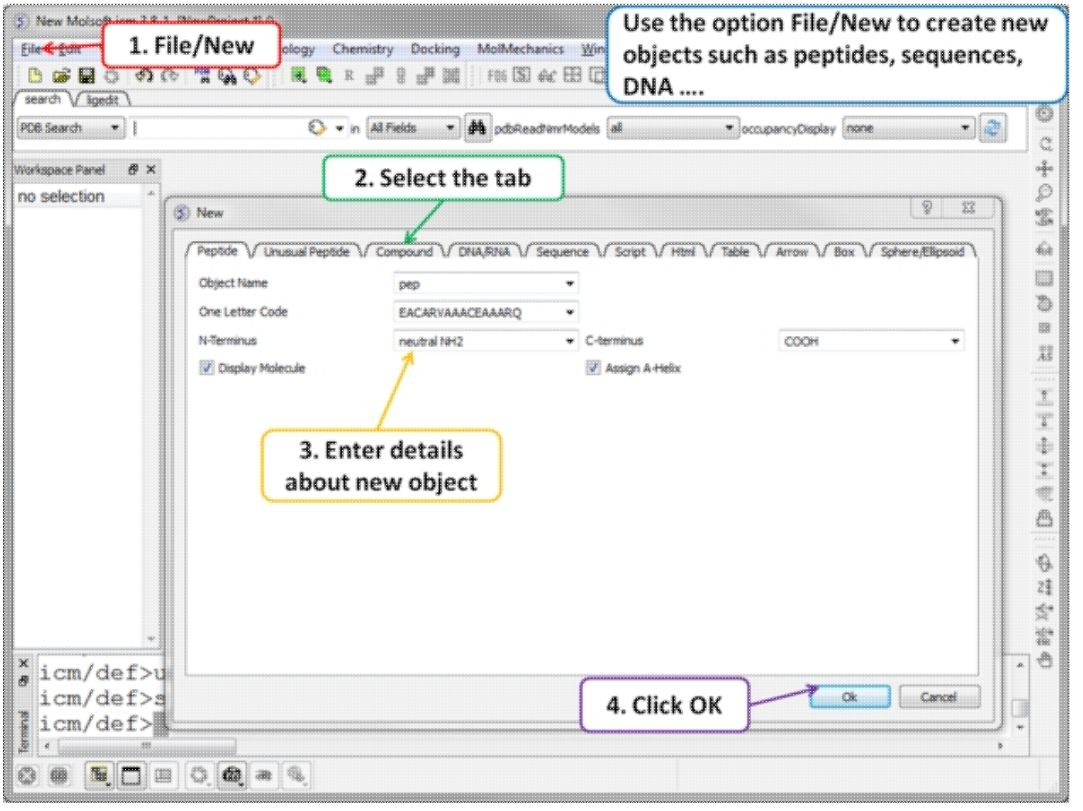
- Click on the search tab and select **PubChem** from the drop down menu.
- Enter a search string and a table of results will be displayed or click on the chemical sketch button and sketch a substructure. When you close the chemical sketch window the smiles string will be added to the keyword search panel.
- Click on the "binocular" button and run the search.
- A table of hits will be displayed.

3.2 Create New Objects

Available in the following product(s): `ICM-Browser` | `ICM-Browser-Pro` | `ICM-Pro` | `ICM-Chemist`

In the File menu there is an option called New. This option can be used to create new objects of the following types:

- Peptide
- Unusual Peptide
- Compound
- DNA and RNA
- Sequence
- Script
- HTML
- Table
- Arrow
- Box
- Sphere/Ellipsoid



3.3 Open and Read Files

Available in the following product(s): `ICM-Browser` | `ICM-Browser-Pro` | `ICM-Pro` | `ICM-Chemist`

Any file that ICM can understand can be opened by:

- Selecting File/Open.

A file with an extension .icb is an ICM binary file and can be viewed in the GUI. A .icb file can contain many objects such as sequences, meshes, protein objects, alignments, tables etc...

3.3.1 Open with Password

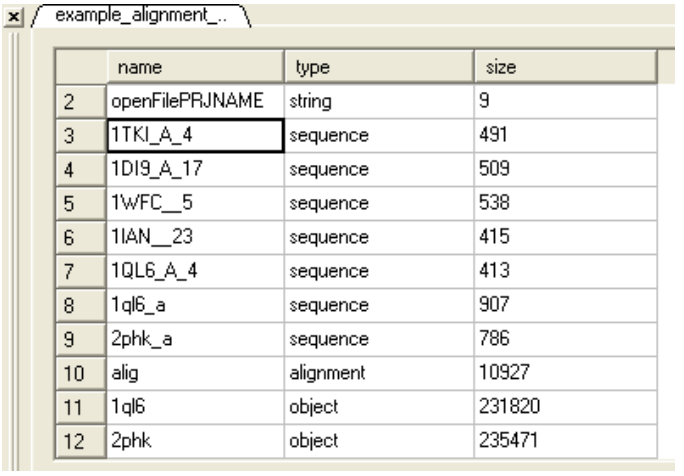
To open a file that is password `protected`:

- File/Open with Password

3.3.2 Extract from icb file

An **icb** file is an `icm project file`, in some instances you may want to take objects saved in an icb file and load it in your current ICM session. This option allows you to view a tabulated list of what a icb file contains and load individual object files from it.

- 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 object from the icb file.


example_alignment_..

	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

3.4 Saving Files

Available in the following product(s): `ICM-Browser` | `ICM-Browser-Pro` | `ICM-Pro` | `ICM-Chemist`

Anything you have displayed in an ICM graphics session can be conveniently stored in a single file called an .icb file. To do this:

- File/Save Project

or

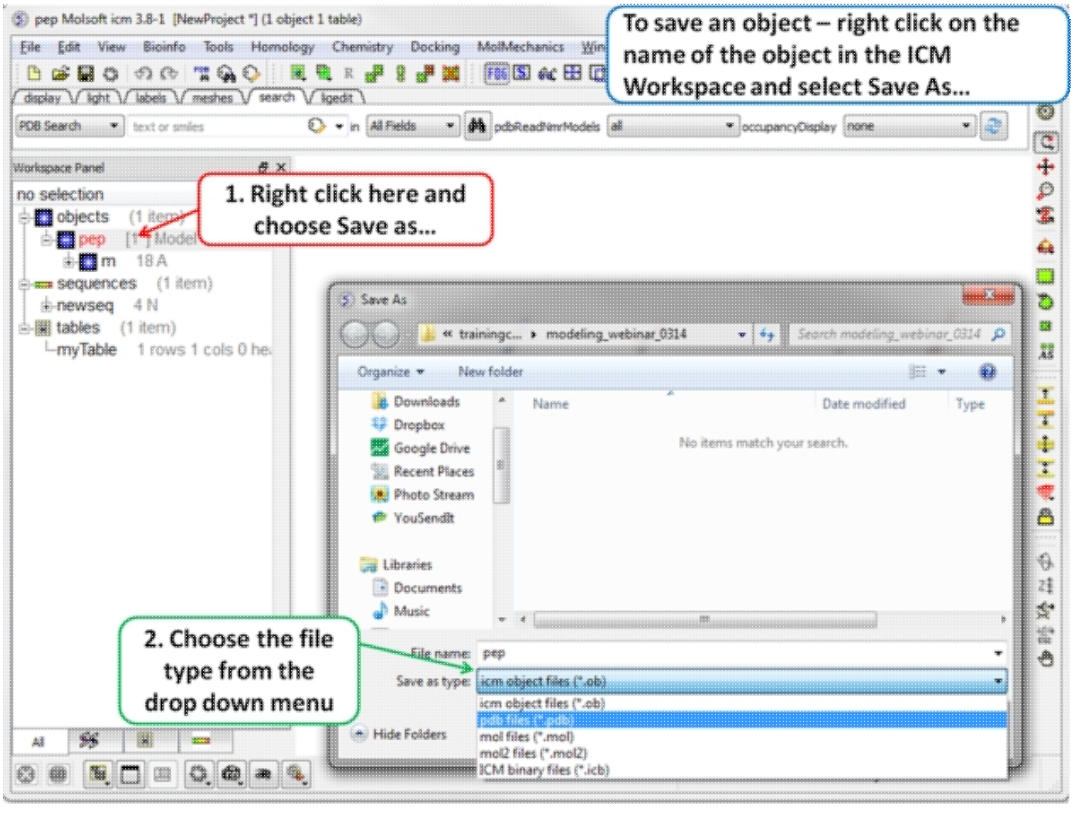
- File/Save Project As

A .icb file can be password protected by:

- 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 .

Any object (e.g. protein,table, alignment...) inside the ICM GUI can be saved by:

- Right click on the name of the object in the ICM Workspace.
- Select "Save As"
- Choose the file format from the "Save as Type" drop down dialog.

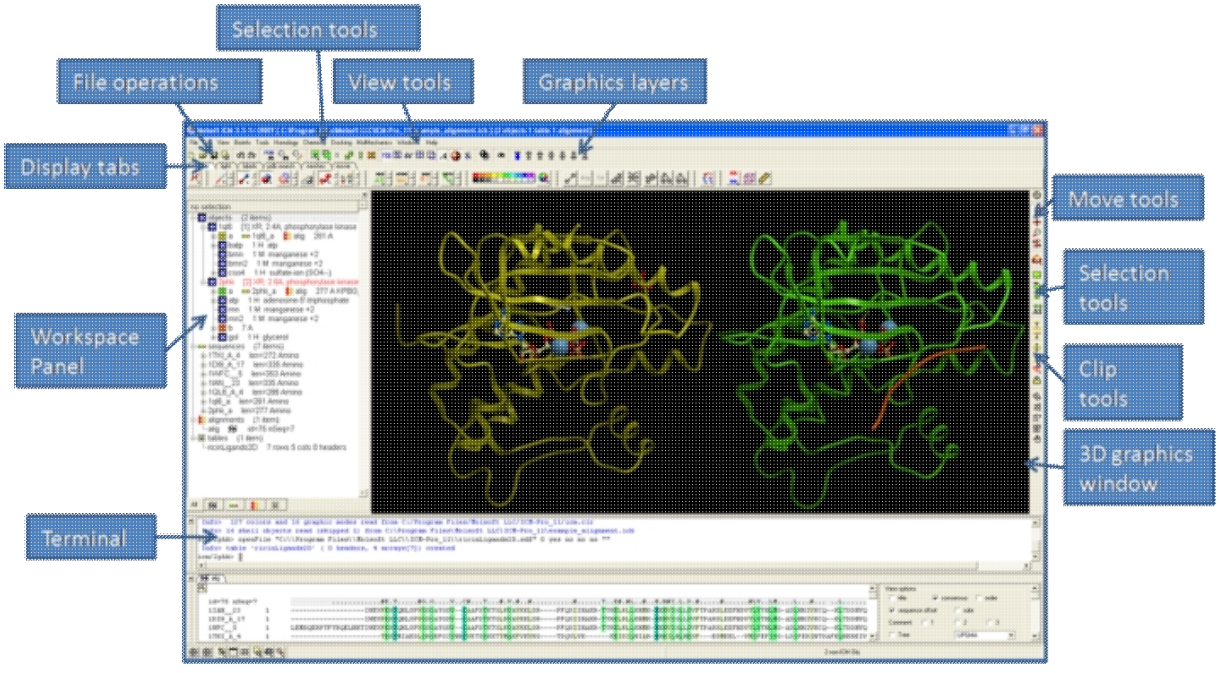


3.5 How to Use the Graphical Display

Available in the following product(s): `ICM-Browser` | `ICM-Browser-Pro` | `ICM-Pro` | `ICM-Chemist`

3.5.1 The Components of the GUI

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

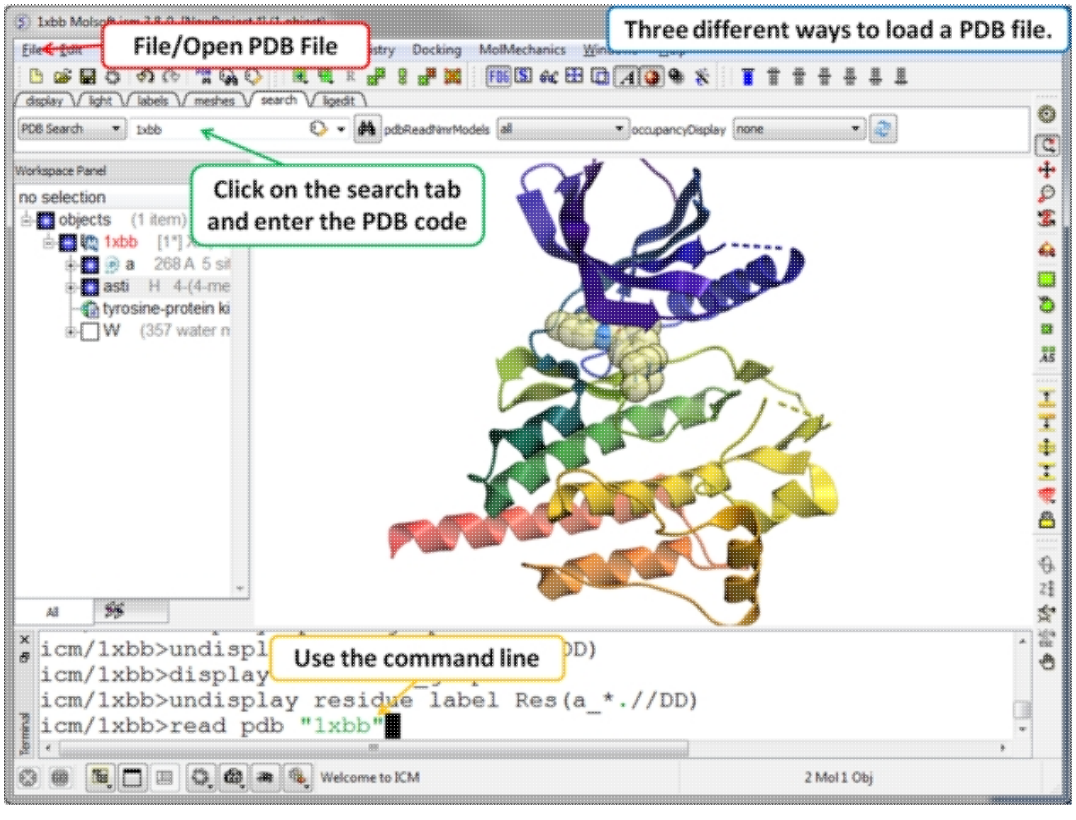


3.5.2 How to load a PDB Structure

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

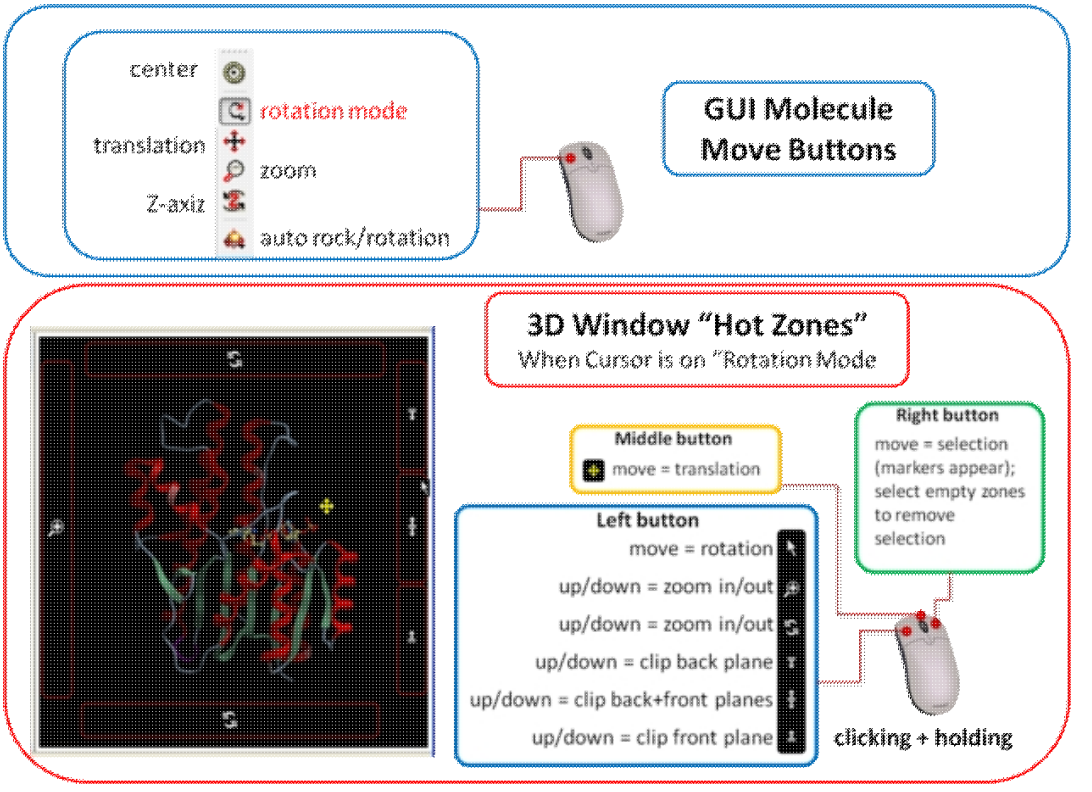
1. Using the command line.
2. Using File/Open button
3. Using the PDB Search tab

Other PDB search options are described in more detail in the `PDB Search` section of this manual.



3.5.3 How to Move a Structure in the Graphical Display

Available buttons and options for moving molecules around the graphical display window. This is described in more detail in the section entitled `Move Buttons`.



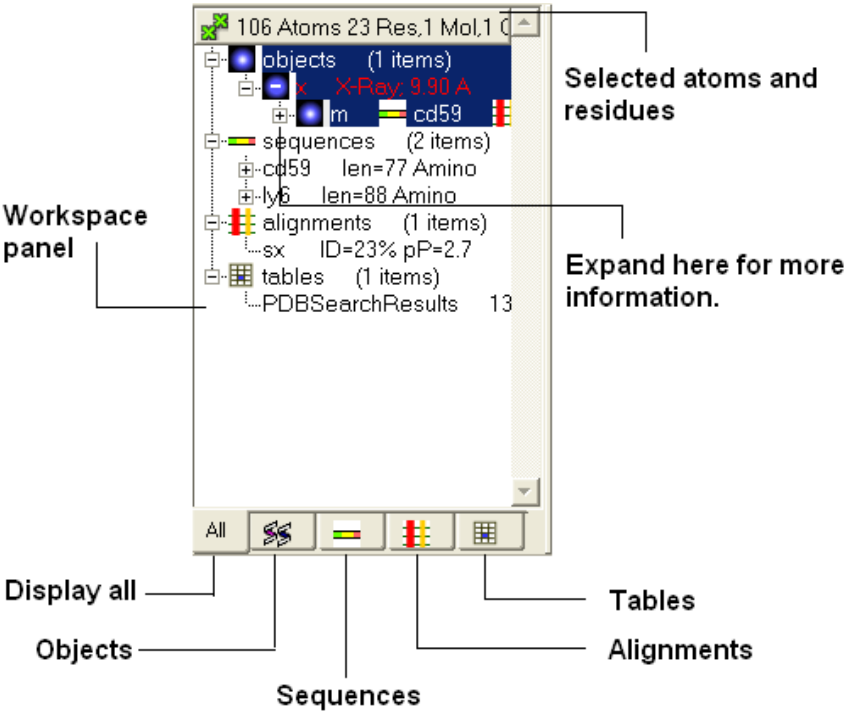
How to use the Graphics window controls

In the graphics window you can use various `tools` described elsewhere but it is helpful to know the following things:

- **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.

3.5.4 How to Display Molecules using the ICM Workspace Panel

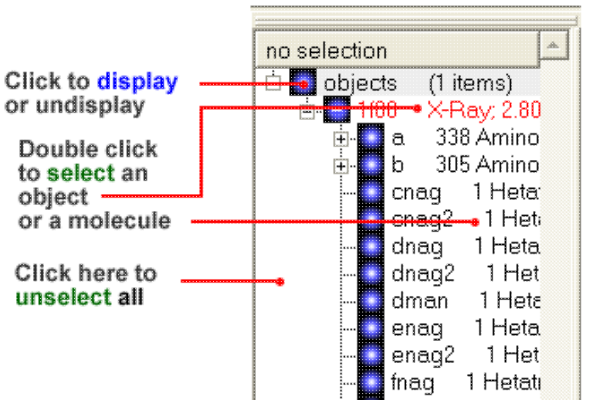
The workspace panel (located on the left hand side panel of the gui) is an important place within the graphical user interface because it displays which sequences, structures, objects, tables and alignments are currently loaded into ICM. From the ICM Workspace panel you can make graphical selections and display and undisplay molecules.



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.

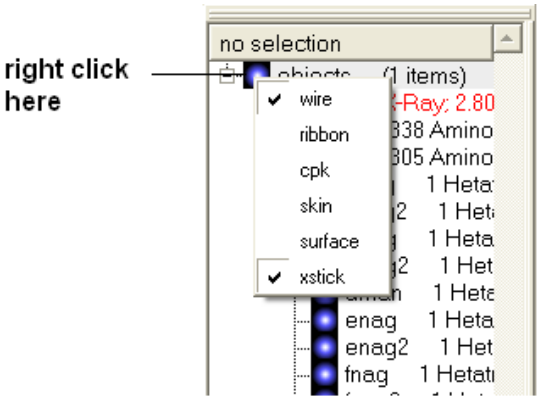
To display every component of the object except for binding sites and water atoms:

- 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 selected regions of the molecule in wire, ribbon, cpk, skin, surface and xstick representations:

- Right click on the appropriate box in the **ICM** workspace. A menu will be displayed and select the representation you would like to use (e.g. wire, ribbon etc...)

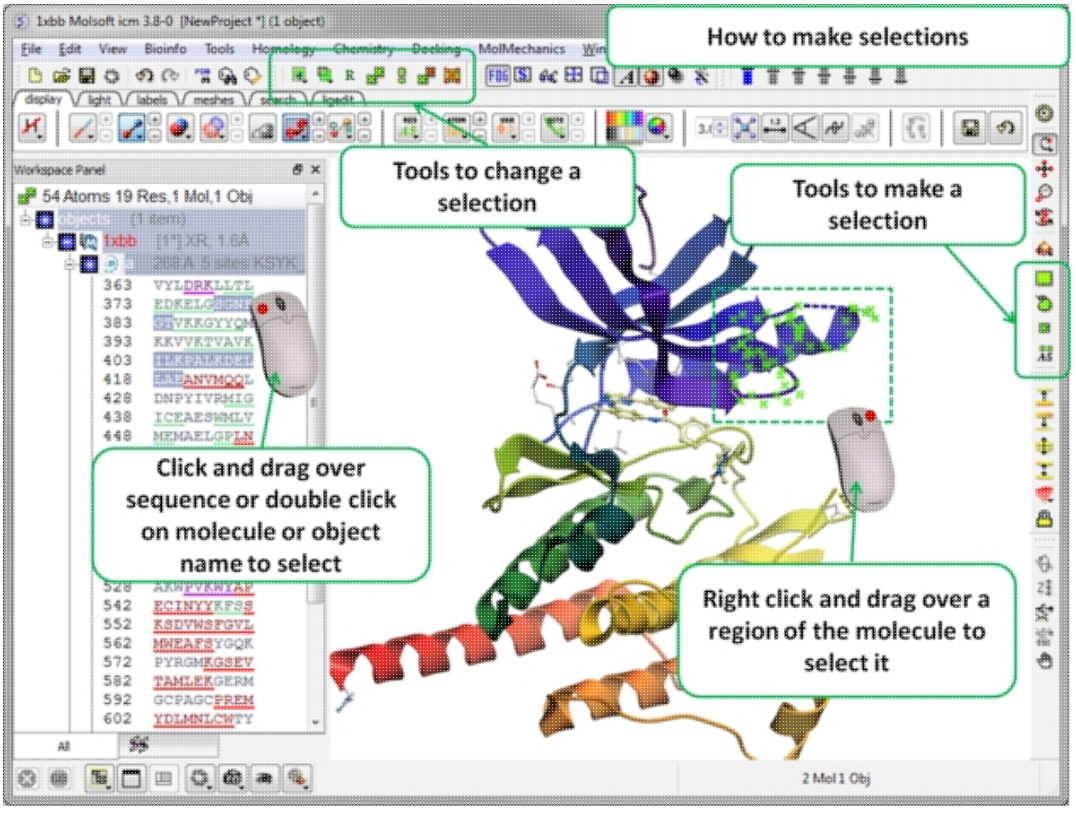
3.5.5 How to Make Selections

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.

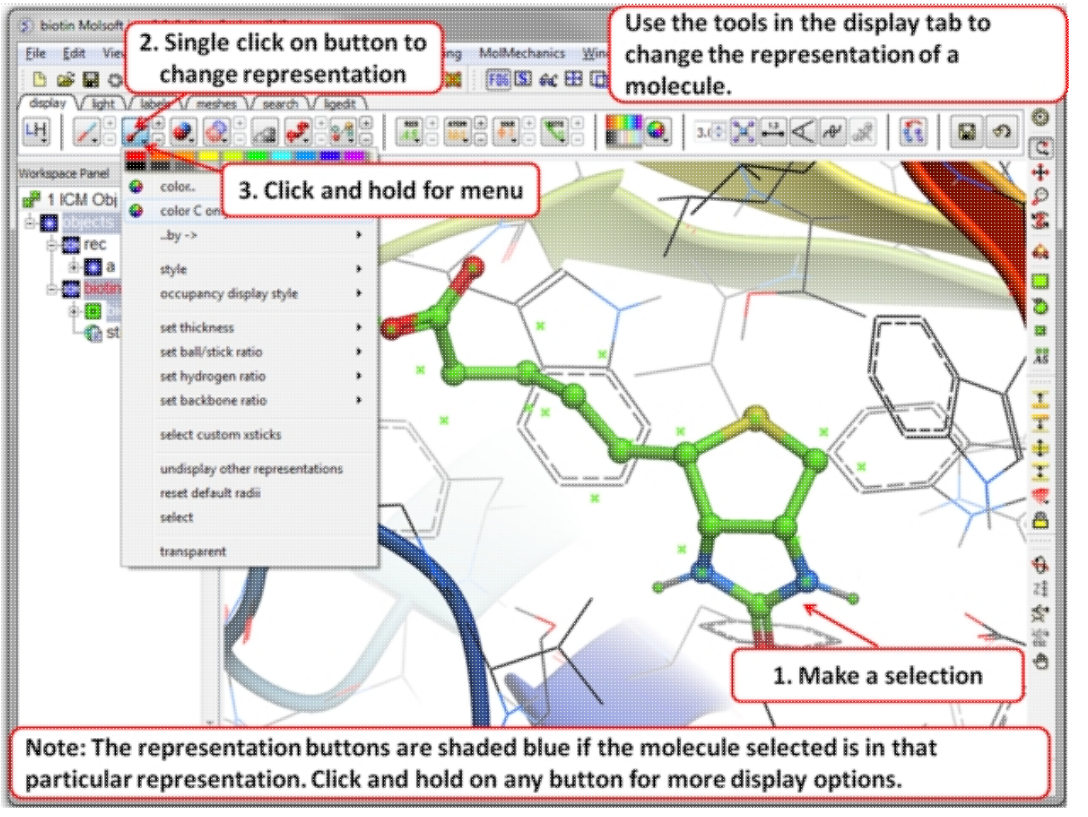


3.5.6 How to Change Protein Representation

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

There are 6 main types of representation:

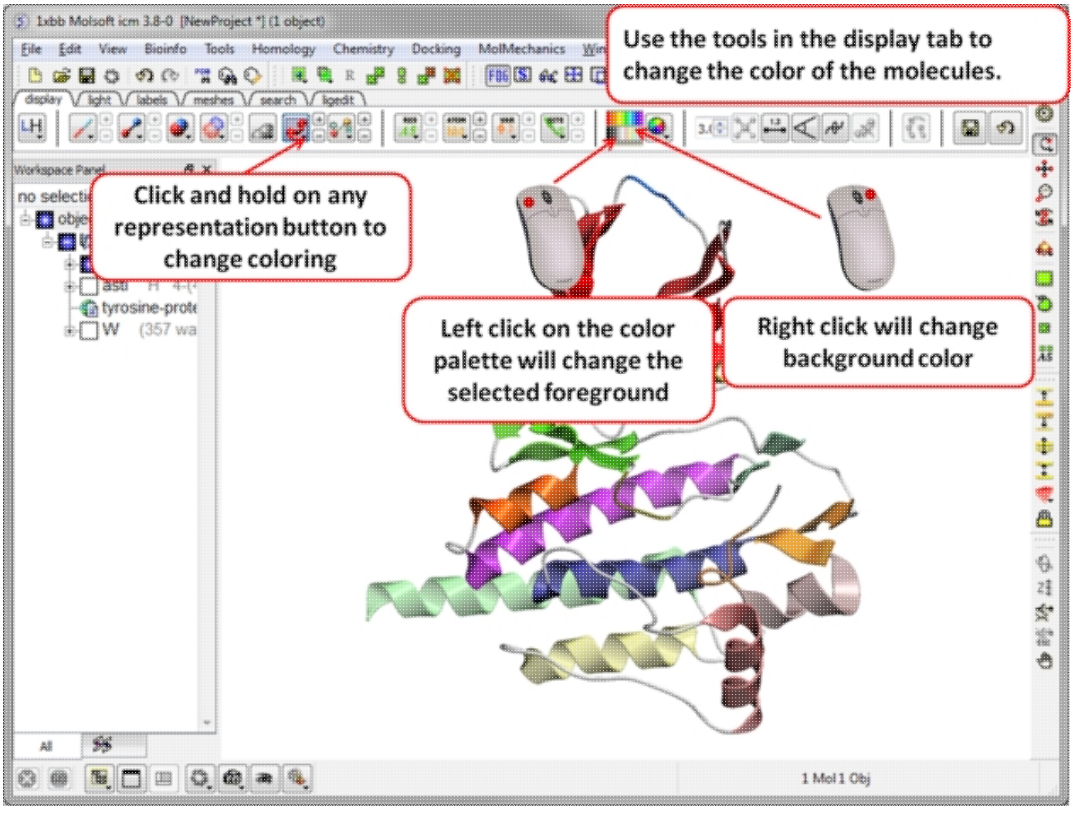
- **Wire:** Wires connecting covalently bound atoms of a molecule. This representation has no defined thickness as such will not make shadows. Useful for showing the chemical structure of a small molecule.
- **Xstick:** Covalent bonds are represented as cylinders whilst atoms are represented as small 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 Kultun.
- **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



3.5.7 How to Color

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

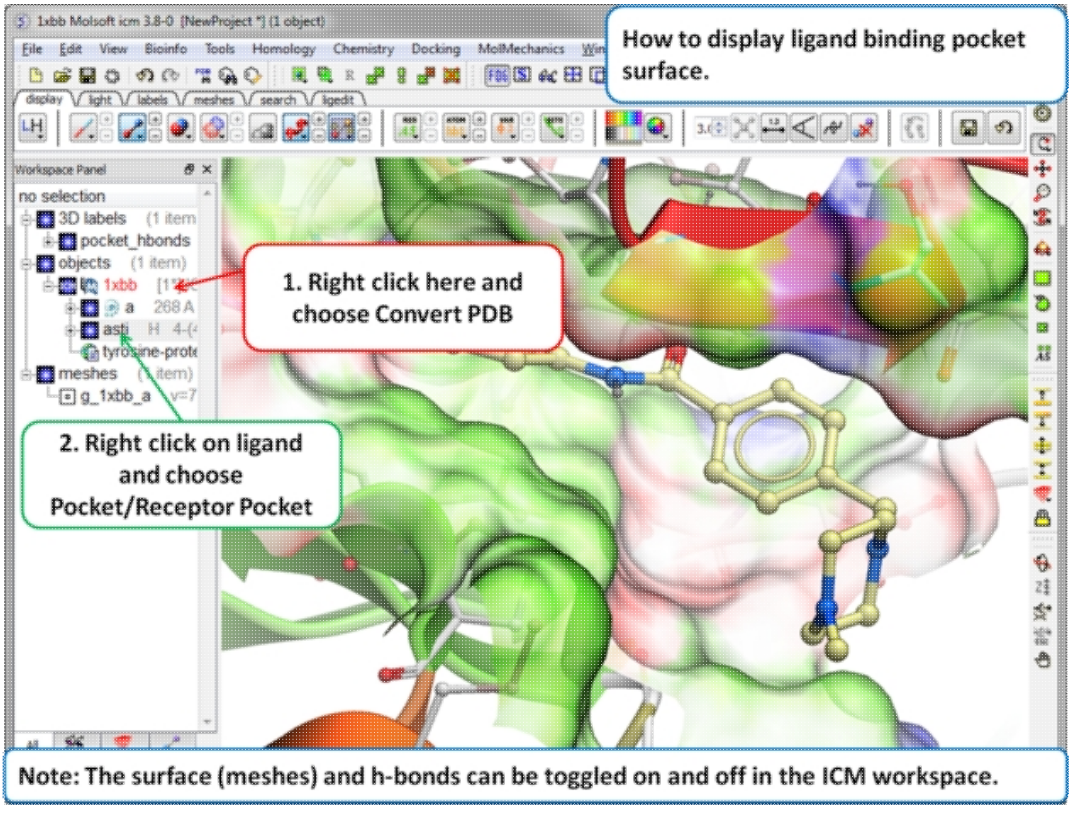
Changing the colour of a representation works in much the same way as displaying the representation itself. The selection rationale is the same followed by clicking on a colour in the palette in the `display tab`. It is also possible to colour different representations of the same selection independently by clicking and holding on the representation buttons in the `display tab`.



3.5.8 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**.

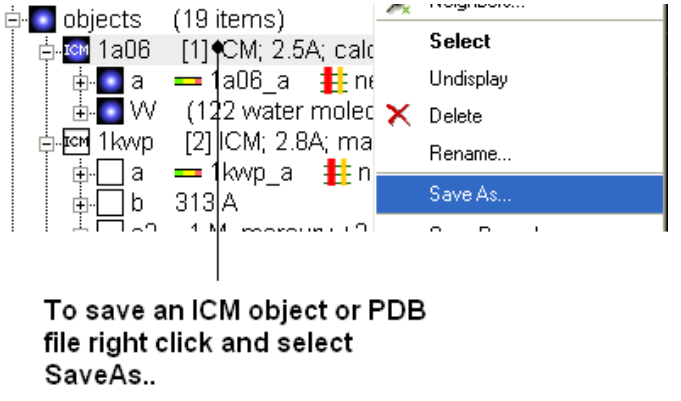


3.5.9 How to Save an ICM Object

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.



3.5.10 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**.

3.5.11 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.

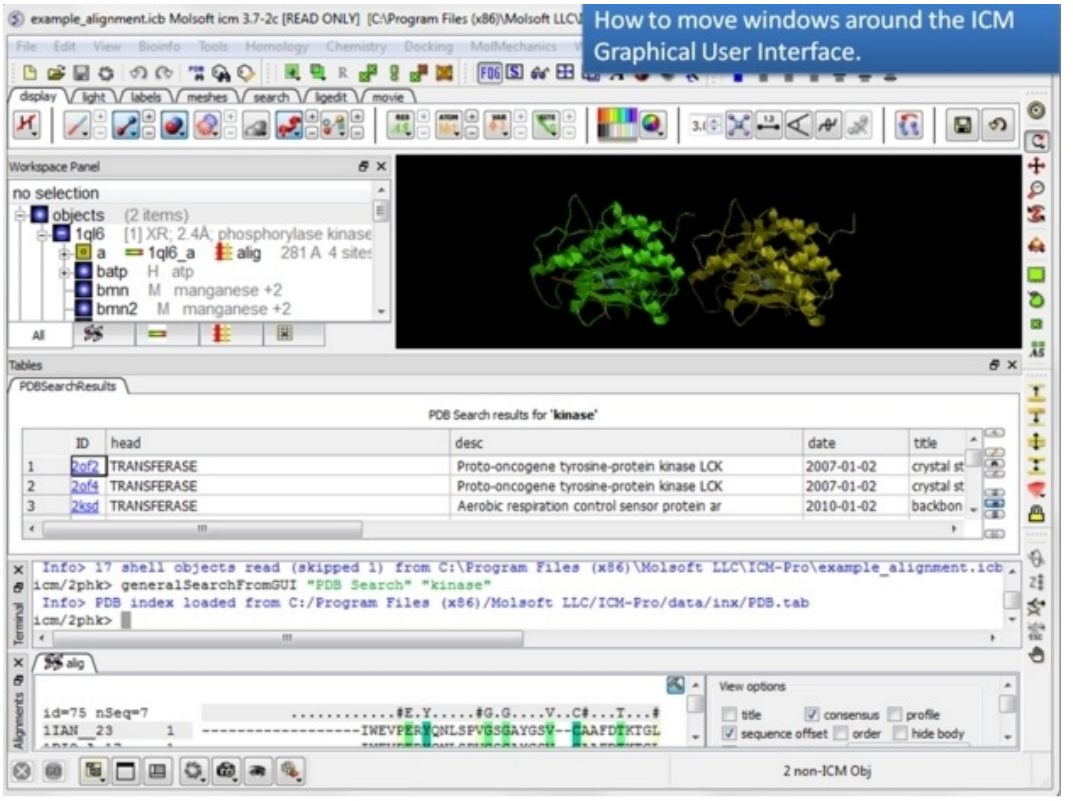
3.5.12 How to: Right Click Options

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

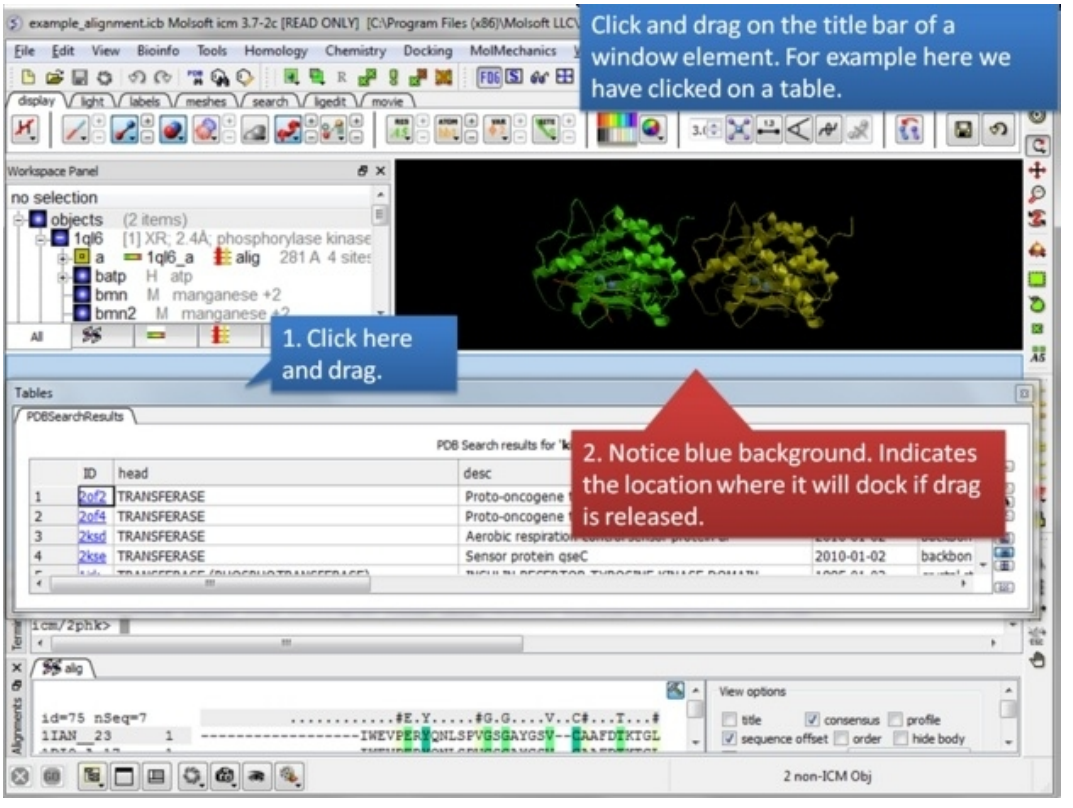
The right click mouse option can be used throughout the graphical user interface. It is a very useful means of opening up a whole new world of menus and options. Most of these options are described in this book. However, when using the graphical user interface it is always a good idea to try right clicking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

3.5.13 How to Move Windows

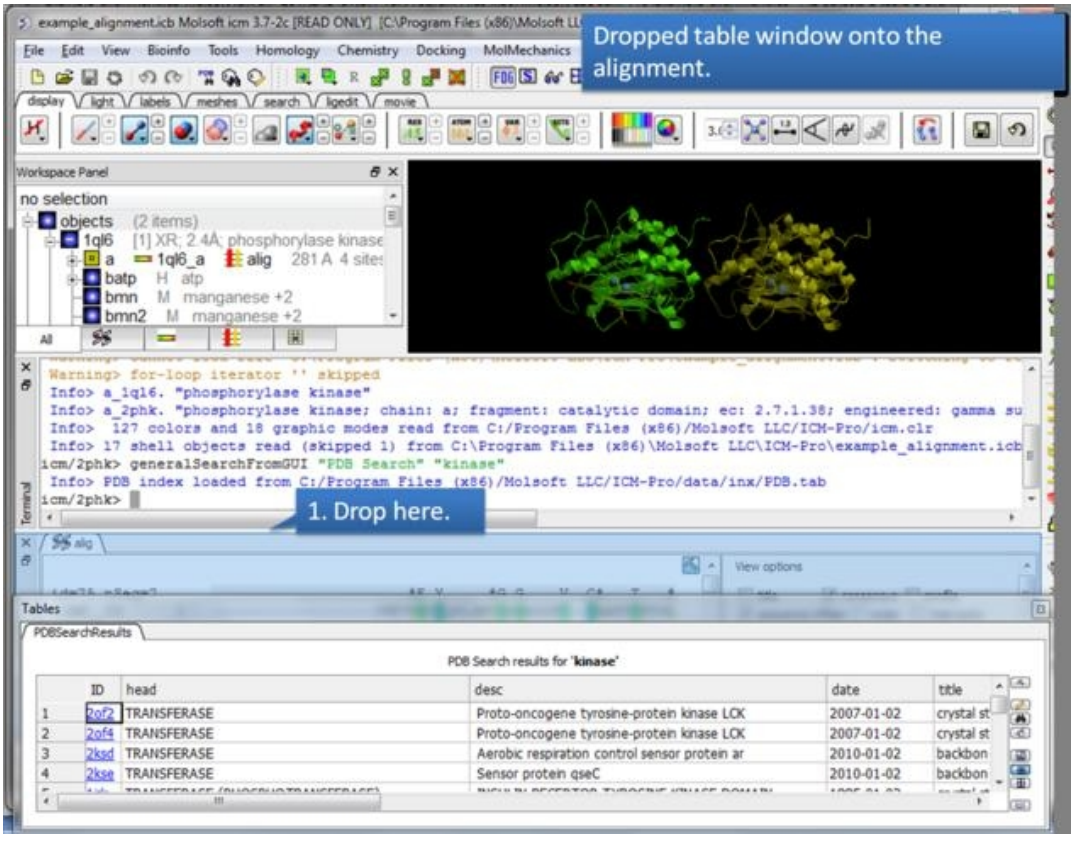
Is your graphical user interface looking a bit messy? Do you have tables, alignments, plots all over the place? Here we show you how to arrange everything to make a clearer GUI environment.



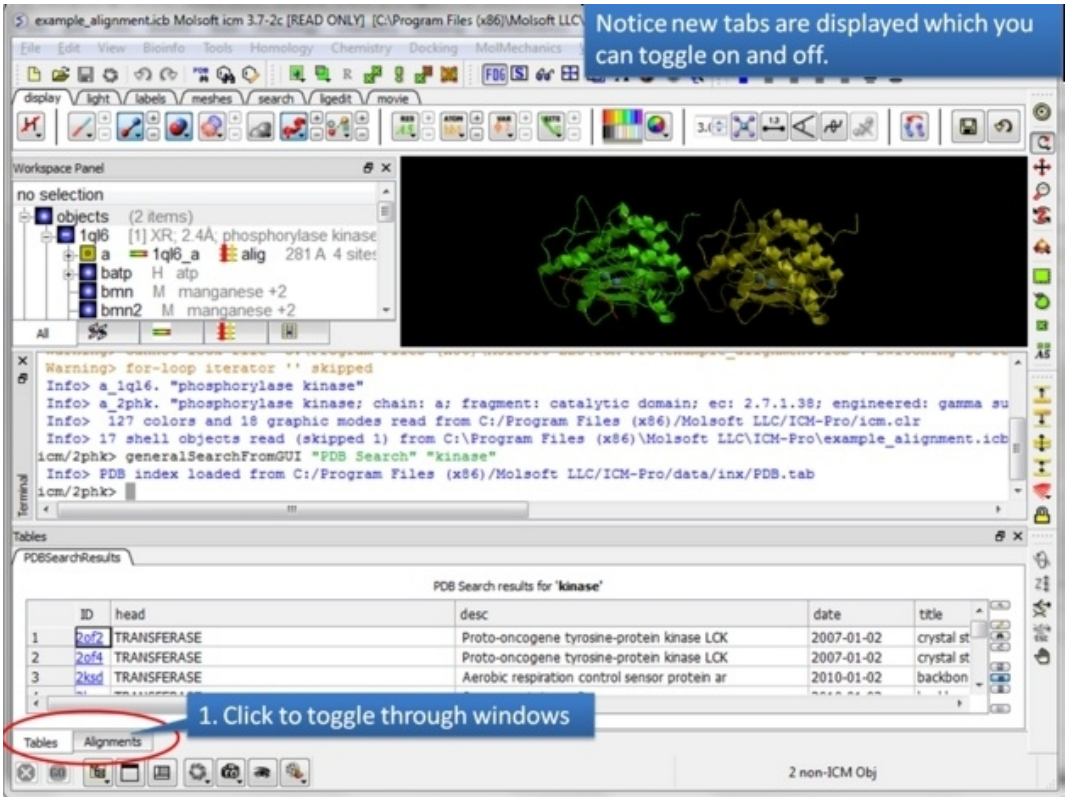
1. Too many windows in your GUI? You can move them around to make viewing easier.



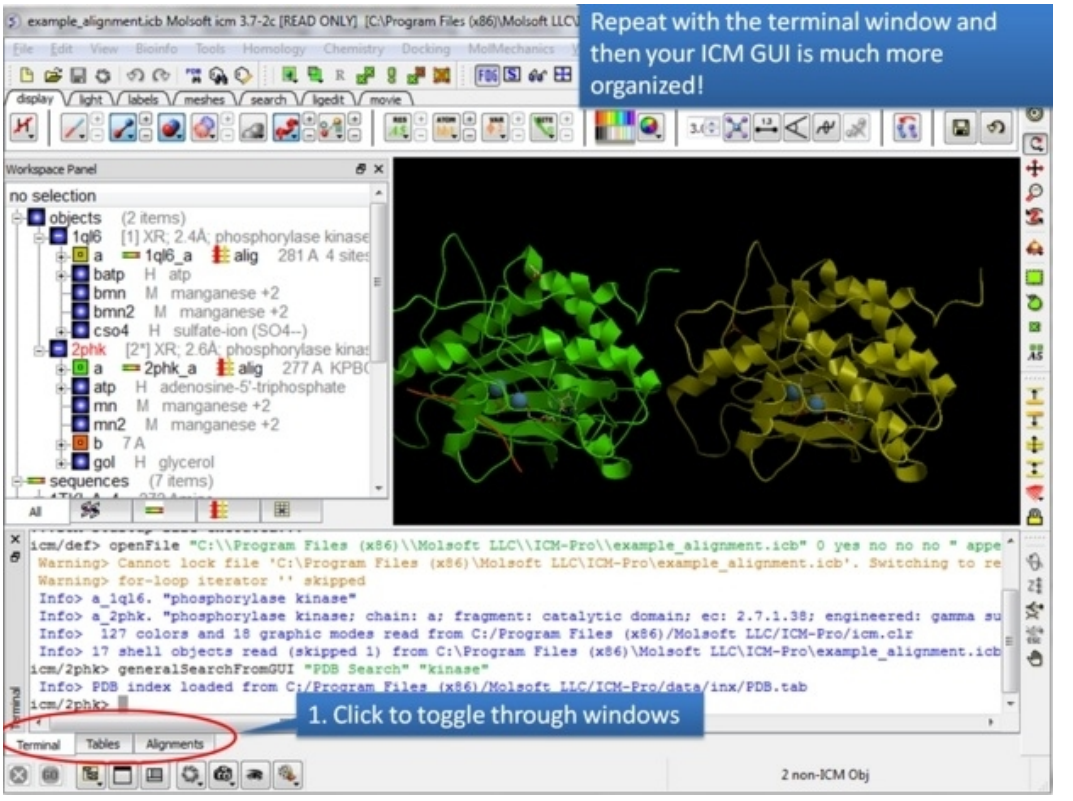
2. Click and drag on a window title bar to move it.



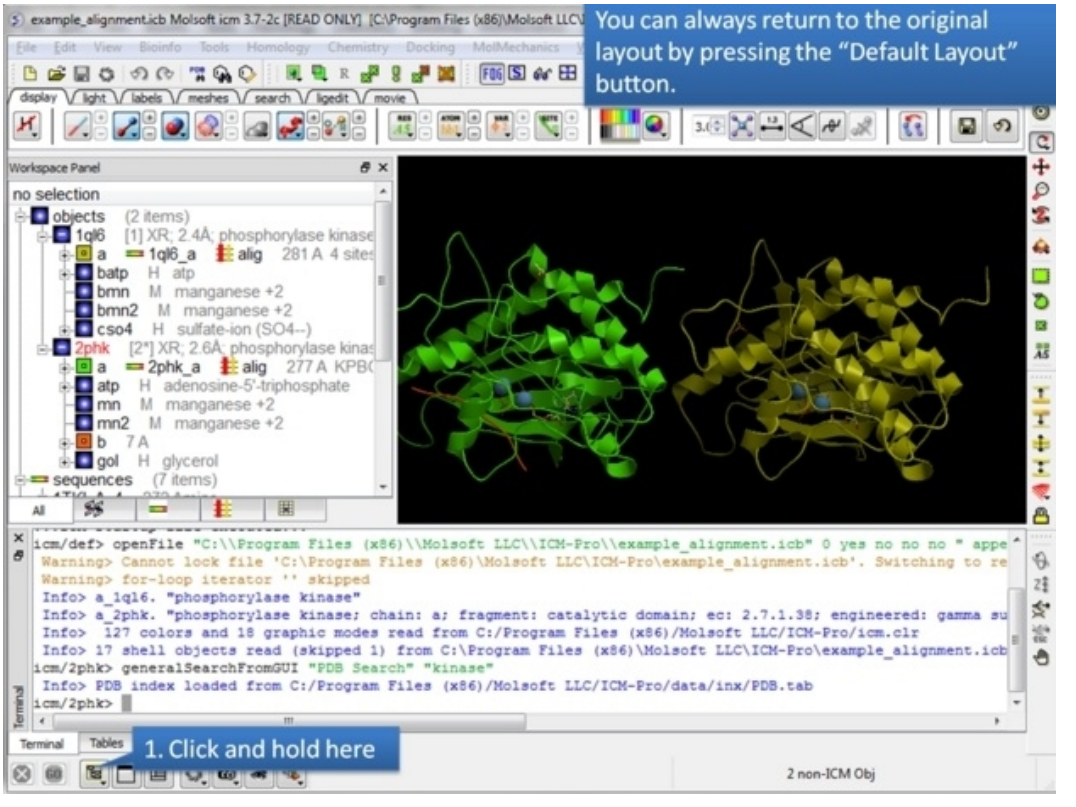
3. Drop one window on another one to dock it.



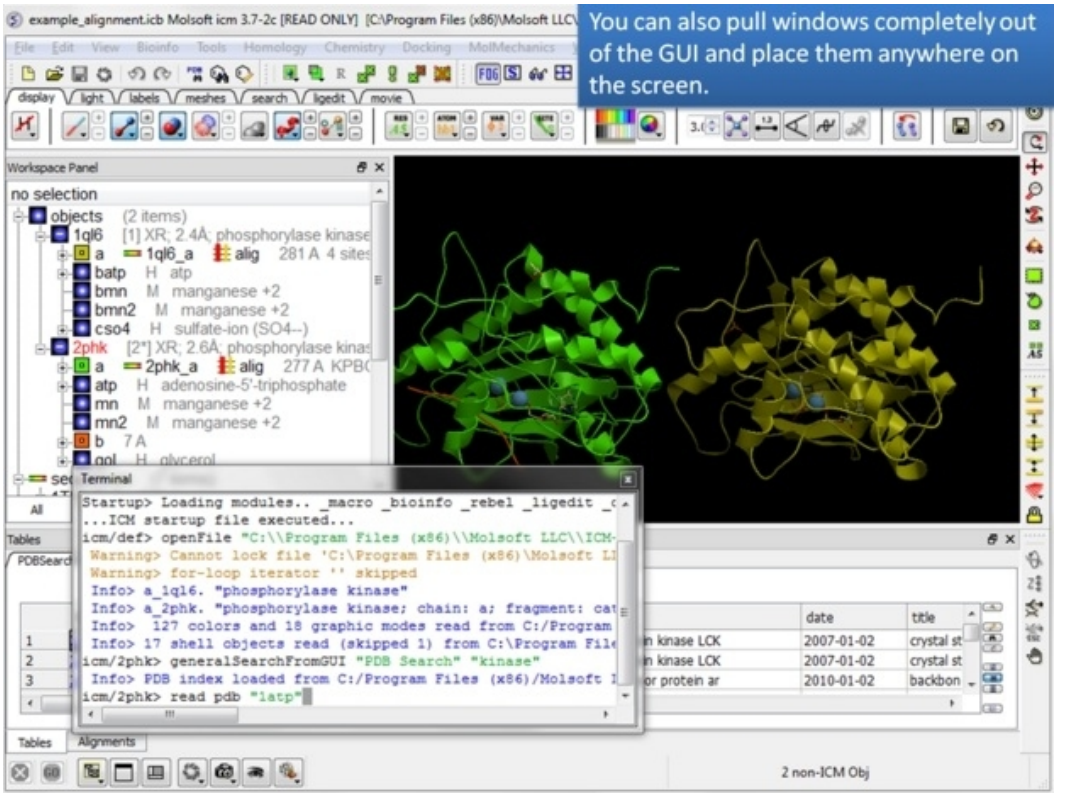
4. You can access each window by clicking on the tabs.



5. In this example we have the table, alignment, and terminal all in the same panel



6. There is a quick way to return the windows to their original location.

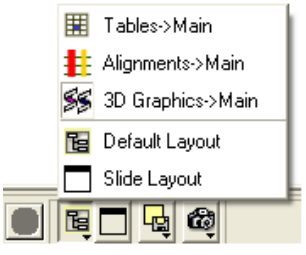


7. You can also move a window to any part of your screen.

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

OR

Click the default layout icon.



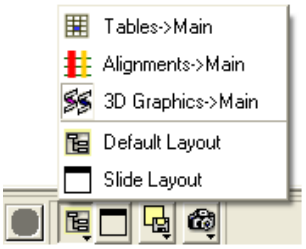
Some options can be accessed at the bottom of the GUI.

OR

Double click on the window header.

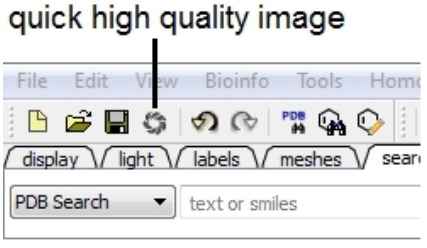
3.5.13.1 How to Arrange Windows

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.



3.5.14 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 button in the view tools panel (see image below).



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`.

3.6 Making Selections

Available in the following product(s): `ICM-Browser` | `ICM-Browser-Pro` | `ICM-Pro` | `ICM-Chemist`

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 want to display a particular region or molecule contained within your protein structure 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 isnt.

There are four basic levels of selection

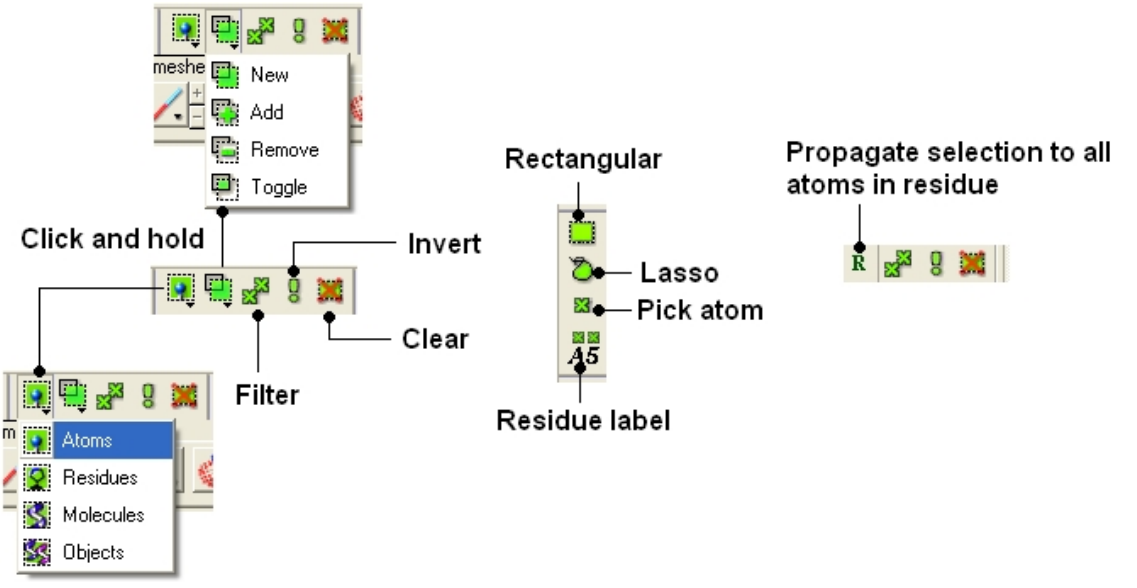
1. Object (eg a PDB structure or ICM object)
2. Molecule
3. Residue
4. Atom

You can make selections in:

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

3.6.1 Graphical Selection Tools

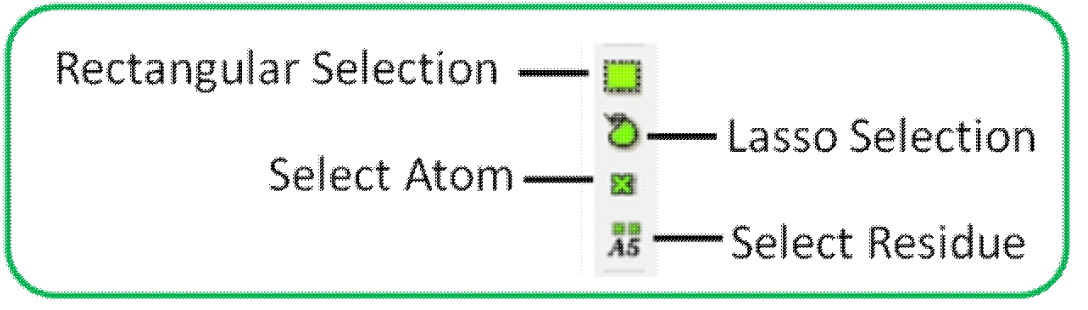
The following buttons can be used to make a selection once a structure is displayed.



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

3.6.2 Quick Selection

To make a quick selection the following buttons can be used.



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:

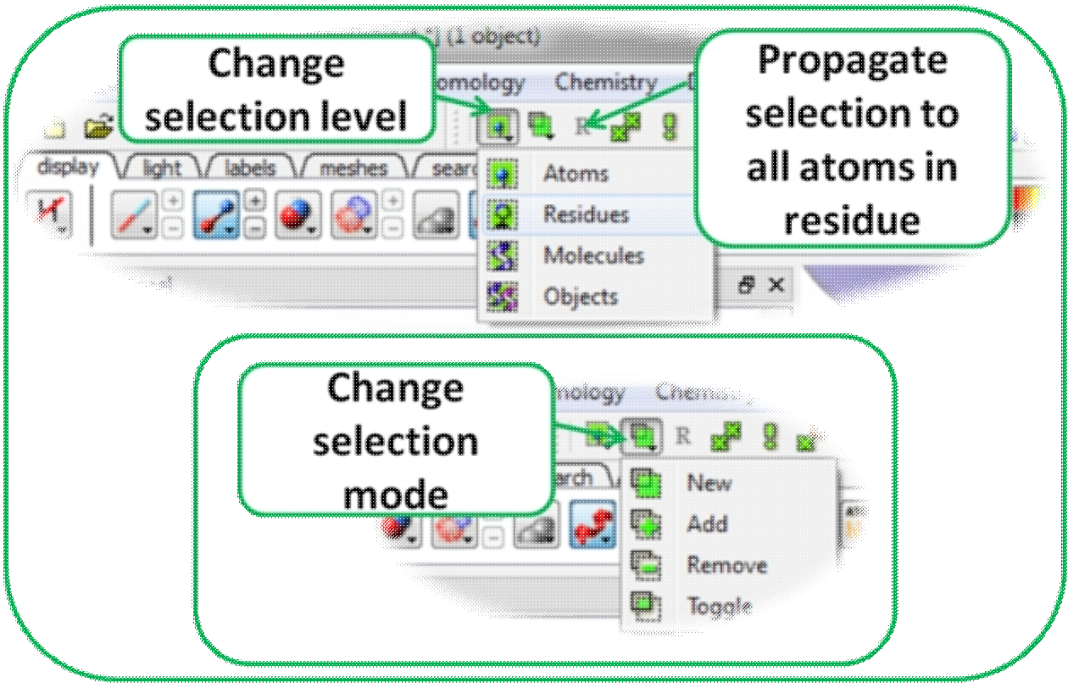
- Click on the 'pick atom' button

3.6.3 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 button can be used to do this (see image below).

For example, a C-alpha of a residue is selected but one would like to select all atoms in the residue. You can change the level to **Residues.** This selection can then be changed into all atoms of the residue by then selecting the **Atoms** level again. Or you can use the **Propagate Selection to all Atoms** button (see image below).

- 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.

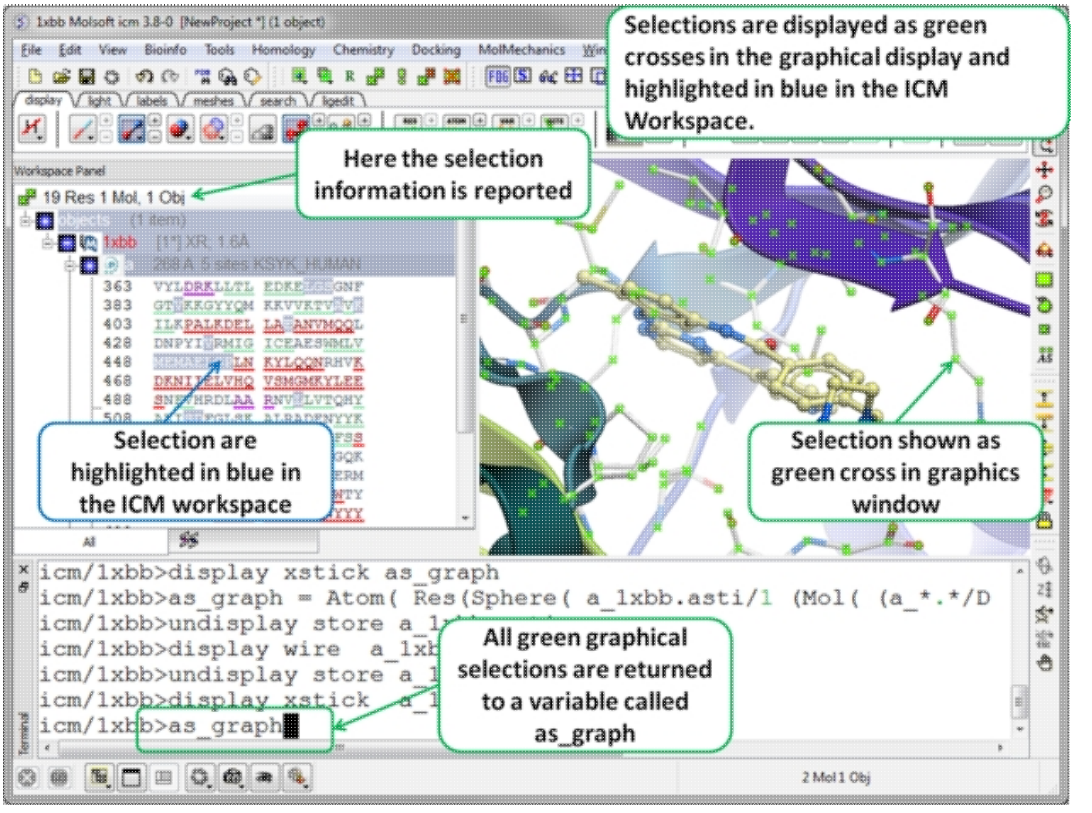


It is also important to observe the selection mode that is being used. There are four modes:

- 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 hasnï¿½t been selected, wilbe selected

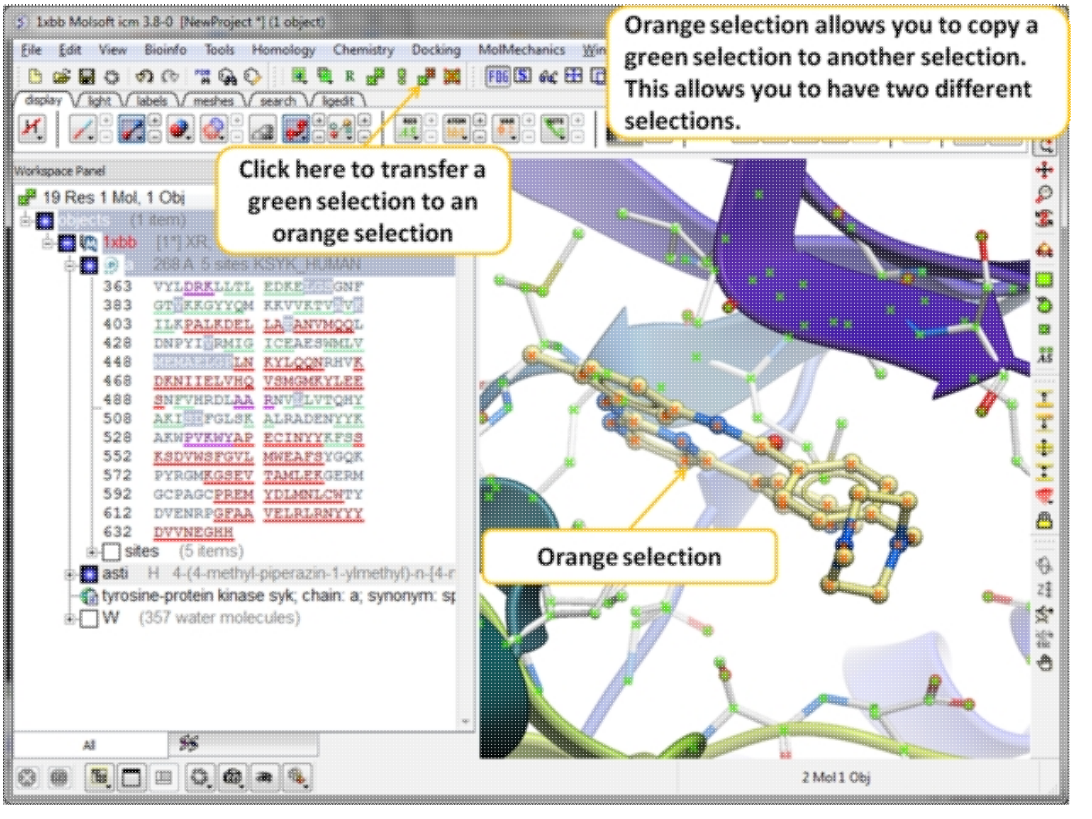
3.6.4 How to check what is selected.

All selections are displayed as green crosses in the graphical display and blue in the ICM Workspace. All green selections are returned to a variable called as_graph.



3.6.5 Orange Selection

Sometimes it is necesary to have two different selections. The Orange selection allows you to do this it is useful for such operations as superposition and more technical procedures such as designing a protein loop. The orange selection is returned to a variable called as2_graph.



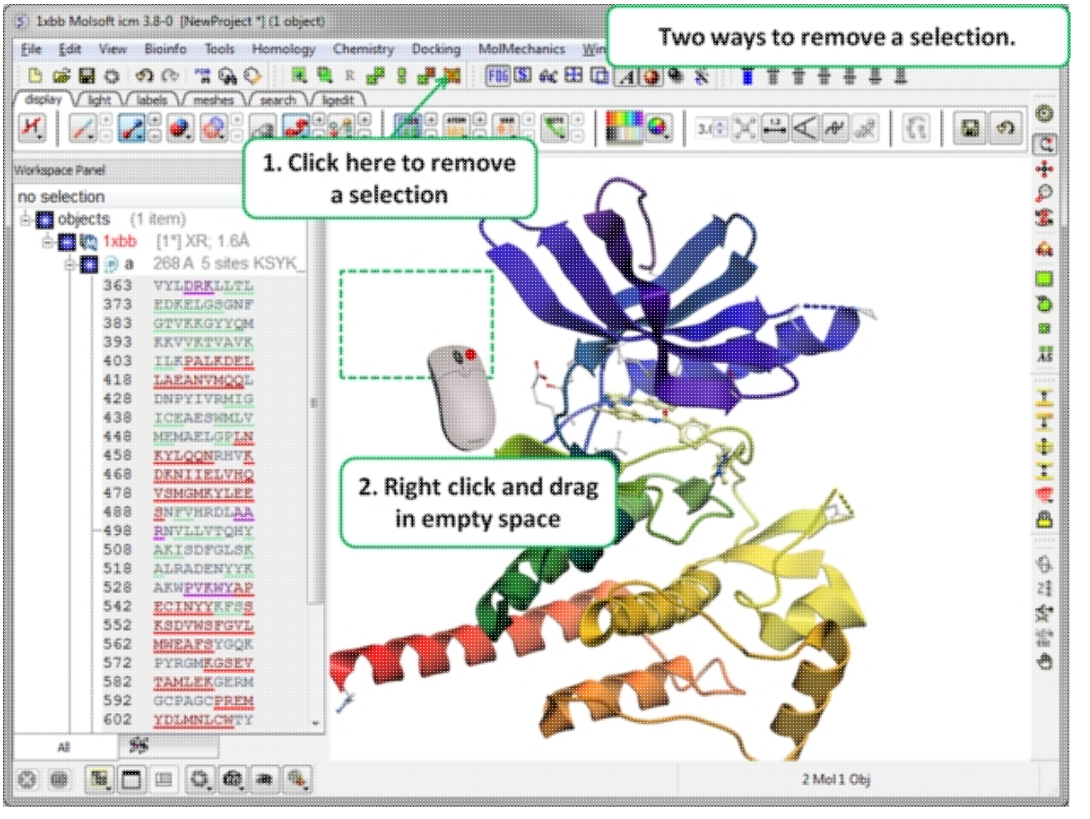
3.6.6 Clear Selection

To unselect everything you have previously selected:

- Simply click on the **Clear Selection** button on the selection toolbar.

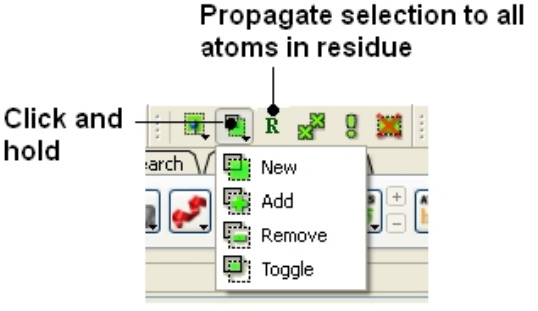
OR

- Right click and drag away from the displayed structure.



3.6.7 Changing 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.

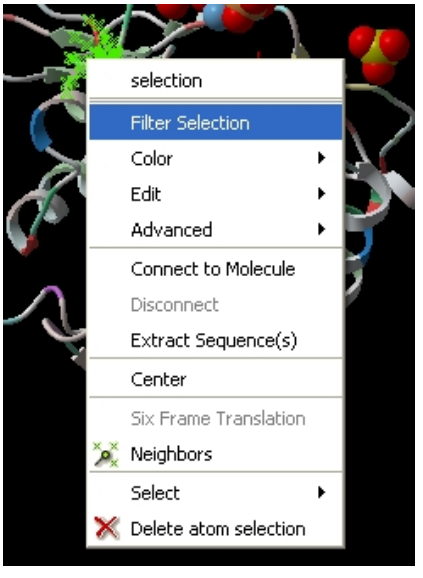
3.6.8 Filter Selection

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

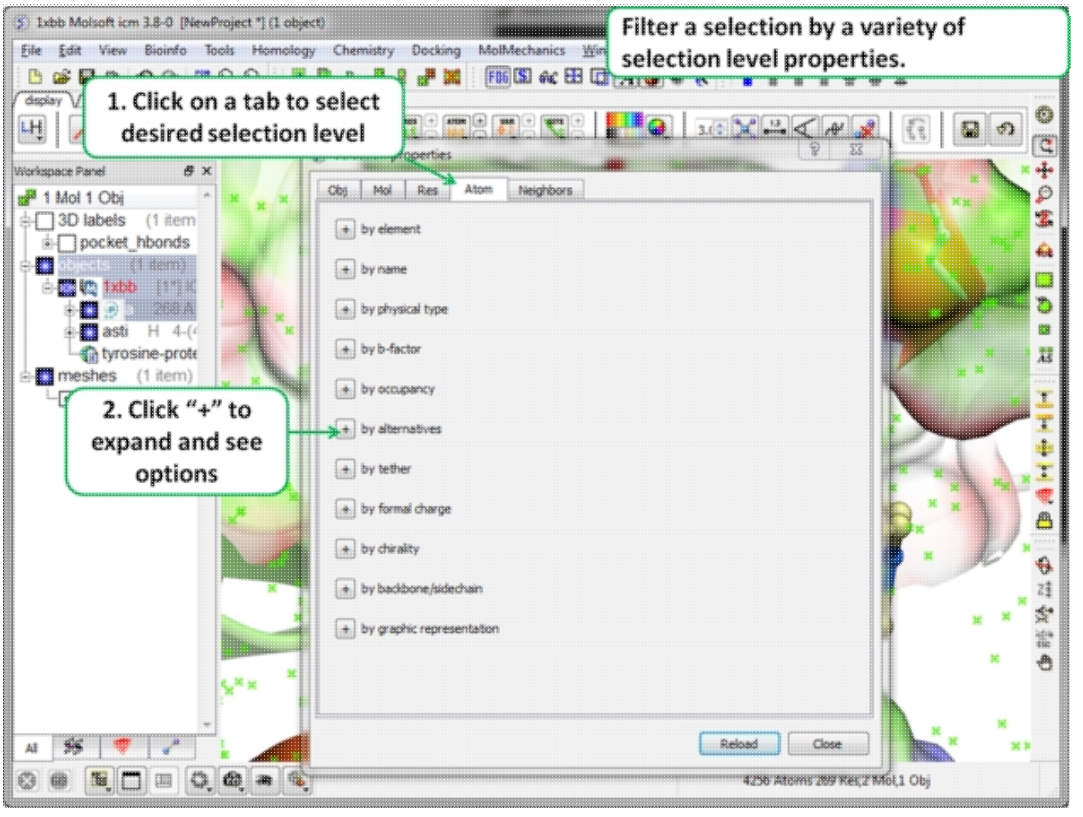
The button shown below enables you to filter your selection:

Or

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

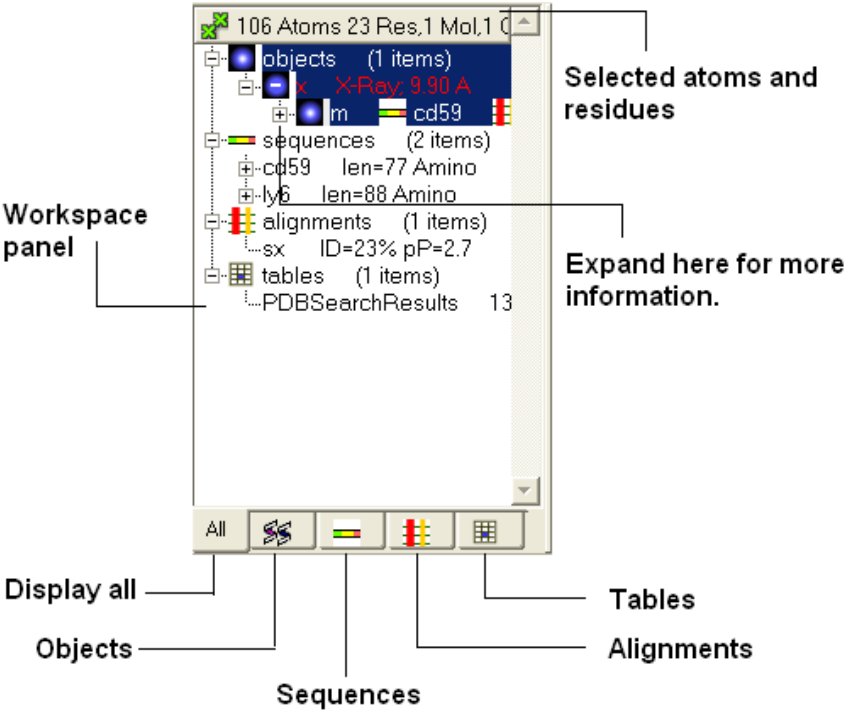


- Select the Filter Selection option.
- A dialog box will be displayed as shown below.



3.6.9 Workspace Selections

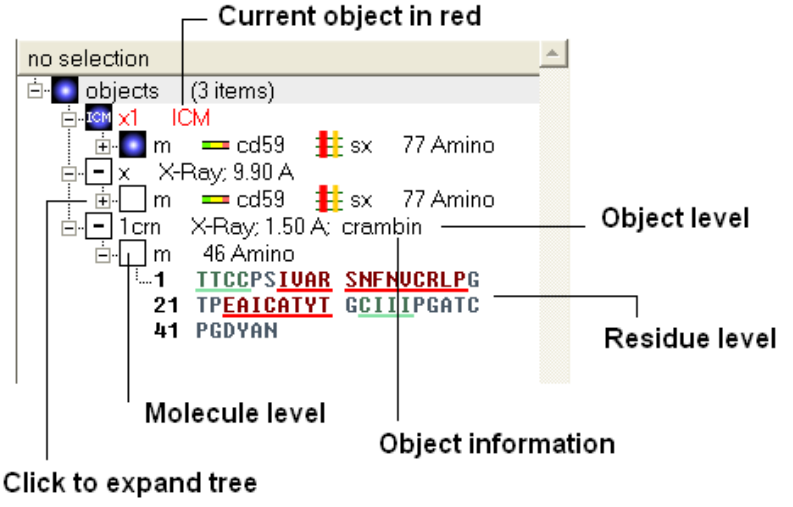
In the default GUI layout the workspace panel is located to the left of the 3D graphics display. It is a great tool for keeping track of all your sequences, pdb structures, objects, tables and alignments. As you will see in this section it also provides a way of making selections.



3.6.10 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.

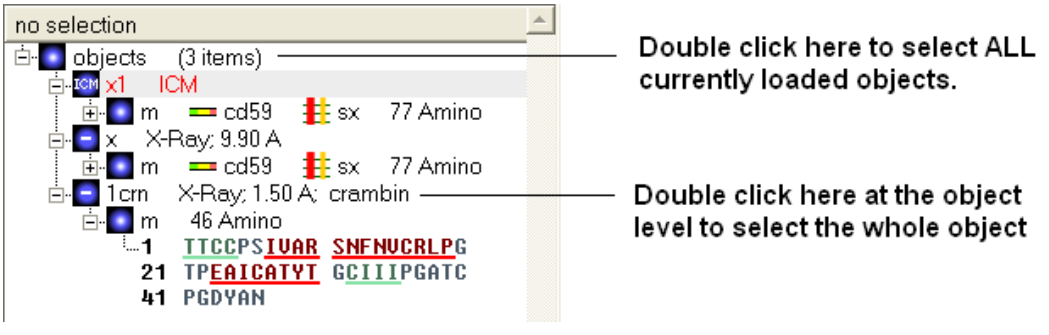


NOTE: You can expand each level of the ICM workspace by clicking the "+" button as shown above.

3.6.11 How to Select an Object

To select the whole object:

- Double click on the object level.

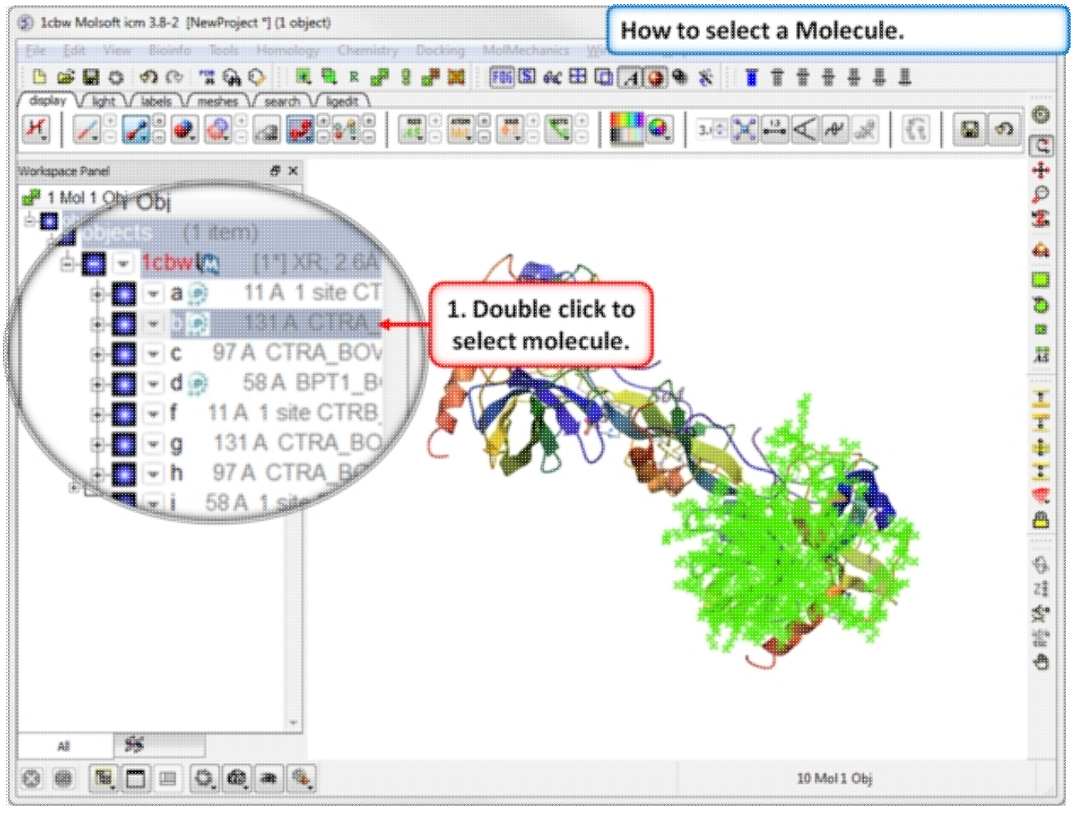


Use the CTRL button to select multiple non-contiguous objects or if they are continuous you can use double click and hold the tab button.

3.6.12 How to select a Molecule

To select a molecule(s):

- Double click on the molecule in the ICM workspace.



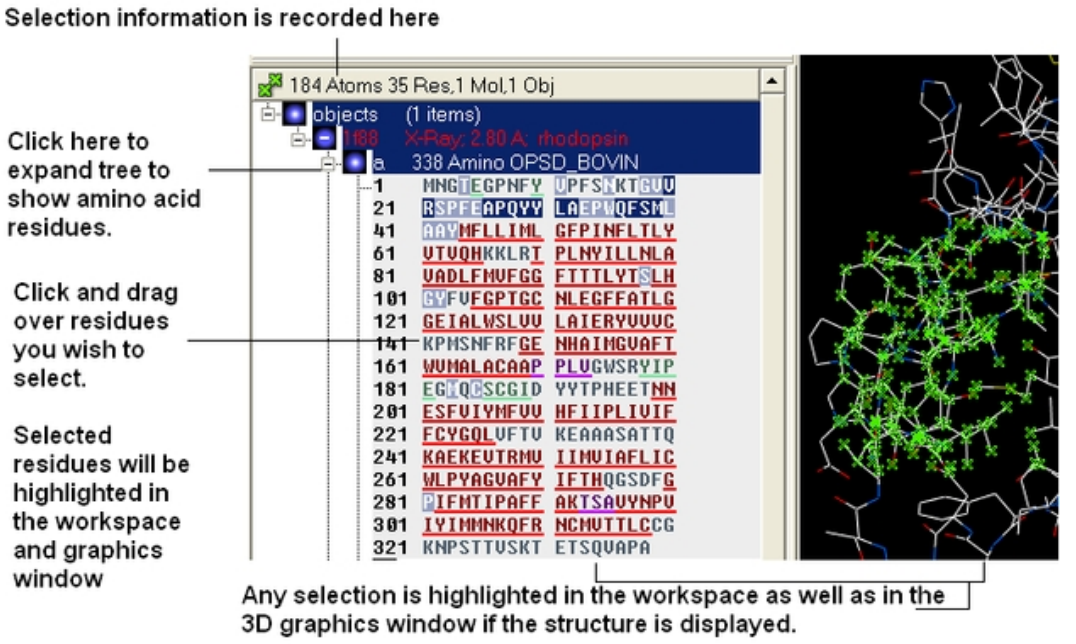
Use the CTRL button to select multiple non-contiguous molecules or if they are continuous you can use double click and hold the tab button.

3.6.13 How to select Residues

There are different options to select 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.

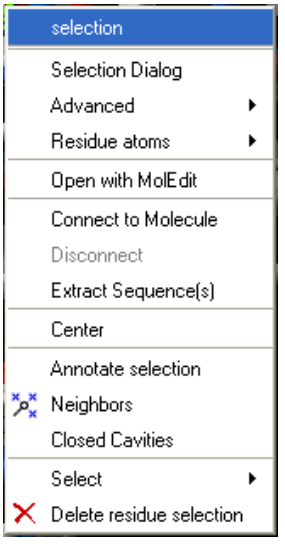


OPTION 2:

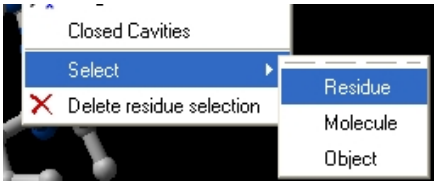
- Click on the **rectangular selection** icon or **lasso selection** icon on the toolbar.
- Click and drag around the residues you wish to select. Selected residues will be displayed by green crosses on the graphical display and blue in the ICM workspace.
- Use the `propagate selection to residue level`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

OPTION 3:

- Right click on the a 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.**



OPTION 4:

Use the select `residue button`.

3.6.14 Select All

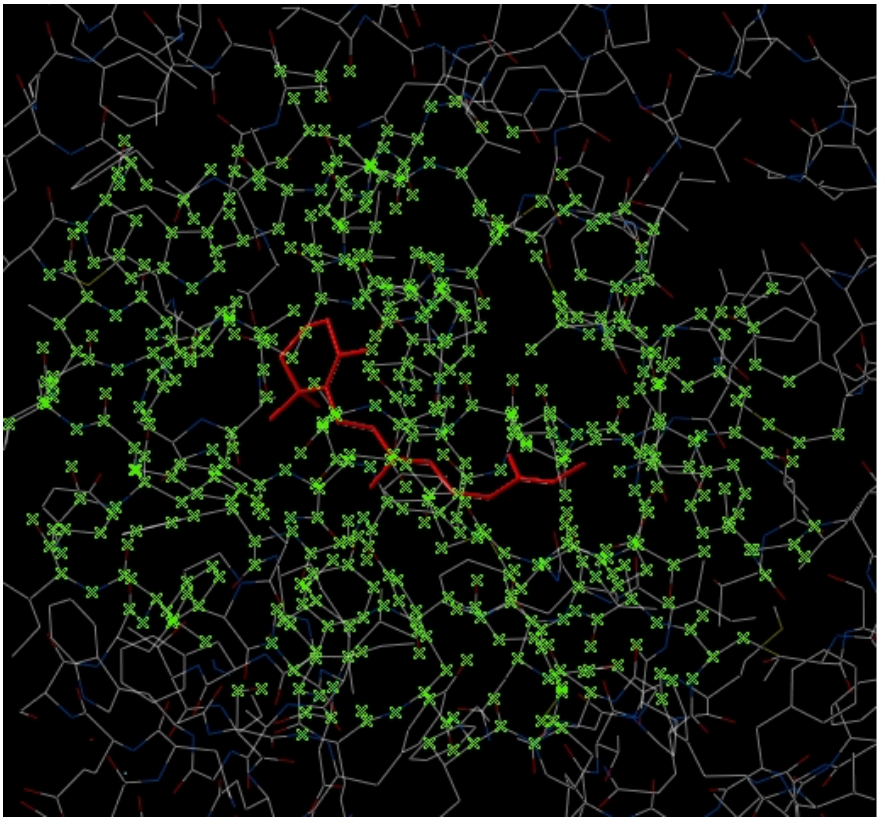
Ctrl + A will select everything in the ICM workspace, and Ctrl + Shift + A will unselect your objects.

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

3.6.15 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 shpere of a defined radius.

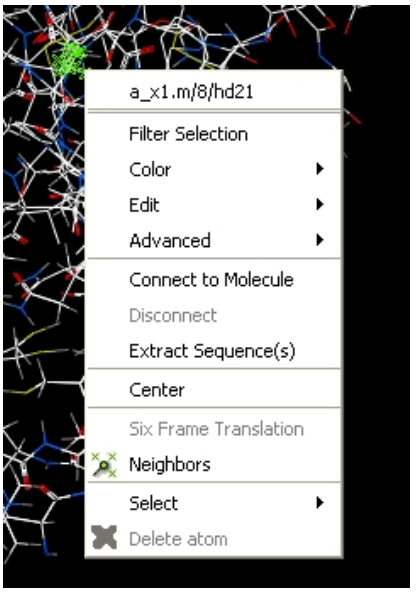
There are two ways of selecting neighbours to a particular atom or residue in ICM. Either by right clicking on the atom or residue in the graphical display or by right clicking in the ICM workspace.



3.6.16 Selecting Neighbors: Graphical

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

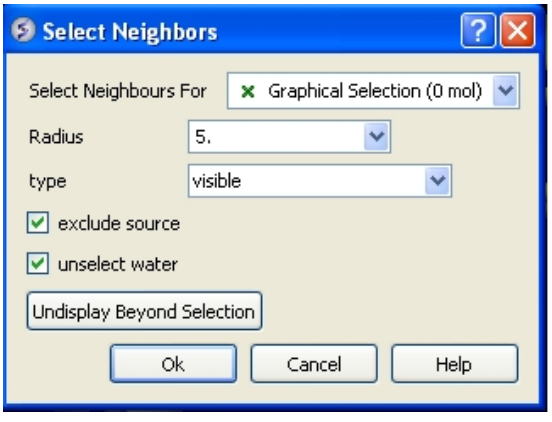
- First select the residue(s) or atom(s) around which you wish to select neighbors. (See the `Selection Toolbar Section`)
- Right click on the selection and a menu as shown below will be displayed or choose Tools/Geometry/Neighbors.



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

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.

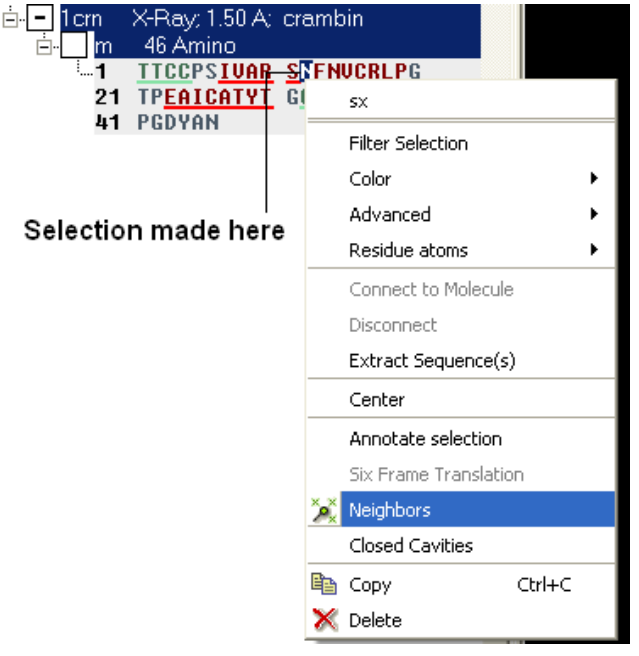
- **unselect water** if checked will not select water molecules
- **Undisplay Beyond Selection** will only display the atoms selected.

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 Workspace.

3.6.17 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 Neigbors 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

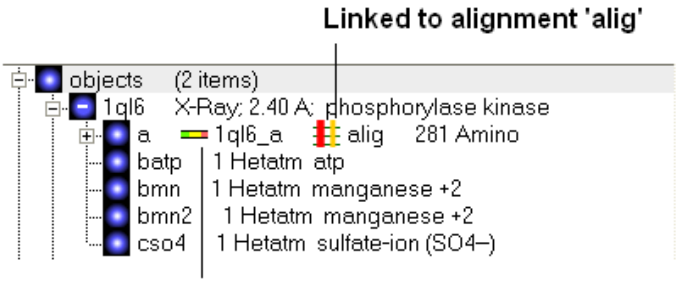
3.6.18 Alignment and Table Selections

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

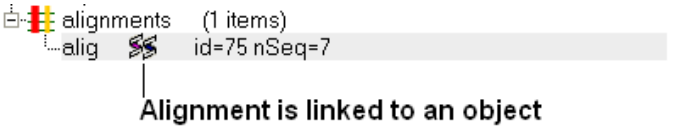
3.6.19 Making Links

It is sometimes necesary 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 transfered 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'.



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.

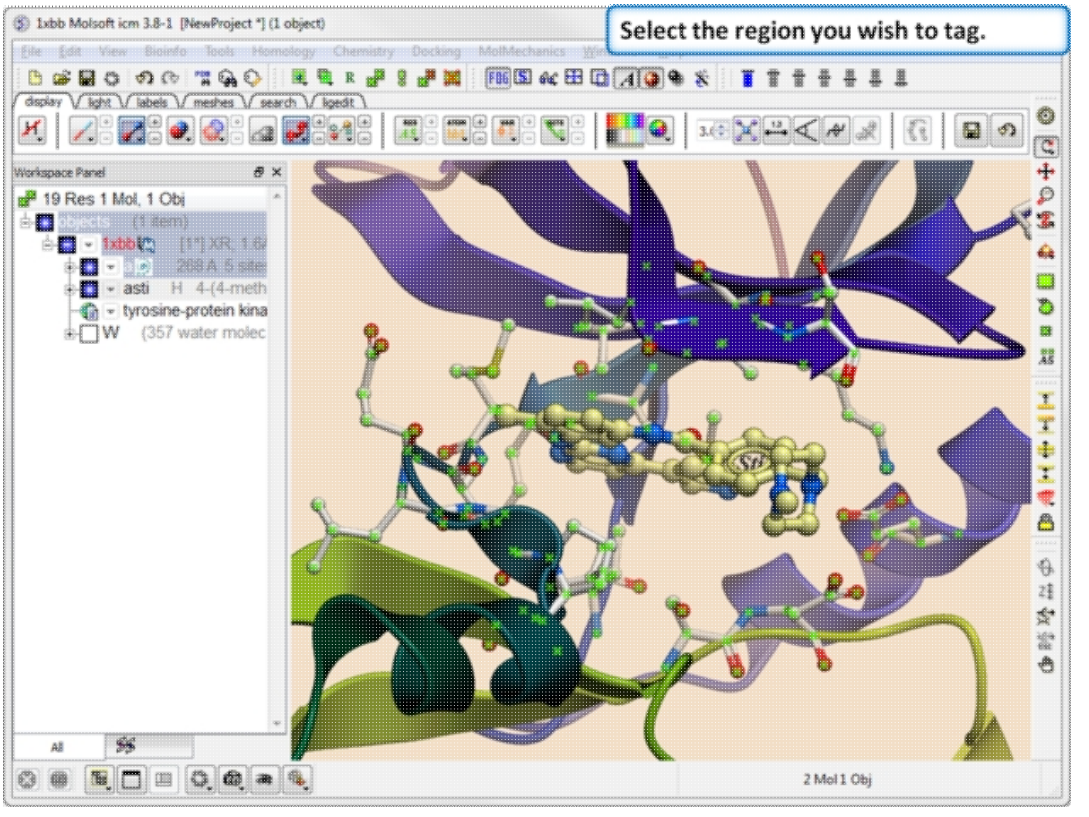
Use the extracted sequence as described above to build your alignment.

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

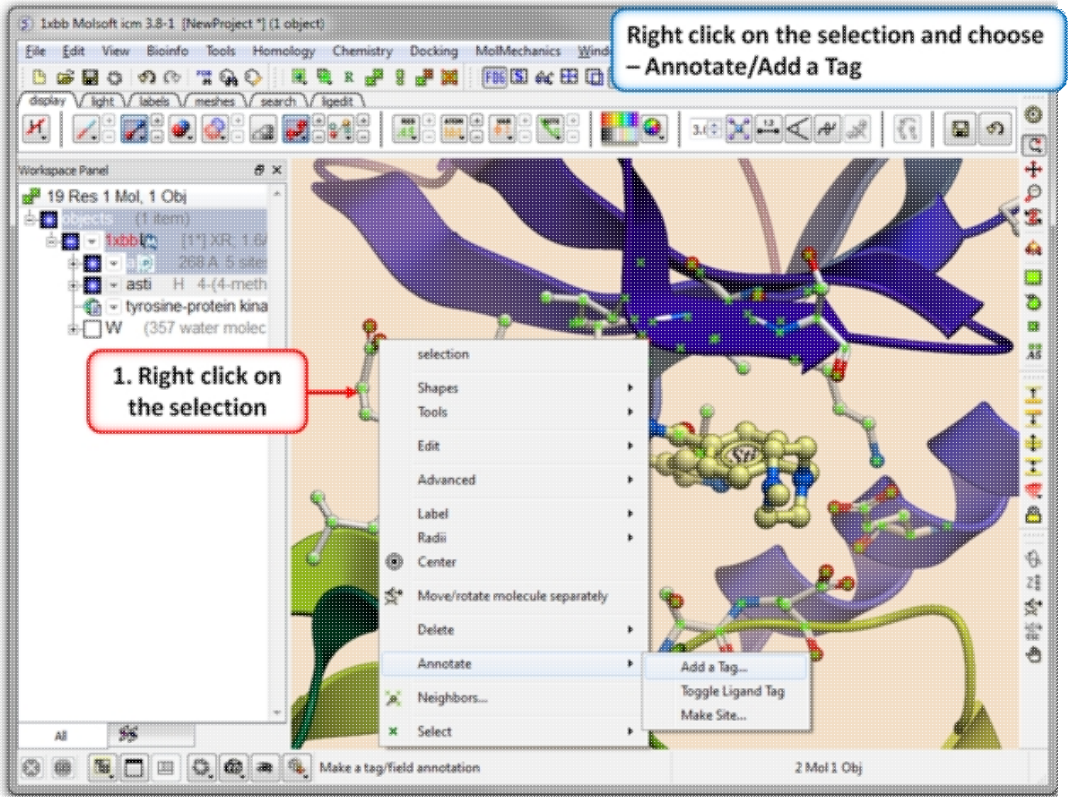
- Bioinfo/Link to Structure.
- Enter alignment name.
- OK

3.6.20 Tags

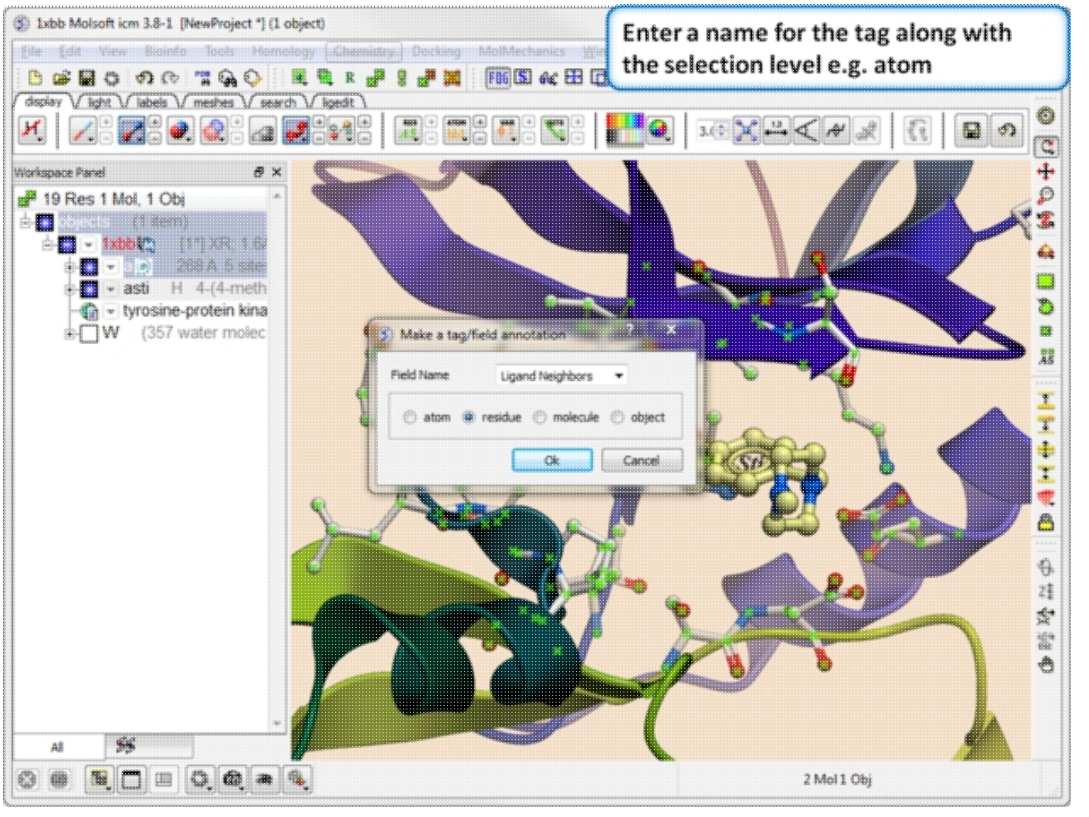
It is sometimes convenient to tag selections so you can come back and use them at a later date. To do this:



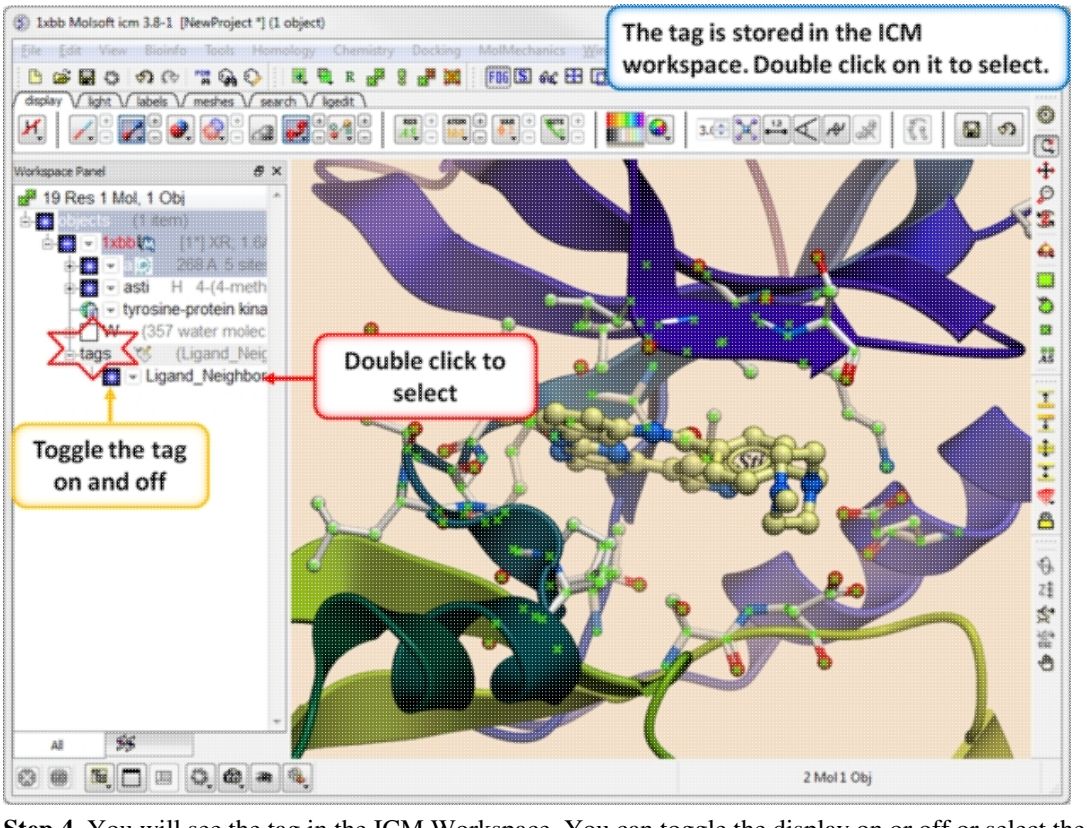
Step 1. `Select` the region you wish to tag.



Step 2. Right click on the selection and choose Annotation/Add a Tag.



Step 3. Give the tag a name and choose the selection level (atom, residue, molecule, or object).



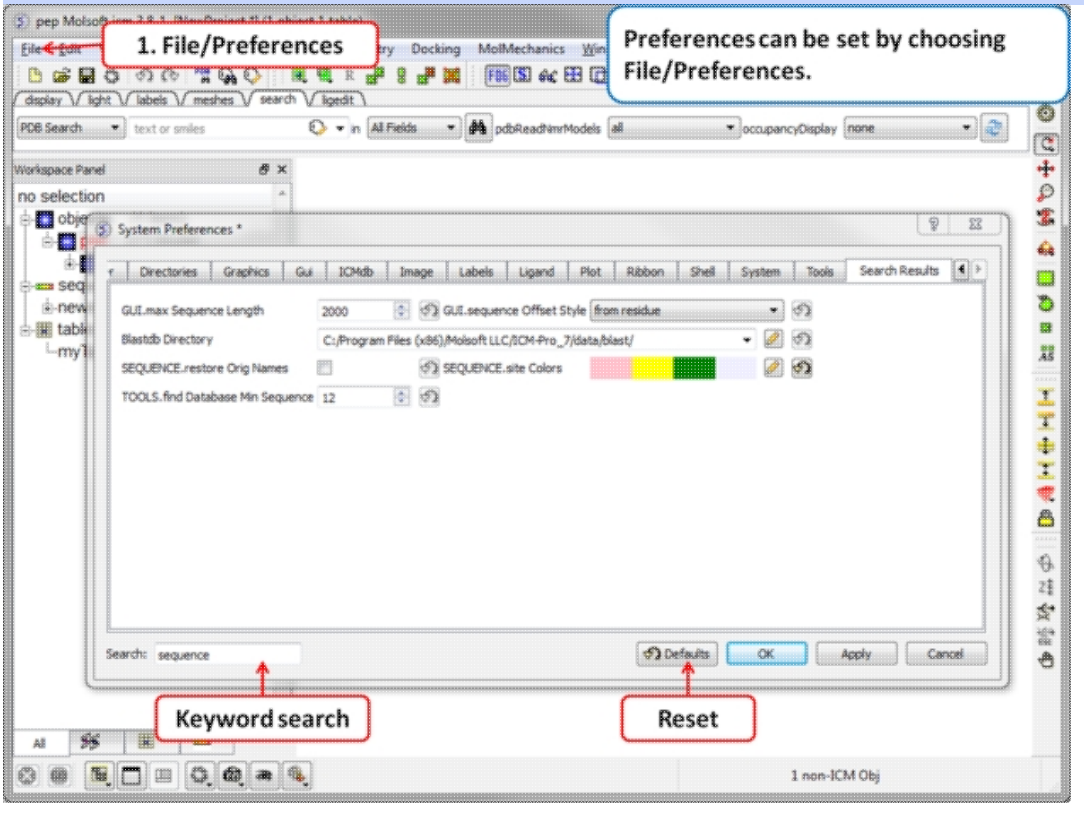
Step 4. You will see the tag in the ICM Workspace. You can toggle the display on or off or select the tag by double clicking on it in the ICM Workspace.

3.7 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 and also a search option.



3.7.1 Bonds Preferences

To change Bond Preferences:

- Select File/Preferences.
- Choose the **Bonds** tab.

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"  #
```

3.7.2 Directories Preferences

DIRECTORIES TAB:

To change Directory Preferences:

- Select File/Preferences.
- Choose the **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 fil es

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
3. = "all stack" : creates one object and loads all other models as a stored cartesian stac
```

3.7.3 Graphics Preferences

To change Graphics Preferences:

- Select File/Preferences.
- Choose the **Graphics** tab.

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 posiion 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 partical or zero atom occupancies are displayed. The abnormal occupanices 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 lable 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). 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 thich 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 becames equivalent to the solvent accessible surface with a probe of 1.4A

GROB.arrowRadius - a real arrow radius in Angstoms 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_eds 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 partical 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.

3.7.4 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 resoltuion of the movie

SEQUENCE.site Colors - Controls coloring of squence 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`.

3.7.5 GUI Preferences

To change GUI Preferences:

- Select File/Preferences.
- Choose the **GUI** 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 hydorgens 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 - adius 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 [arealvolume] skin
- display skin while vwExpand is used in
- show [arealvolume] 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 Lenght 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 an
```

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.

3.7.6 Image Preferences

To change Image Preferences:

- Select File/Preferences.
- Choose the **Image** 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 documnents.

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.

3.7.7 Label Preferences

To change Label Preferences:

- Select File/Preferences.
- Choose the **Labels** 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.

3.7.8 Plot Preferences

To change Plot Preferences:

- Select File/Preferences.
- Choose the **Plot** tab.

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 plor 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.

3.7.9 Ribbon Preferences

To change Ribbon Preferences:

- Select File/Preferences.
- Choose the **Ribbon** tab.

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 DN
3 = "alignment" if there is an alignment linked to a protein, color gapped backbone regions gr
4 = "reliability"       3D gaussian averaging with selectSphereRadius of alignment strength in
If ribbonColorStyle equals to 4, the conserved areas will be colored blue, while the most dive
```

3.7.10 Shell Preferences

To change Shell Preferences:

- Select File/Preferences.
- Choose the **Shell** tab.

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 Angstoms 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

3.7.11 System Preferences

To change System Preferences:

- Select File/Preferences.

- Choose the **System** tab.

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 - Maximu 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.enumberation Memory Limit - memory limit for enumeration operations.

GUI.splash Screen Delay

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

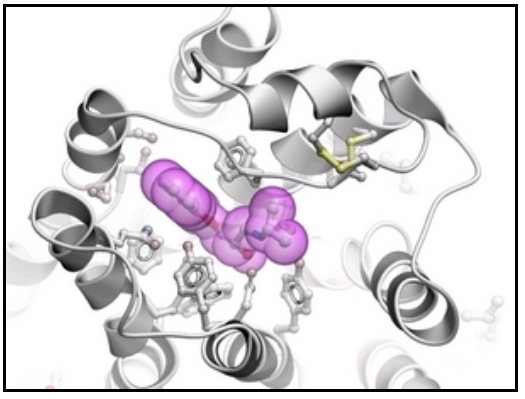
HTTP.timeout - timeout in seconds

Http Read Style icm or lynx

Force Auto Bond Typing - yes/no

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

4 Protein Structure



Chapter Contents:

- How to Convert Proteins and Chemicals to ICM Objects.
- Binding Site Display Tools.
- Crystallographic Analysis Tools.
- Protein Superposition.
- Protein Structure Analysis.
- Protein Structure Prediction Tools e.g. ICM Pocket Finder.

4.1 Convert to ICM Object

Available in the following product(s): ICM-Browser | ICM-Browser-Pro | ICM-Pro | ICM-Chemist

4.1.1 Load a Protein Structure

There are a couple of ways to read into ICM a protein structure.

1. Search the PDB using the Search Tab.
2. Load in a PDB file that you have saved on your computer using File/Open.

4.1.2 Converting PDB Files Into ICM Objects

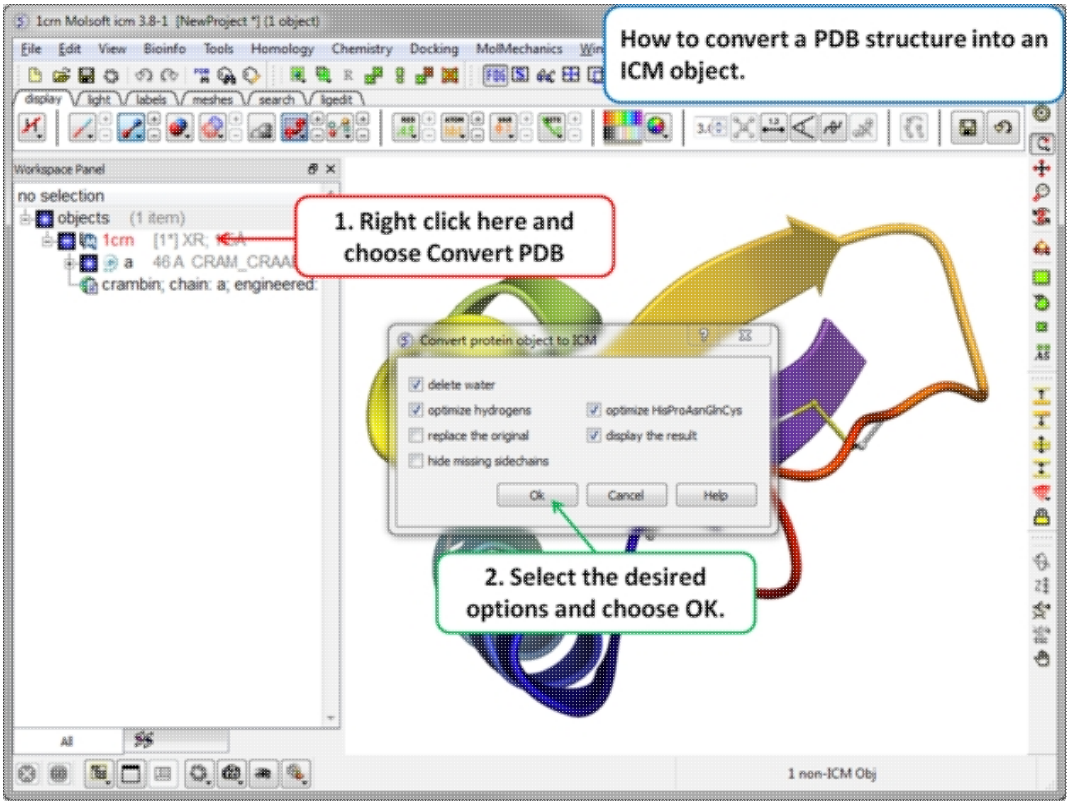
If you are going to make any type of energy calculation in ICM (eg docking, display H-bonds, display electrostatic and binding property surfaces etc..) it is necesary to convert a protein or chemical into an ICM object. Be aware that upon conversion ICM adds missing side-chain atoms (but wont try to build missing loops) due to the nature of the internal-coordinate system. The list of residues/ atoms added is presented in the command line shell and can be reviewed. For reference, the original PDB entry is kept in the system. See the command line manual for a more complete description of what the conversion process does.

NOTE: Before converting a protein structure to an ICM object make sure that the chemicals contained within the structure (e.g. ligands) are correct. If an error is found you can edit the ligand as described here.

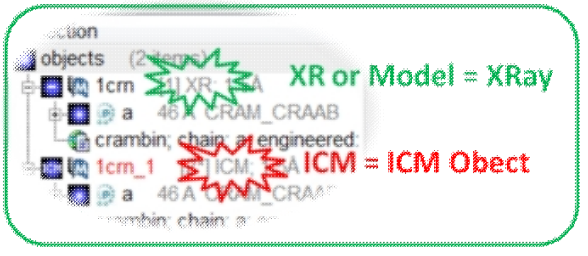
To convert a PDB structure into an ICM object follow the steps shown below:

- Right click on the name of the protein you wish to convert in the ICM Workspace.
- A dialog box will be displayed as shown below.
- If you want to delete the water molecules select **Delete Waters**
- If you want to optimize hydrogen atoms (recommended for important work) select **Optimize Hydrogens**. This option performs global optimization of hydrogens to find the best hydrogen bonding network.

- If you want to optimize the orientation of His, Pro, Asn, Gln, Cys residues then choose **optimizeHisProAsnGlnCys.** The following residues will be further optimized: His - three protonation states and two rotations will be tried and the residue will be renamed according to its subtype: hie (epsilon tautomer) or hip (+). Asn and Gln - (a 180 deg. flip will be tried). Cys - in the vicinity of Zn, Cu, Fe and Co to cym.
- If you want to keep a copy of your PDB file uncheck the option **replace original**.
- The converted structure can be displayed immediately by checking **display the result**
- **Uncheck** the box **hide missing side chains** if you want ICM to build missing heavy atoms that are not reported in the PDB (due to the lack of density), they will be added according to the residue name and assigned zero occupancies. **Check** this box if you want residues missing heavy atoms to be hidden.



If your object is an ICM object it will display **ICM** next to the molecule in the ICM Workspace.



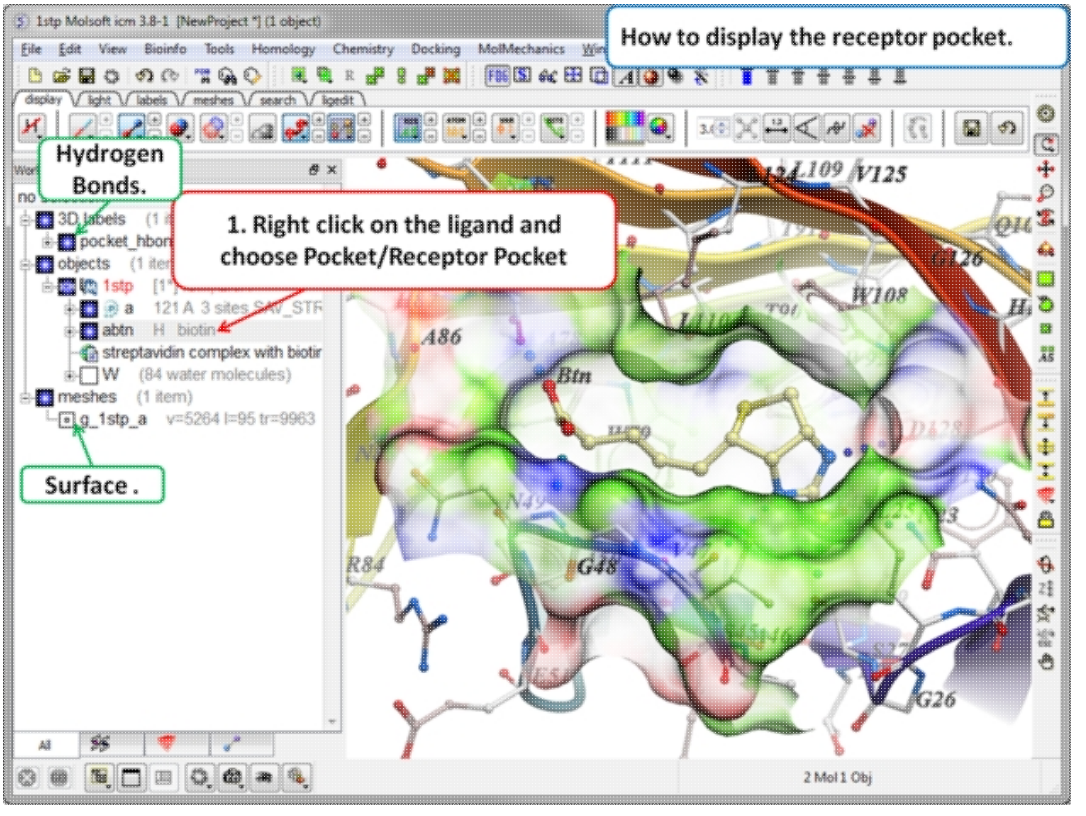
4.2 Pocket Display

Available in the following product(s): `ICM-Browser` | `ICM-Browser-Pro` | `ICM-Pro`

4.2.1 Receptor Pocket Surface.

To display the Receptor Pocket Surface:

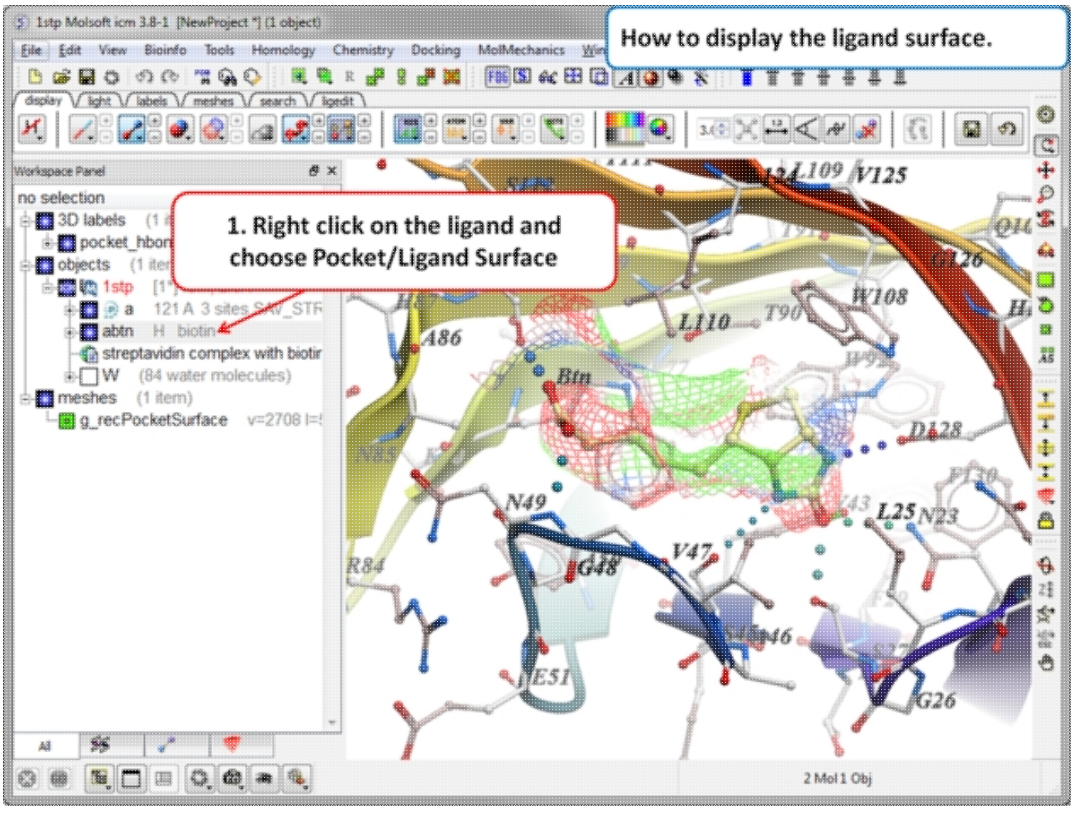
- As an example we will use the PDB structure 1STP. Type 1STP in the `pdb search tab` and press return.
- `Convert` the protein to an ICM object. If you do not convert a generic surface will be displayed that is not colored by binding property.
- Right click on the ligand "abtn" and select **Pocket/Receptor Pocket**.
- Select whether you would like to display side-chain hydrogen bonds and label.
- The receptor pocket will be displayed colored by binding property - White=neutral surface Green=hydrophobic surface Red=hydrogen bonding acceptor potential Blue=hydrogen bond donor potential.
- The surface can be toggled on and off by selecting in the ICM Workspace in the **meshes** section.



4.2.2 Ligand Surface.

The Ligand Surface option allows you to visualize cavities that are open for ligand modifications. To display the Ligand Surface:

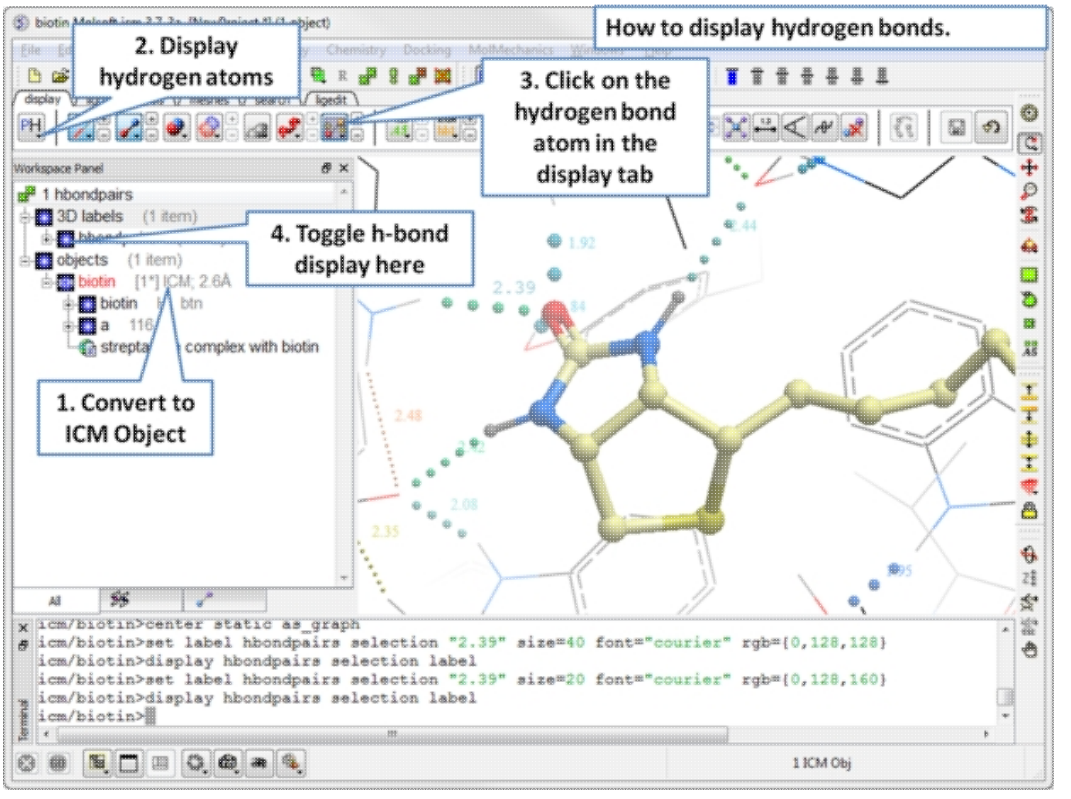
- As an example we will use the PDB structure 1STP. Type 1STP in the `pdb search tab` and press return.
- `Convert` the protein to an ICM object. If you do not convert a generic surface will be displayed that is not colored by binding property.
- Right click on the ligand "abtn" and select **Pocket/Ligand Surface**.
- The Ligand Surface will be displayed colored by binding property - White=neutral surface Green=hydrophobic surface Blue=hydrogen bonding acceptor potential Red=hydrogen bond donor potential.



4.2.3 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.

- 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.

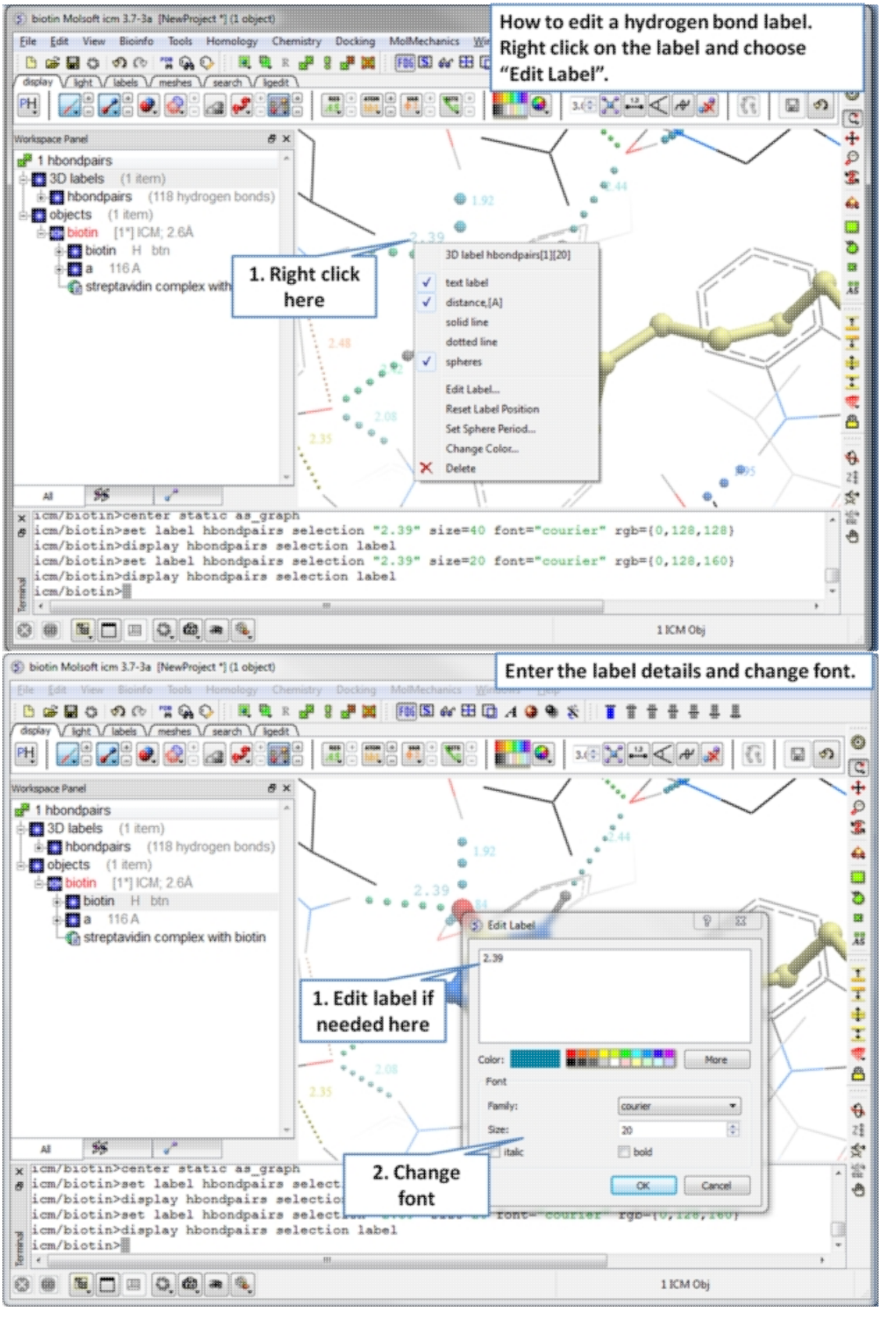


NOTE: Different options for displaying the H-bond can be accessed by clicking and holding on the H-bond button in the "Display" tab. The coloring of the H-bonds are red (strong - thick spheres) to blue (weak - thin spheres). Once the hydrogen bonds have been displayed they can be displayed and undisplayed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

4.2.3.1 Edit Hydrogen Bond Label

To edit a hydrogen bond label

- Right click on the label.
- Choose Edit Label.
- Make changes in the dialog box and press OK.

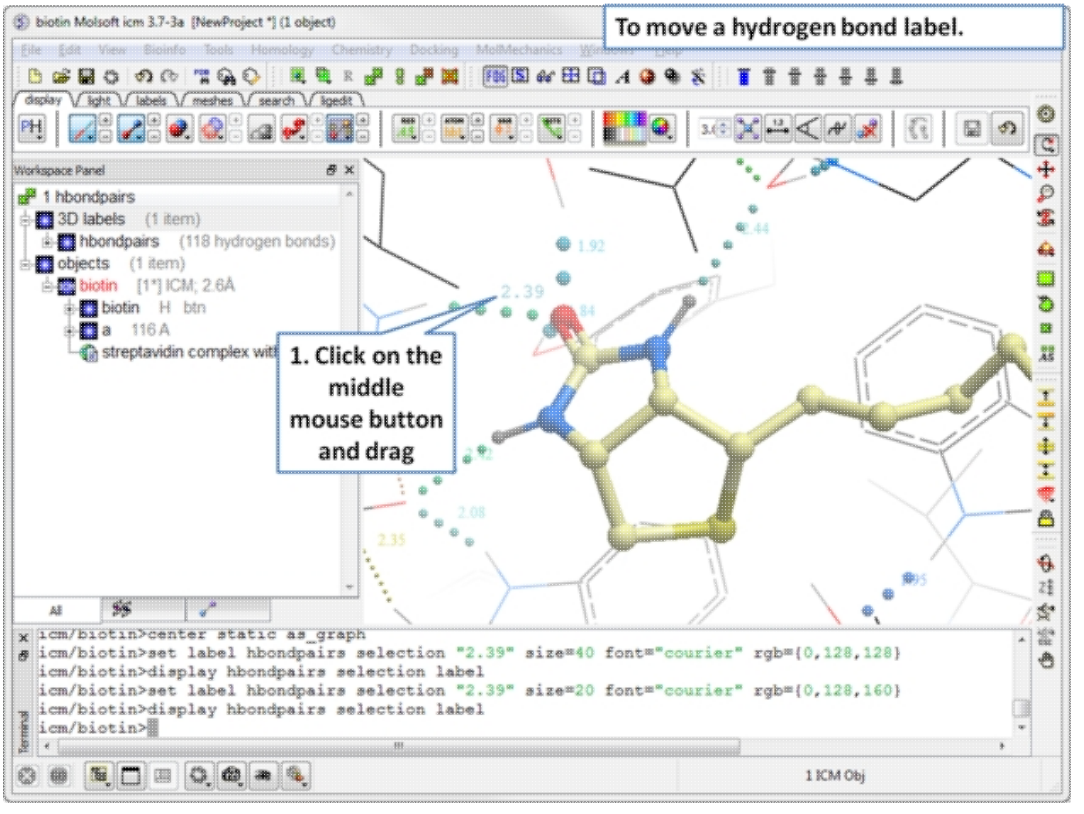


4.2.3.2 Move Hydrogen Bond Label

To move a hydrogen bond label

- Right click on the label.
- Click on the label using the middle mouse button.

- Hold the middle mouse button down and drag.



4.3 Crystallographic Analysis

Available in the following product(s): `ICM-Browser-Pro` | `ICM-Pro`

4.3.1 Crystallographic Neighbor

Theory

Molecular objects and 3D density maps may contain information about crystallographic symmetry. It consists of the following parameters:

1. Crystallographic group eg. P2121 that determine N (depends on a group) transformations for the atoms in the asymetric unit.
2. Crystallographic cell parameters A, B, C, Alpha, Beta and Gamma

To generate the coordinates within one cell one needs to apply N transformations and then to generate neigboring cells the content of one cell needs to be translated in space according to the cell position.

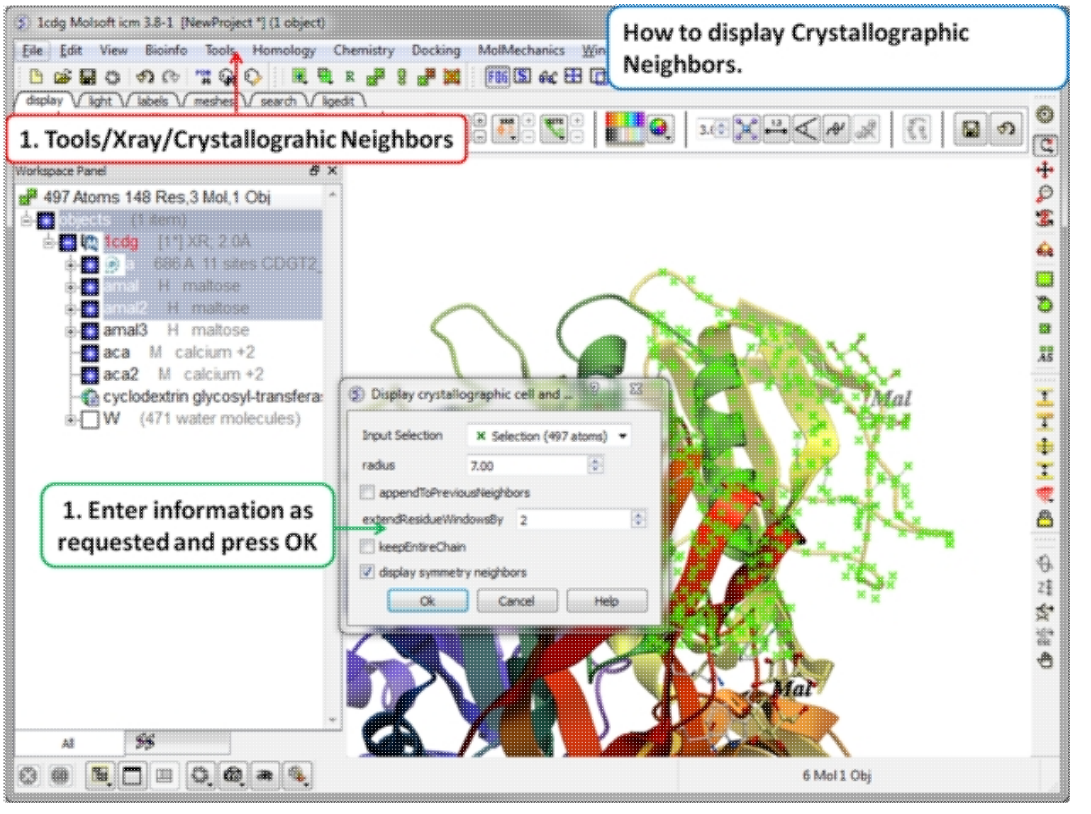
ICM has a function which generates crystallographic neighbors for the selected atoms. For large proteins it is impractical to generate neighbors for the whole molecule due to the high number of atoms in all neighboring molecules.

This information allows to generate symmetry related parts of the density or molecular objects.

To generate symmetry related molecules around a selection of atoms:

- Read a PDB file into ICM. For instruction see the section entitled `Search PDB`.
- Display the structure and select the residues around which the symmetry will be generated. For information on how to select residues see the `Making Graphical Selections` section.
- Select the menu Tools/Xray/Crystallograhic Neighbors.

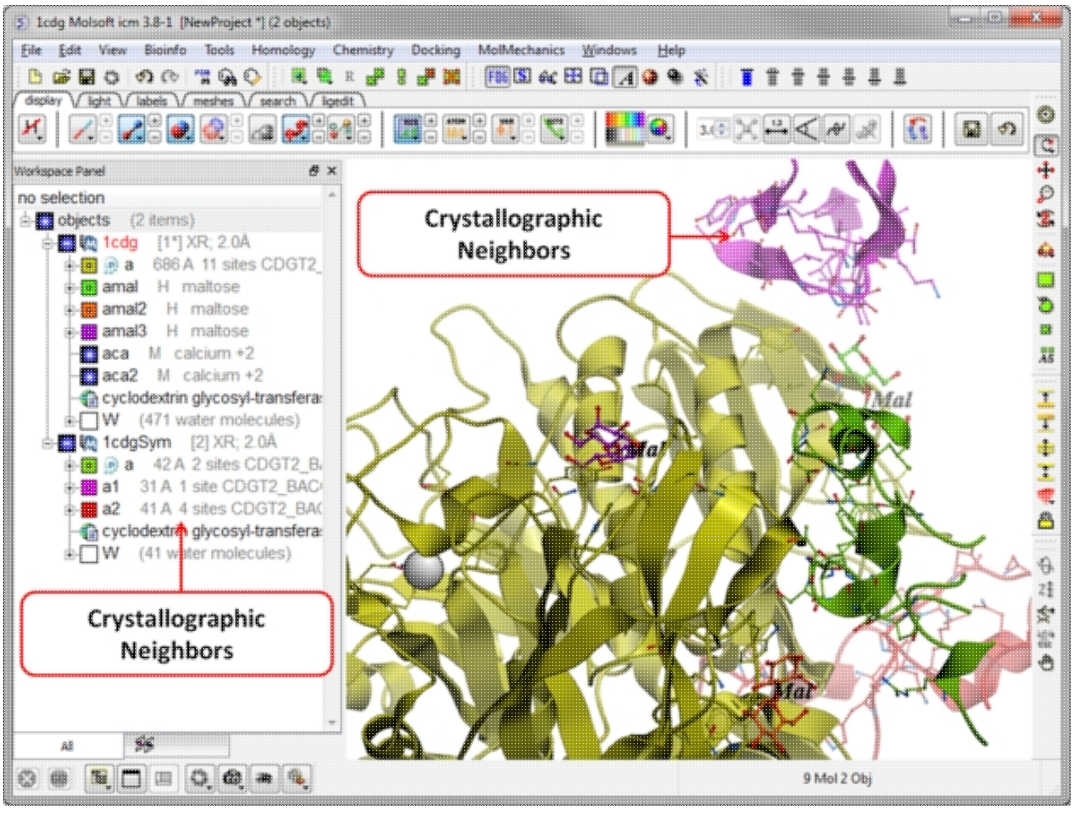
A data entry box as shown below will be displayed.



- Check that the selection is correct in the **Input Selection** box.
- Enter the radius around your selction from which you wish to construct the symmetry related molecules.
- If you have made symmetry related molecules previously you can select **appendToPreviousNeighbors** otherwise leave unchecked.
- The **extendResidueWindowsBy** option will allow a window of residues outside of the selection radius selected above to be displayed
- If you leave the **keepEntireChain** unchecked then a fragment of each neighbor will be created. If you check this box the full neighbor will be generated
- Check display symmmetry neighbors to display them in the graphics window. The nearest neighbor residues will be displayed in xstick representation and the each neighbor colored by molecule.
- Click OK.

The crystallographic symmetry neighbors will be displayed in the Workspace. By default the object will have the object name + "Sym" and each of the neighbors will be individual molecules.

For packing analysis and display you can color each symmetry unit a different color as described in the `Structural Representations Color section`. This is shown in the picture below.



4.3.2 Crystallographic Cell

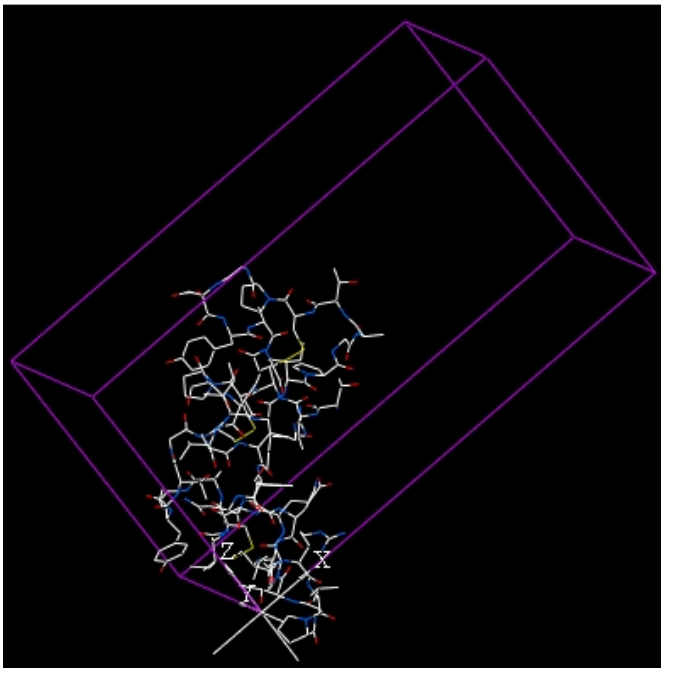
Theory

The crystal structure of a protein is often discussed in terms of its unit cell. The unit cell is a box containing one or more motifs, a spatial arrangement of atoms. The units cells are tiled in three-dimensional space to describe the crystal. The unit cell is given by its lattice parameters, the length of the cell edges and the angles between them, while the positions of the atoms inside the unit cell are described by the set of atomic positions measured from a lattice point.

To display the crystal cell of a PDB structure:

- Read a PDB file into ICM. For instruction see the section entitled `Search PDB`.
- Select the whole object. You can do this by double clicking on the name of the structure in the ICM Workspace (a selection is highlighted blue in the ICM Workspace and green crosses in the graphical display) or you can use the right-click button and drag it over the whole structure in the graphical display.
- Select the menu Tools/Xray/Crystallograhic Cell and a data entry box will be displayed.
- Click OK

The crystallographic cell will be displayed as a box as shown below.



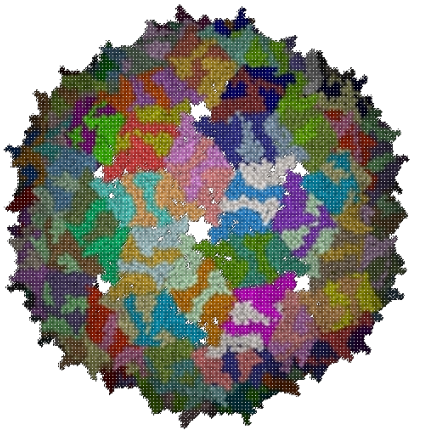
4.3.3 Biomolecule Generator

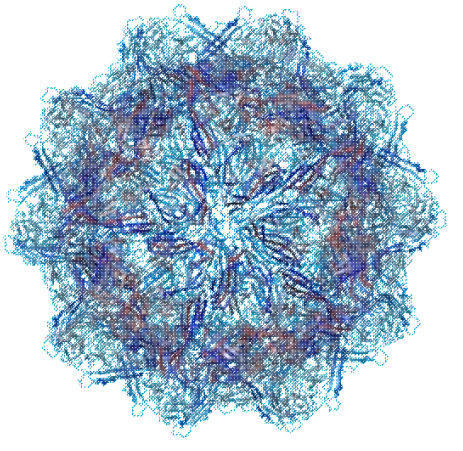
Theory

It is very useful to know how a protein from the PDB may look in a biological environment. The PDB entries solved by X-ray crystallography and deposited in the PDB contain the information about the crystal structure rather than the biologically relevant structure. For example, for a viral capsid only one instance of capsid protein complex will be deposited and only one or two molecules of haemoglobin that is a tetramer in solution maybe deposited.

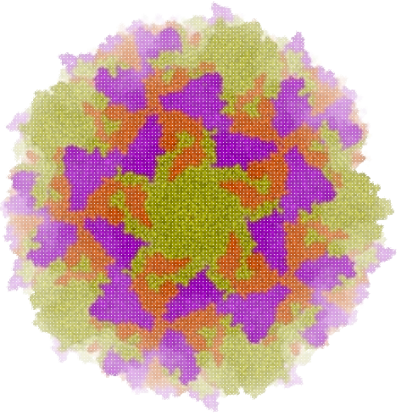
In some other cases the asymetric unit may contain more than one copy of a biologically monomeric protein. ICM reads the biological unit information and has a tool to generate a biological unit. Not every PDB entry has the biological unit information.

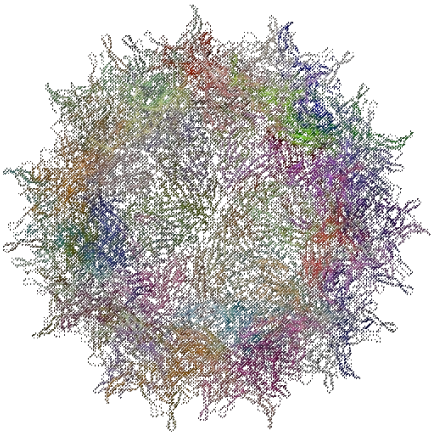
A gallery of images created using the ICM Biomolecule generator is shown below:





Left: PDB: 1DWN Bacteriophage Pp7 From Pseudomonas Aeruginosa At 3.7 A Resolution **Right:** PDB: 1C8E Feline Panleukopenia Virus Empty Capsid Structure At 3.0 A Resolution





Left: PDB: 1AL2 P1/Mahoney Poliovirus, Single Site Mutant V1160I At 2.9 A Resolution **Right:** PDB: 1LP3 Adeno-Associated Virus (Aav-2), A Vector For Human Gene Therapy At 3.0 A Resolution

NOTE: Right click on a PDB structure in the ICM workspace to determine whether a structure from the PDB has biological unit information. If it does have this information then there will be an option in the menu entitiled "Generate Biomolecules" if not the option will be blanked out.

To generate a biological unit with ICM:

- `Select` the object or PDB file.
- Select the menu Tools/Xray/Biomolecule Generator.

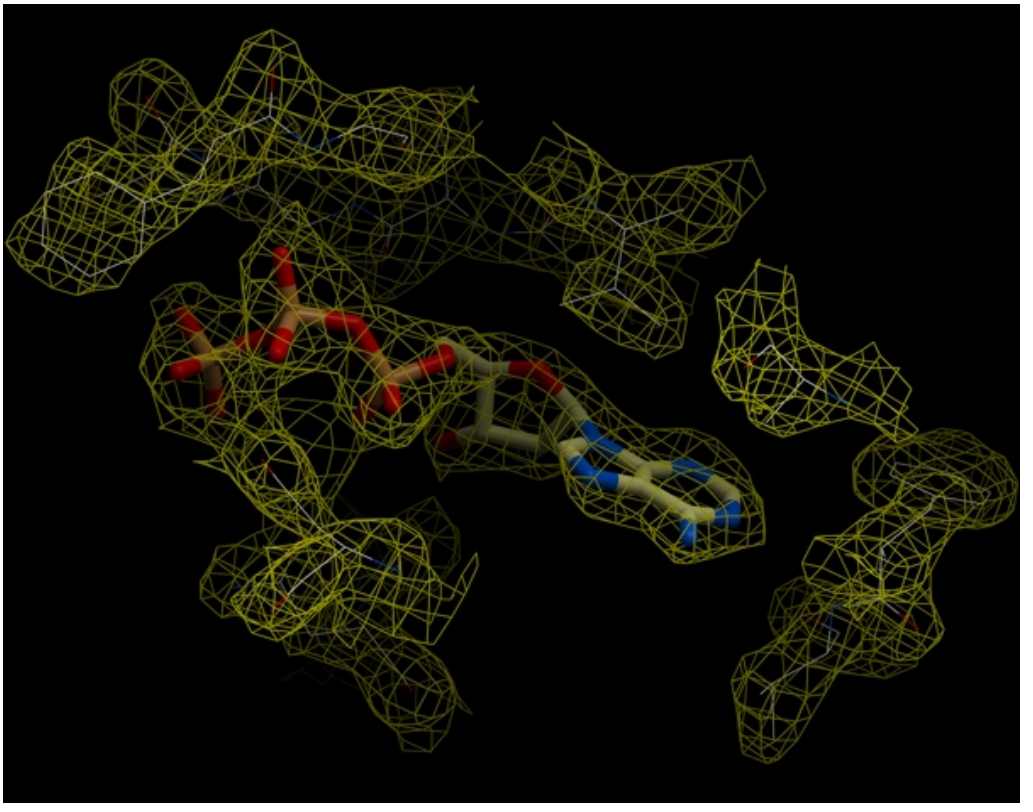
- Tick the **makeAllBiomolecules** box.
- Click OK - with very large molecules the biomolecule generation may take some time.

4.3.4 Get Electron Density Map

Theory

An electron density map is a representation of a crystal structure based on the diffraction data. The map is constructed by a summation of waves of known phase, amplitude and frequency using Fourier transform. The electron density map of a protein can be viewed along with the pdb structure. The easiest way to view the electron density map is to contour and convert it into a graphical object (mesh).

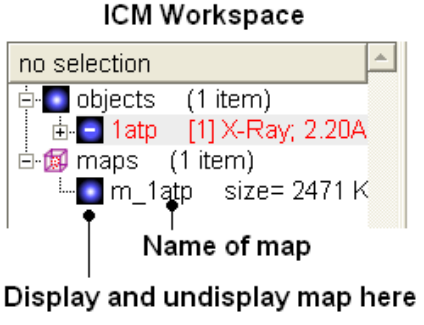
A figure showing the electron density contours surrounding the ATP molecule in pdb entry 1ATP.



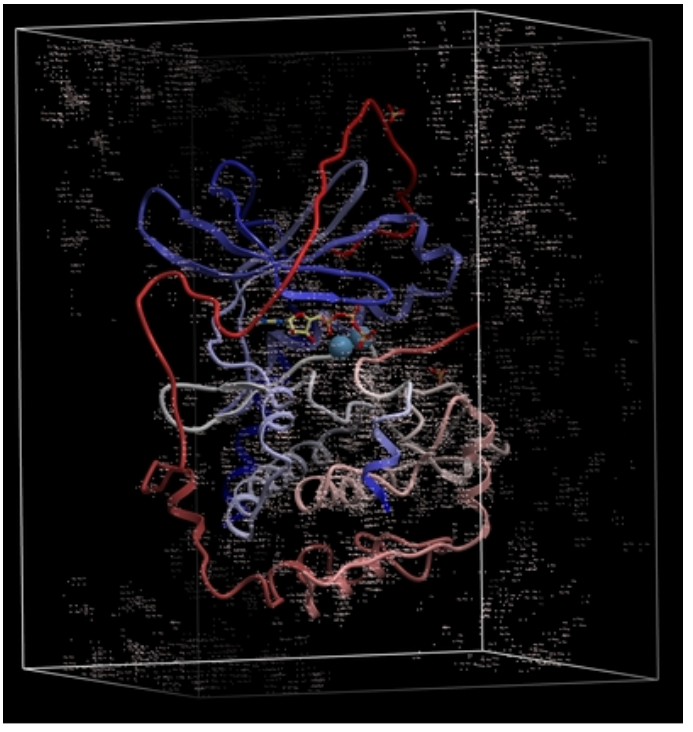
To load an electron density map:

- Tools/Xray/Get Electron Density Map
- Enter the PDB code of the map you would like to view.
- Click OK and the map will be downloaded from the Uppsala Electron Density Server.

The map will be represented in the ICM Workspace as shown below.



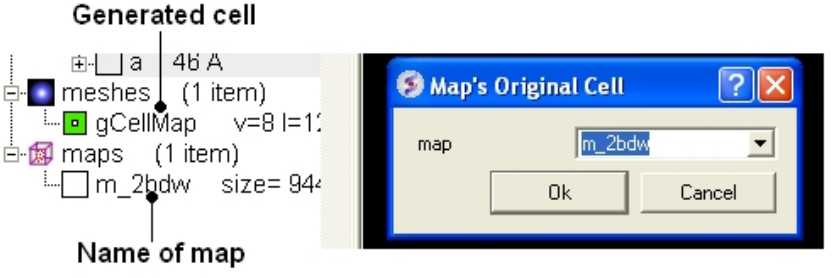
The map can be displayed as shown below however a clearer way of representing the density is to contour the map into a graphical object (mesh) as described in the following section.



4.3.5 Map's Original Cell

To display the original `crystallographic cell` of an electron density map:

- Tools/Xray/Map's Original Cell
- Enter the name of the map or use the drop-down button to locate it. If you do not know the name of the map the name can be located in the ICM Workspace.
- Click OK and the cell will be displayed. The map can be displayed and undisplayed in the **meshes** section of the ICM Workspace.



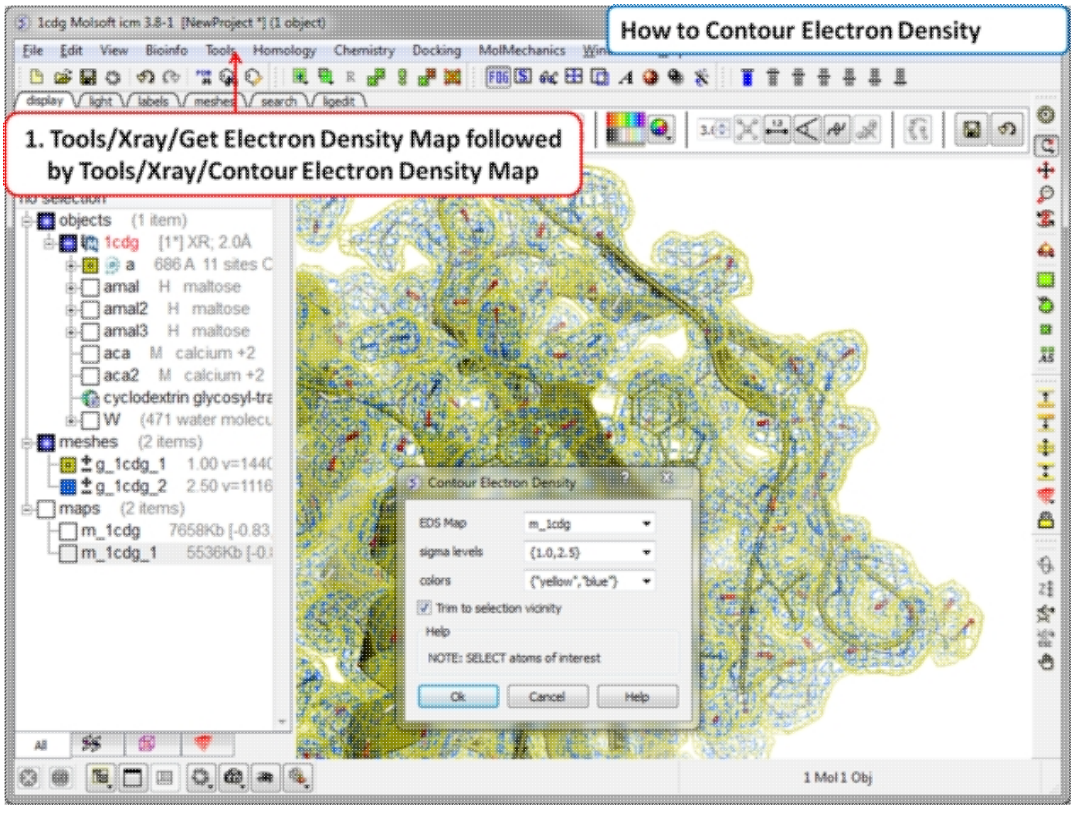
4.3.6 Contour Electron Density Map

To contour an electron density map and display as a graphical object:

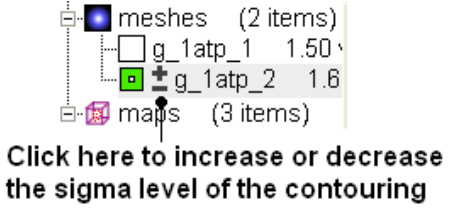
- Load an electron density map as described earlier in the `Load Map` section.
- Read in the PDB file - File/Load PDB or use the PDB search tab.
- Tools/Xray/Contour Electron Density.

- Enter the name of the map e.g. m_1cdg - the name of the map is displayed in the ICM Workspace or use the drop down arrow to locate it.
- If nothing is displayed then the whole map will be contoured. If you only want to contour a particular region of the map then you need to `select` the region to be contoured (e.g.the binding pocket) and then select the option **Trim to Selection Vicinity**.
- Enter a sigmaLevel value for more information see: `http://www.molsoft.com/man/reals.html#mapSigmaLevel`. Once the contoured

map has been created the sigma level can be changed manually using the +/- buttons in the ICM workspace.



The sigma level can be changed interactively in the ICM workspace as shown below.



NOTE: Meshes can be cut away using the `mesh clipping tools`.

4.3.7 Convert Xray Density to Grid

For some applications, such as trying to fit a structure to a density map, you may want to extract a sub map and convert to a grid. You can do this by

- First read into ICM a map (eg File/Open or Tools/X-ray/Get Electron Density Map)
- Tools/X-ray/Convert Xray Density to Grid
- Enter the map name or use the drop down list
- Enter a grid size
- Click OK

4.4 Protein Superposition

Available in the following product(s): `ICM-Browser-Pro` | `ICM-Pro`

One or more proteins can be superimposed. Simply select the molecules or parts of the molecules you wish to superimpose and then use the selection of protein superimpose tools described in this section. A convenient superimpose button can be found in the `Display tab` (see image of button (left).

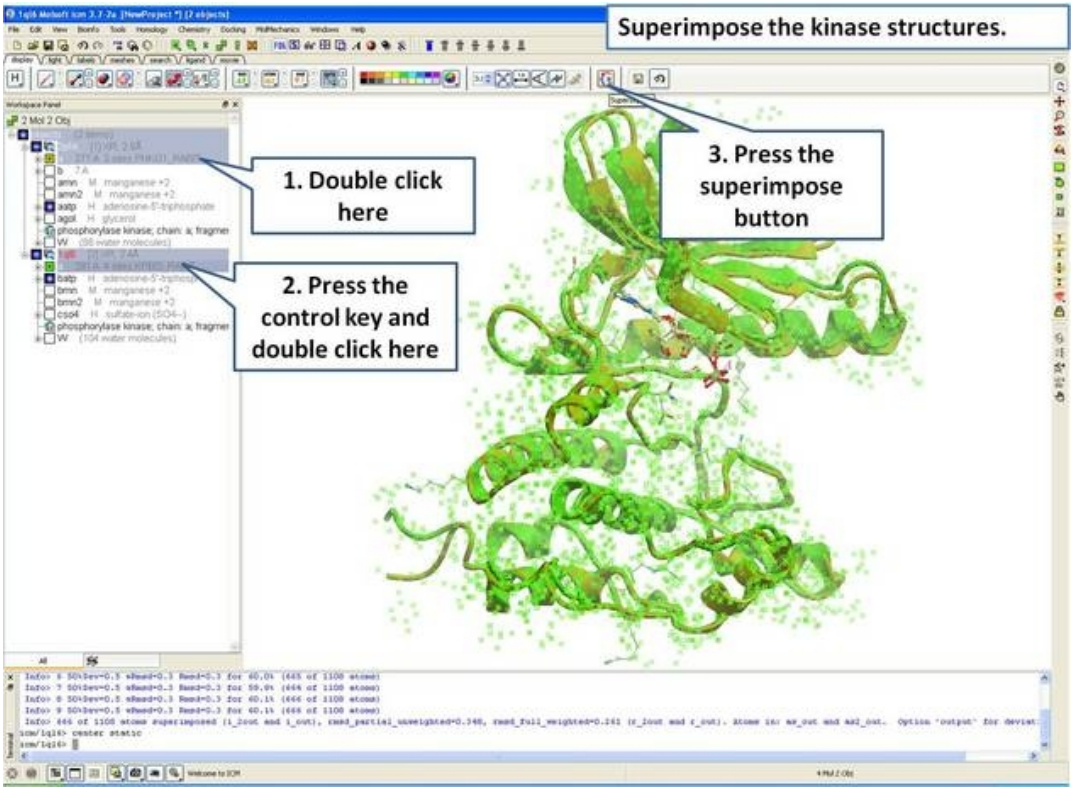
Chapter Contents:

4.4.1 Select Proteins for 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 molecule in the ICM Workspace. To select two molecules 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.



Once the molecules are selected you can then superimpose them using the options described in the next section of this manual.

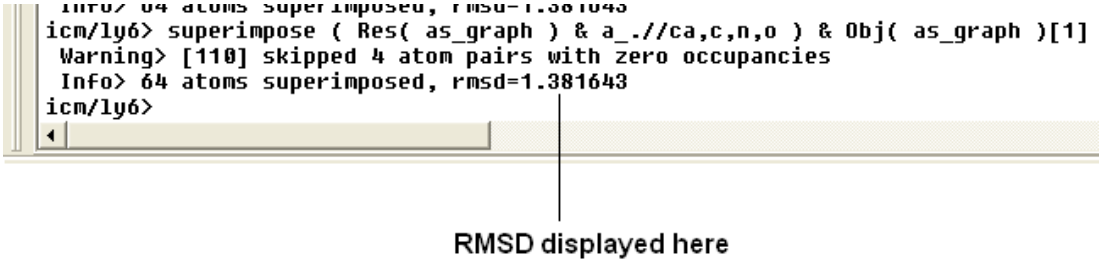
4.4.2 Superimpose Button

A convenient way to superimpose two molecules is 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:

- First load the two structures into ICM.
- Select which parts or all of the two structure you wish to superimpose (see the chapter on `Selections` or the description protein-superposition-select{here}.).
- Select the **display** tab (previously called Advanced tab) at the top of the GUI.
- Select the superimpose button.

The rmsd will be displayed in the terminal window as shown below:

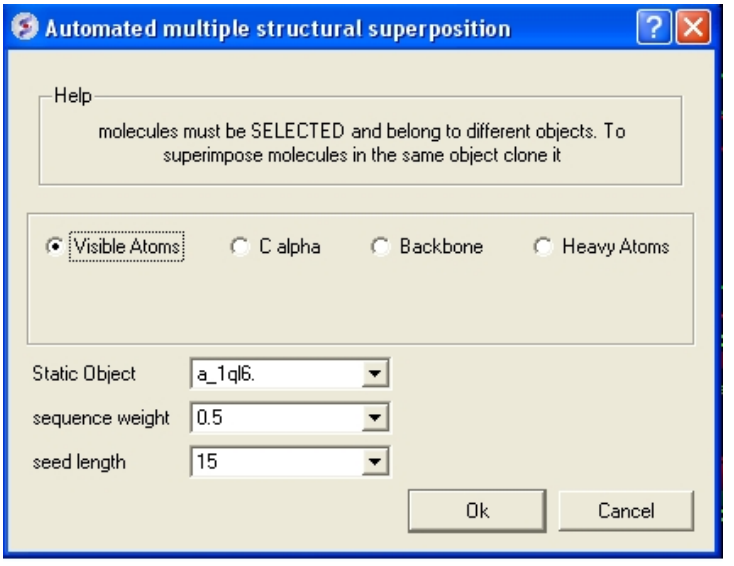


NOTE: You do not need to select the whole molecule, the superimpose button will work on small selections e.g the loop regions or domains.

4.4.3 Superimpose by 3D

To superimpose proteins by 3D:

- First `display and select` the proteins you wish to superimpose by 3D.
- Tools/Superimpose/Proteins by 3D
- A window as shown below will be displayed.

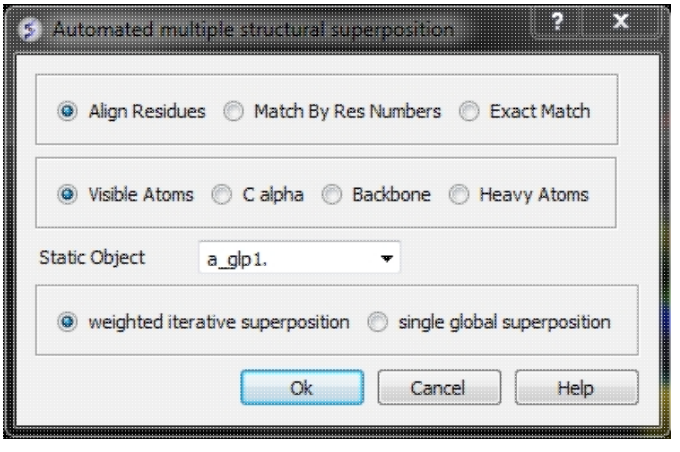


- Select by which atoms you wish to superimpose.
- Enter the ICM selection language description for the protein structure you wish to remain static. You can also use the drop down arrow button to select it.
- Enter the **sequence weight** Average local sequence alignment score.
- Enter the **seed length** This is the similarity window size.

4.4.4 Superimpose Multiple Proteins

To superimpoe multiple proteins:

- First `display and select` the proteins you wish to superimpose by 3D.
- Tools/Superimpose/Multiple Proteins
- A window as shown below will be displayed.



- Select by which method you would like to superimpose

Align Residues - Residue correspondence is established by sequence alignment using the ICM ZEGA alignment Abagyan, Batalov, 1997. Atom alignment: by atom name.

Match by Res Numbers - Residue alignment by residue number.Atom alignment: by atom name for pairs of identical residues or pairs of close residues (F with Y; B with D,N; D with N; E with Q or Z, Q with Z), for other residue pairs only the backbone atoms ca,c,n,o,hn,ha are aligned.

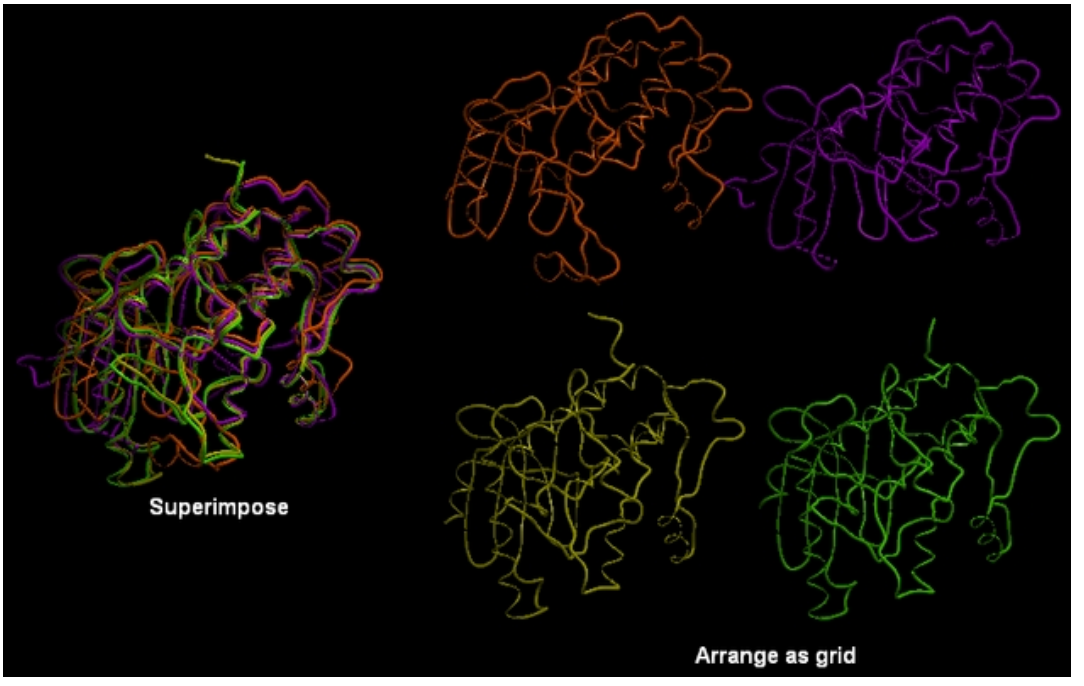
Exact Match - Residue alignment is by the Needleman and Wunsch method. Inside residue atoms are aligned sequentially and regardless of the name.

- Select which atoms you would like to superimpose. Visible Atoms, C alpha, Backbone, or Heavy Atoms.
- Select whether you would like to use **weighted iterative superposition** as described here `http://www.molsoft.com/man/icm-commands.html#superimpose-minimize` or non-iterative **single global superposition**.

4.4.5 Arrange as Grid

To separate superimposed proteins:

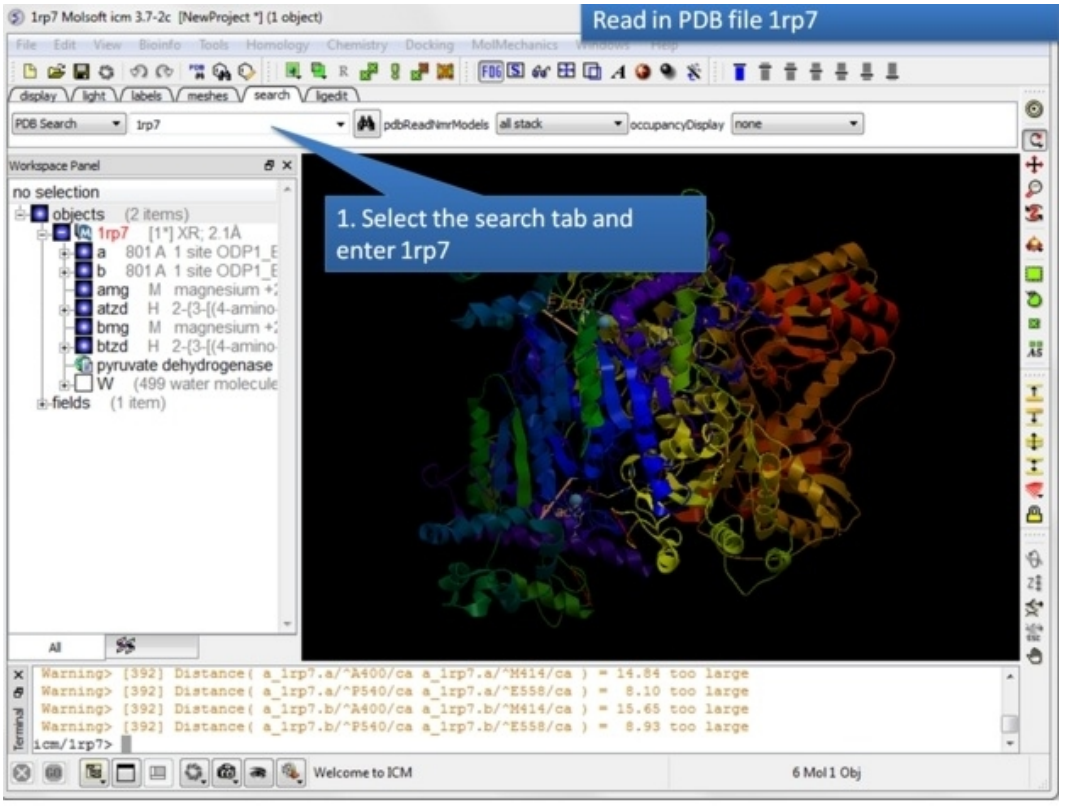
- Tools/Superimpose/Arrange as Grid



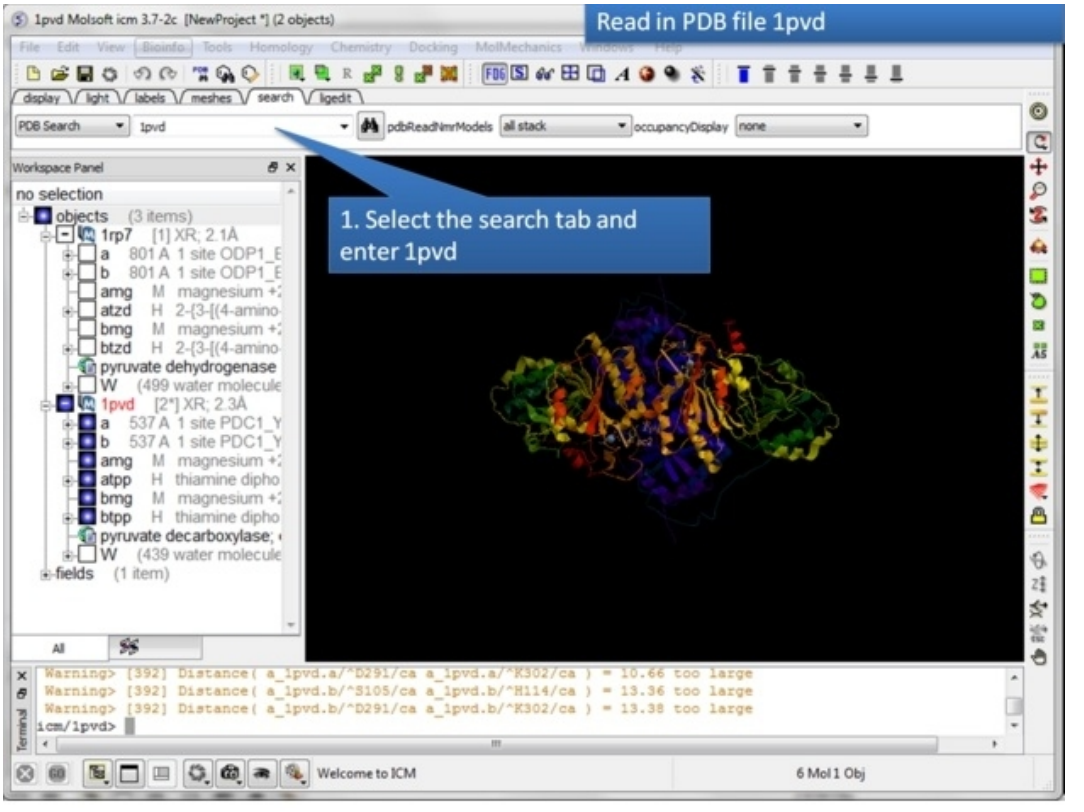
4.4.6 Superimpose Sites by Atomic Property Fields

Here we describe how to superimpose and compare a ligand binding site using Atomic Property Fields. This method is described in more detail in this publication.

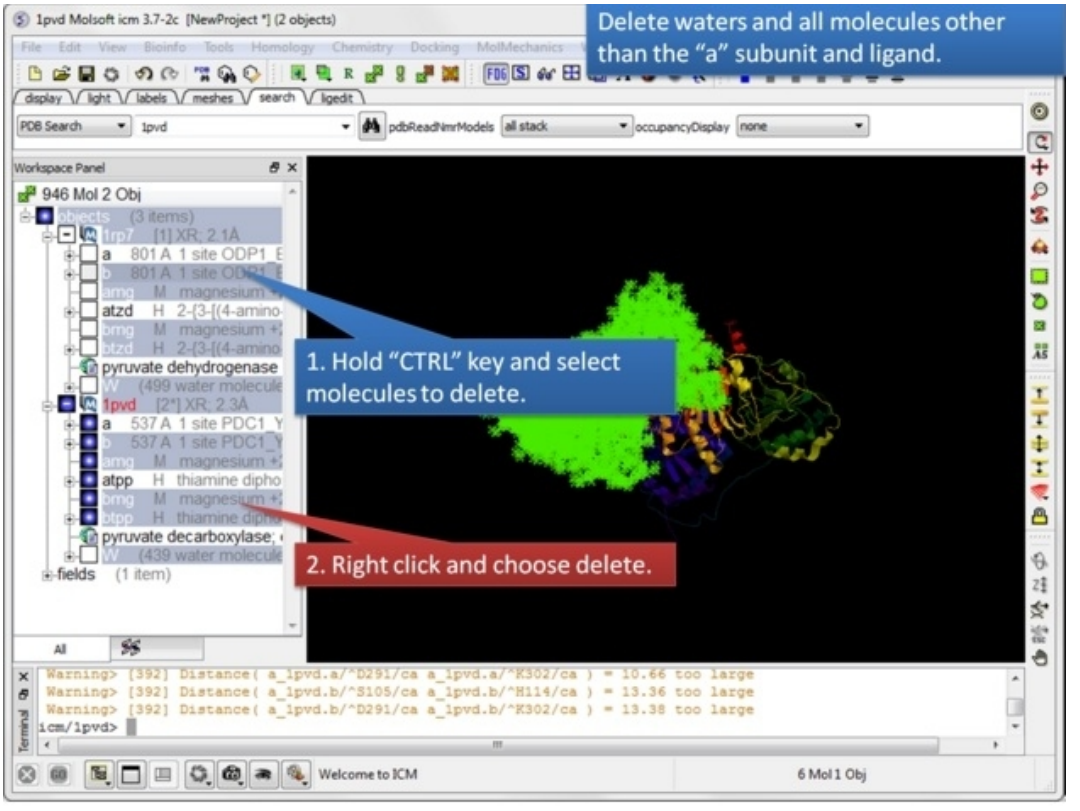
In this example we superimpose the ligand binding pocket of thiamine diphosphate in the binding sites of pyruvate dehydrogenase (pdb code: 1rp7) and pyruvate decarboxylase (pdb code:1pvd).Even though the sequence identity between both proteins is very low (19%) and the secondary structure surrounding the ligand undergoes considerable displacement you will see that the pockets can still be superimposed very well using the APF method.



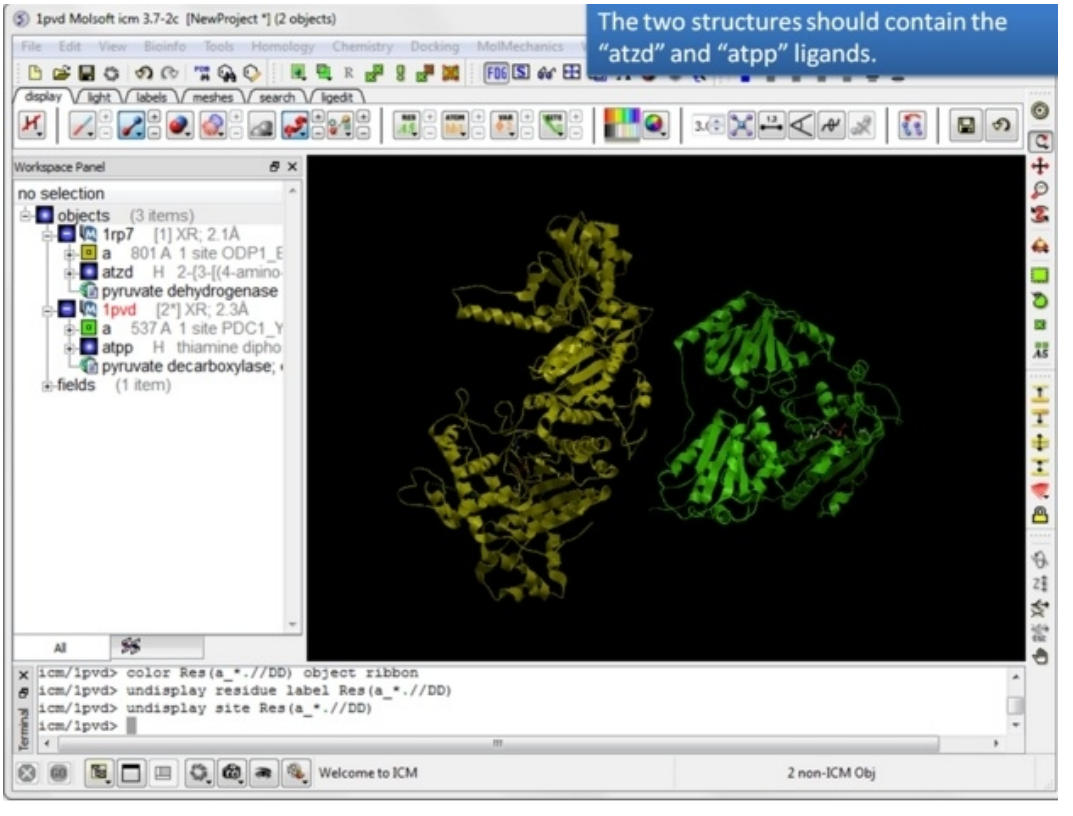
Step 1: Read in the pyruvate dehydrogenase (pdb code: 1rp7) structure.



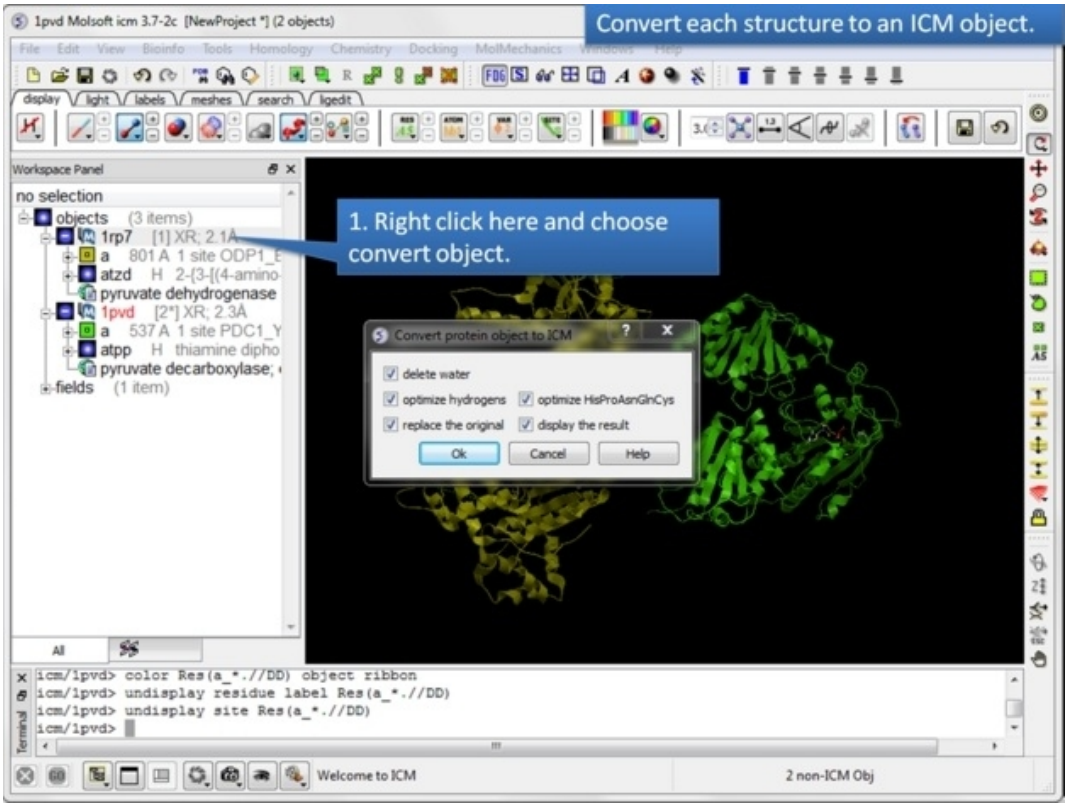
Step 2: Read in the pyruvate decarboxylase (pdb code:1pvd).



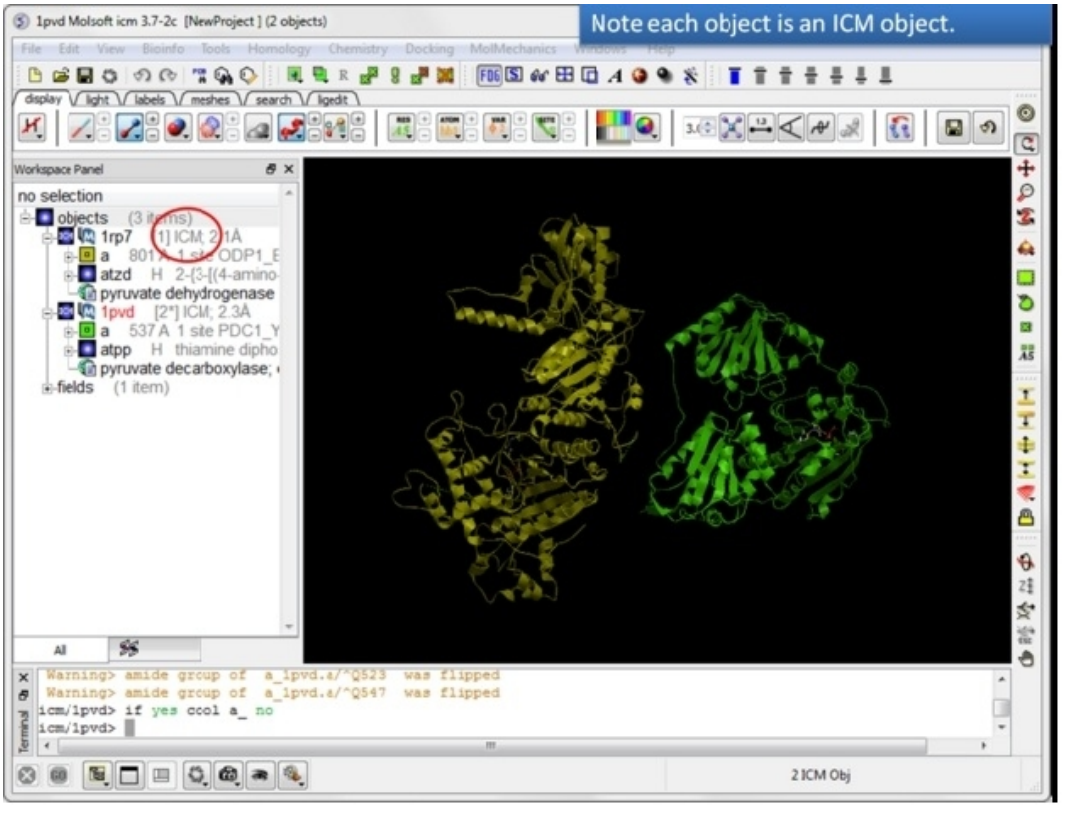
Step 3: Delete unwanted molecules in the b chain and waters.



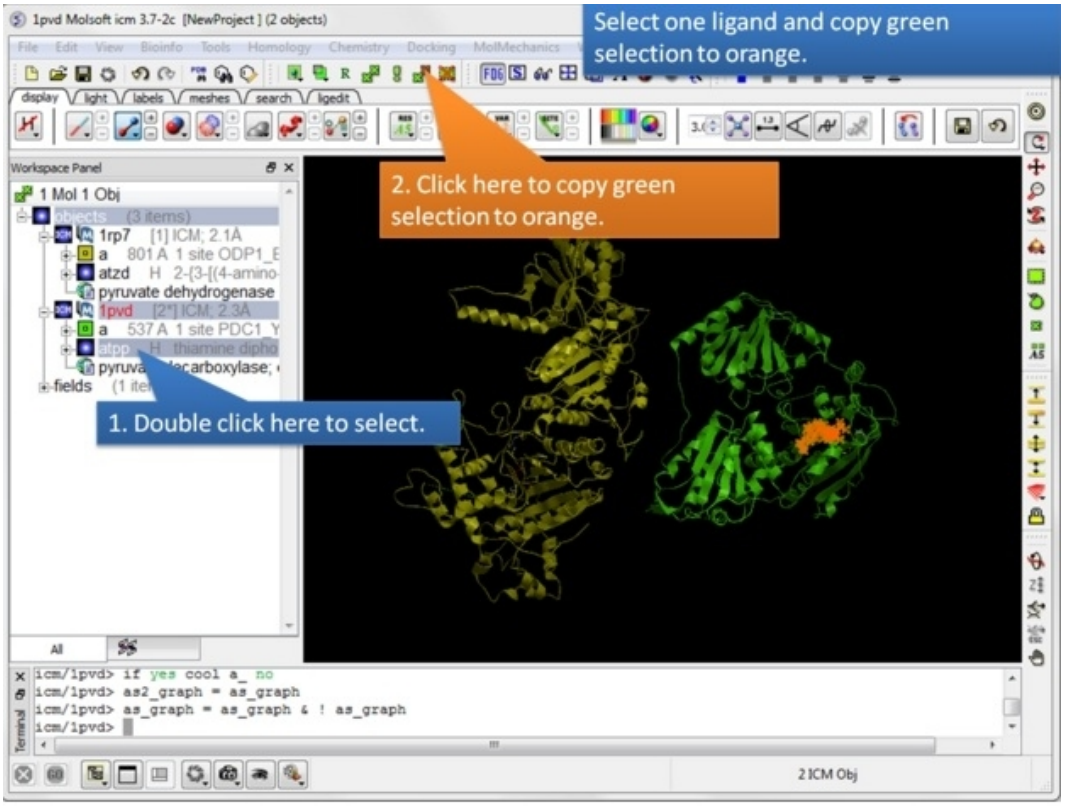
Step 4: You should have two objects containing the protein and ligand.



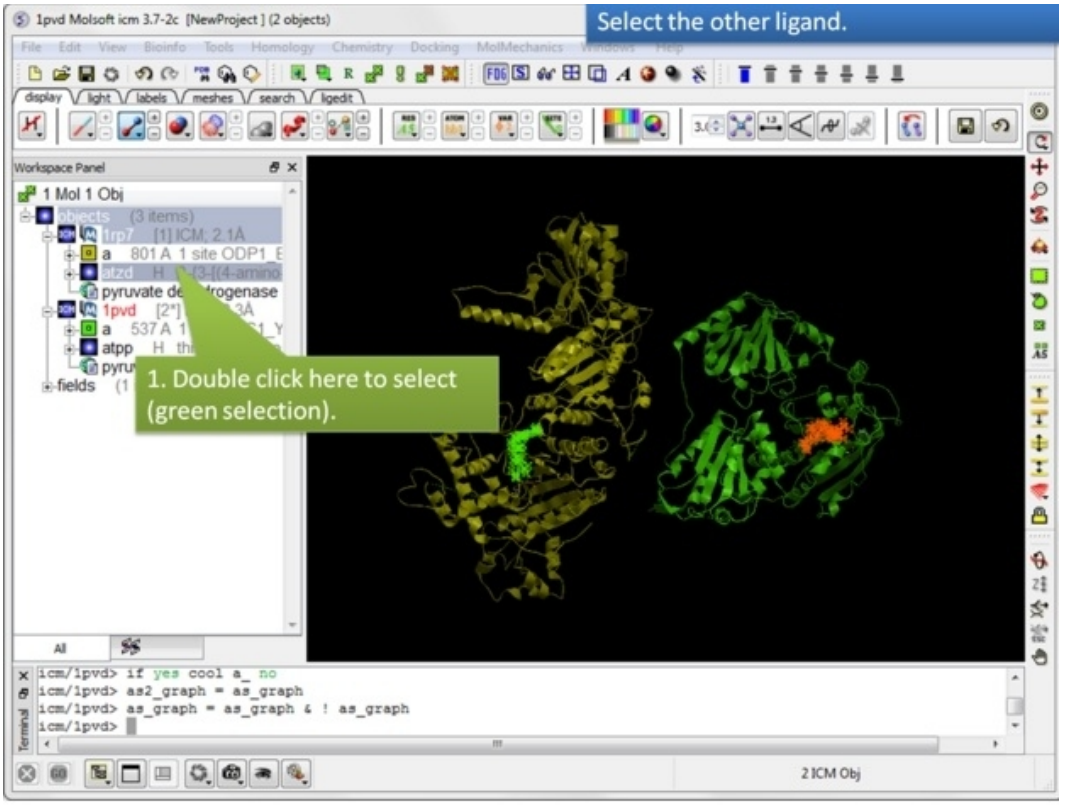
Step 5: Convert both structures to an ICM object.



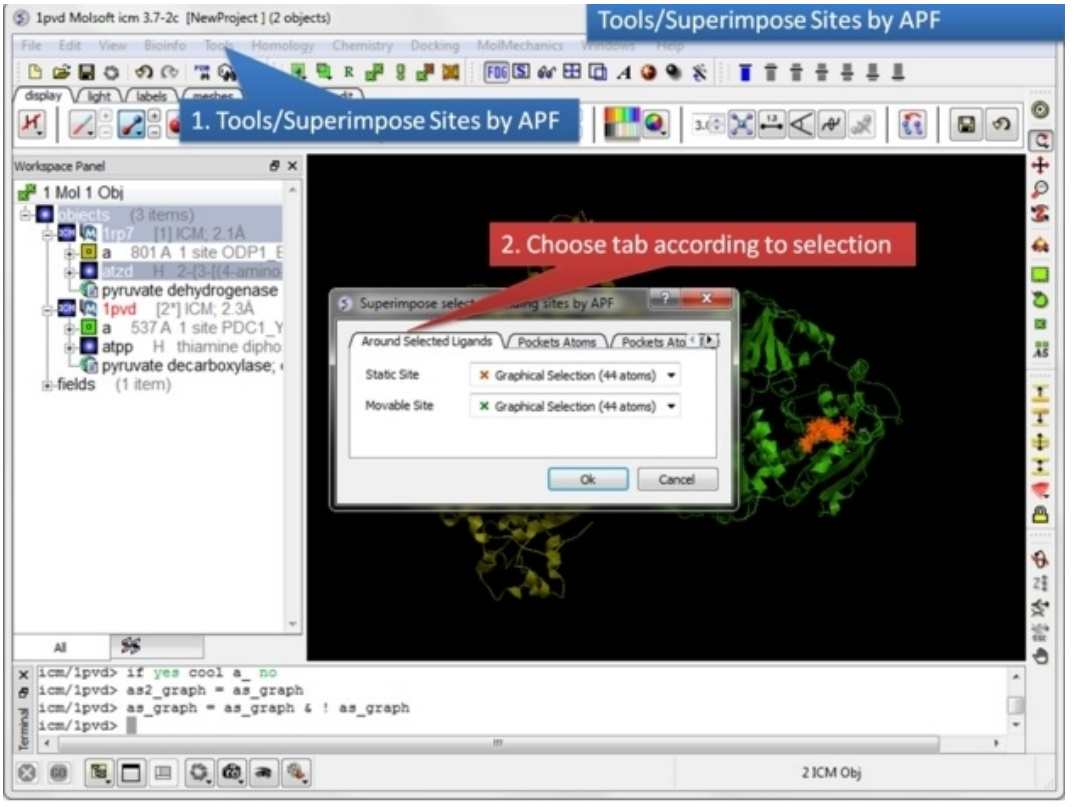
Step 6: If the pdb is converted you will see "ICM" in the workspace.



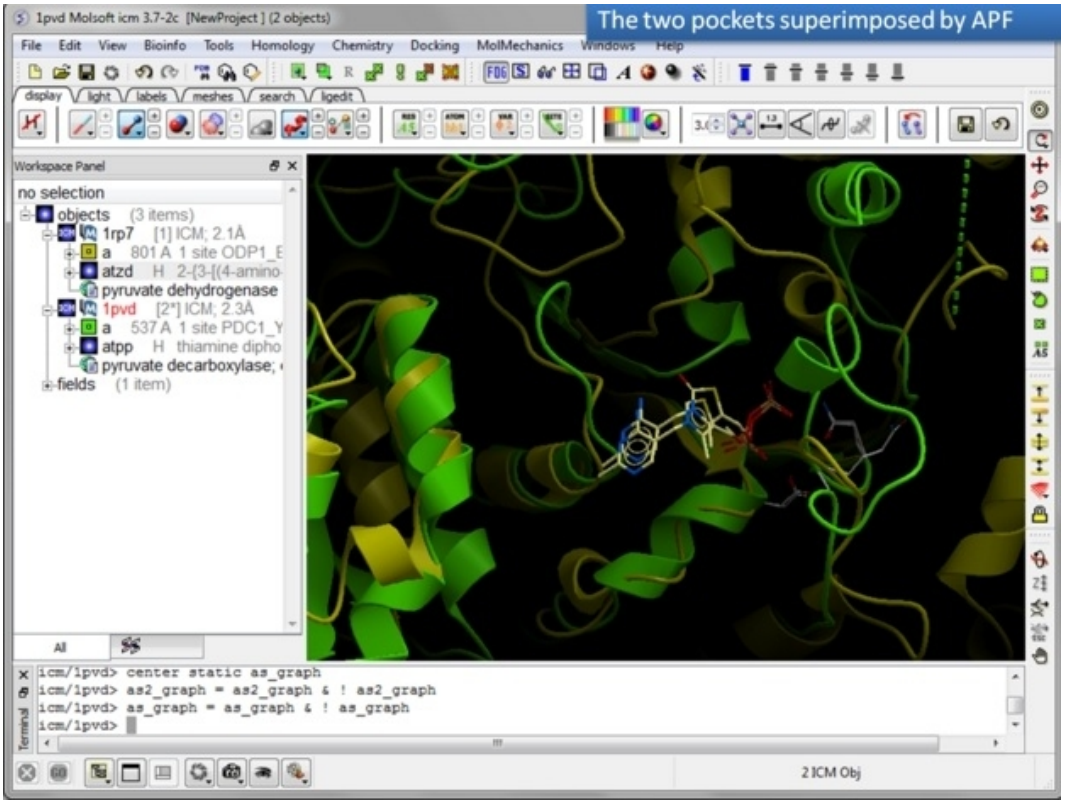
Step 7: Select one ligand and copy the green selection to orange.



Step 8: Select the other ligand (regular green selection).



Step 9: Select the option Tools/Suerpimpose/Sites by APF. Note you can also superimpose pockets - choose the appropriate tabs in the dialog box.



Step 10: Observe the superimposed site.

4.5 Protein Structure Analysis

Available in the following product(s): ICM-Browser-Pro | ICM-Pro

In this chapter we describe the tools available for analyzing protein structure. These tools include calculating RMSD, identifying closed cavities, calculating contact and surface area, measuring anlgles and distances, and generating Ramachandran plots.

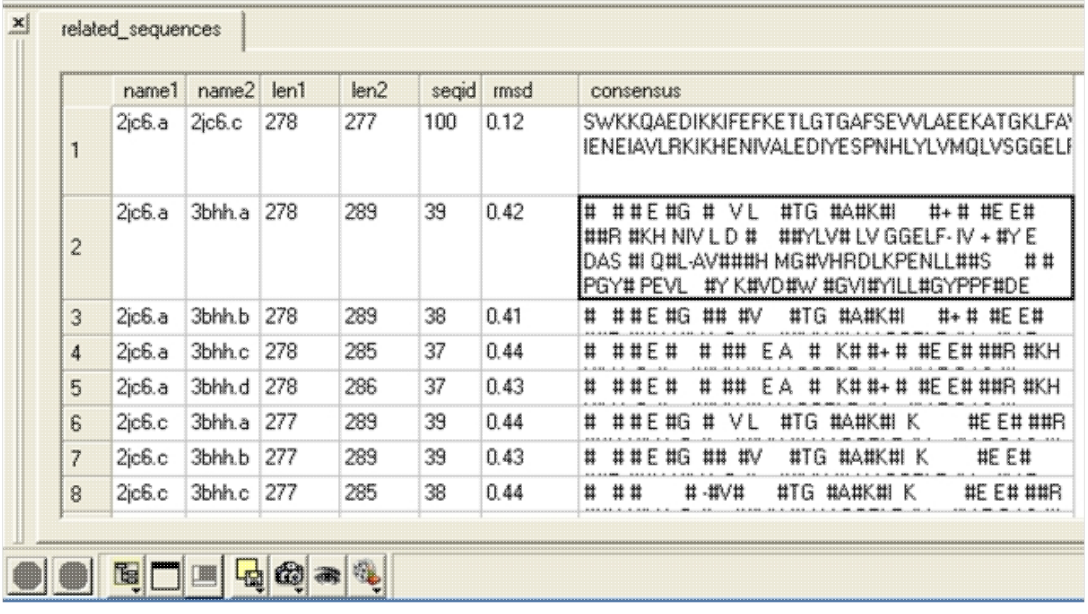
Chapter Contents:

4.5.1 Find Related Chains

This option allows you to search the currently loaded PDB files or ICM objects and identify chains which are similar and/or related.

You can do this by:

- Select the objects or pdb files you want to compare.
- Tools/Analysis/Find Related Chains
- Click OK to confirm the selection you made
- A table as shown below will be displayed.



	name1	name2	len1	len2	seqid	rmsd	consensus
1	2jc6.a	2jc6.c	278	277	100	0.12	SWKKQAEDIKKIFEFKETLGTGAFSEVVLAEEKATGKLFA IENEIAVLRKIKHENIVALEDIYESPNHLYLVMQLVSGGELF
2	2jc6.a	3bhh.a	278	289	39	0.42	# ##E #G # VL #TG #A#K#I #+ # #E E# ##R #KH NIV L D # ##YLV# LV GGELF- IV + #Y E DAS #I Q#L-AV####H MG#VHRDLKPENLL##S # # PGY# PEVL #Y K#VD#W #GVI#YILL#GYPPF#DE
3	2jc6.a	3bhh.b	278	289	38	0.41	# ##E #G ## #V #TG #A#K#I #+ # #E E#
4	2jc6.a	3bhh.c	278	285	37	0.44	# ##E # # ## EA # K# #+ # #E E# ##R #KH
5	2jc6.a	3bhh.d	278	286	37	0.43	# ##E # # ## EA # K# #+ # #E E# ##R #KH
6	2jc6.c	3bhh.a	277	289	39	0.44	# ##E #G # VL #TG #A#K#I K #E E# ##R
7	2jc6.c	3bhh.b	277	289	39	0.43	# ##E #G ## #V #TG #A#K#I K #E E#
8	2jc6.c	3bhh.c	277	285	38	0.44	# ## #-#V# #TG #A#K#I K #E E# ##R

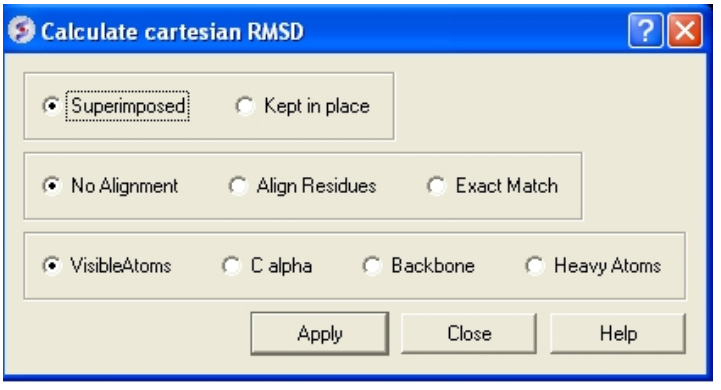
name1 = Name of query structure molecule **name2** = Name of hit **len1** = length of query **len2** = length of hit **seqid** = Sequence identity percentage **consensus** = Consensus sequence

4.5.2 Calculate RMSD

NOTE: This option is for protein structures only not for chemical compounds. You can use the command line options RMSD (http://molsoft.com/man/icm-functions.html#Rmsd) and Srmsd (http://molsoft.com/man/icm-functions.html#Srmsd) for chemicals.

To calculate RMSD between two protein structure:

- Read into ICM the two structures (`File/Open` or `PDB Search` or Read in Chemical) you wish to compare.
- `Select` one of the two molecules you wish to compare, you can do this by double clicking on the name of the structure in the ICM Workspace. Convert this selection to an `Orange Selection`.
- Select the second molecule, and then you should have one orange and one green selection in the graphics display.

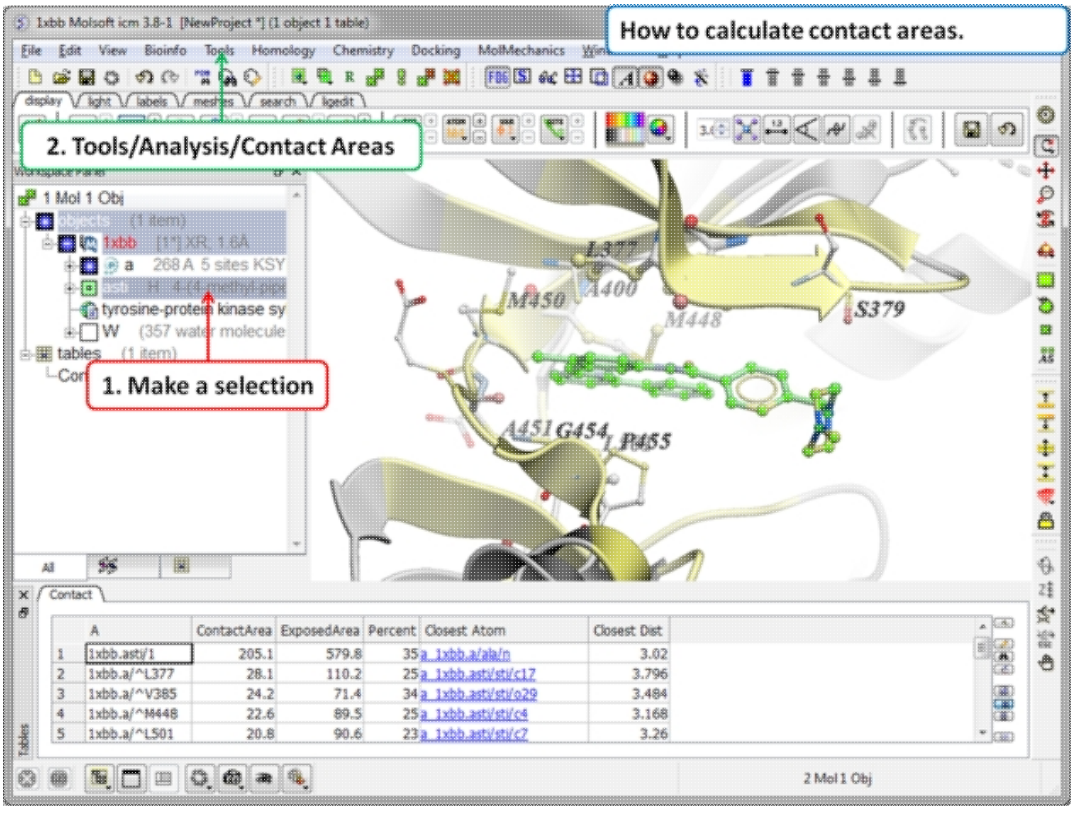


- Select whether you wish the atoms to be superimiposed onto one another or kept in place. The kept in place option would be ideal for comparing docked structures.
- Choose whether you wish to make the superposition by alignment or exactly matching the atom names.
- Select which atom types you wish to superimpose.

The **RMSD** value will be displayed in the terminal window.

4.5.3 Contact Areas

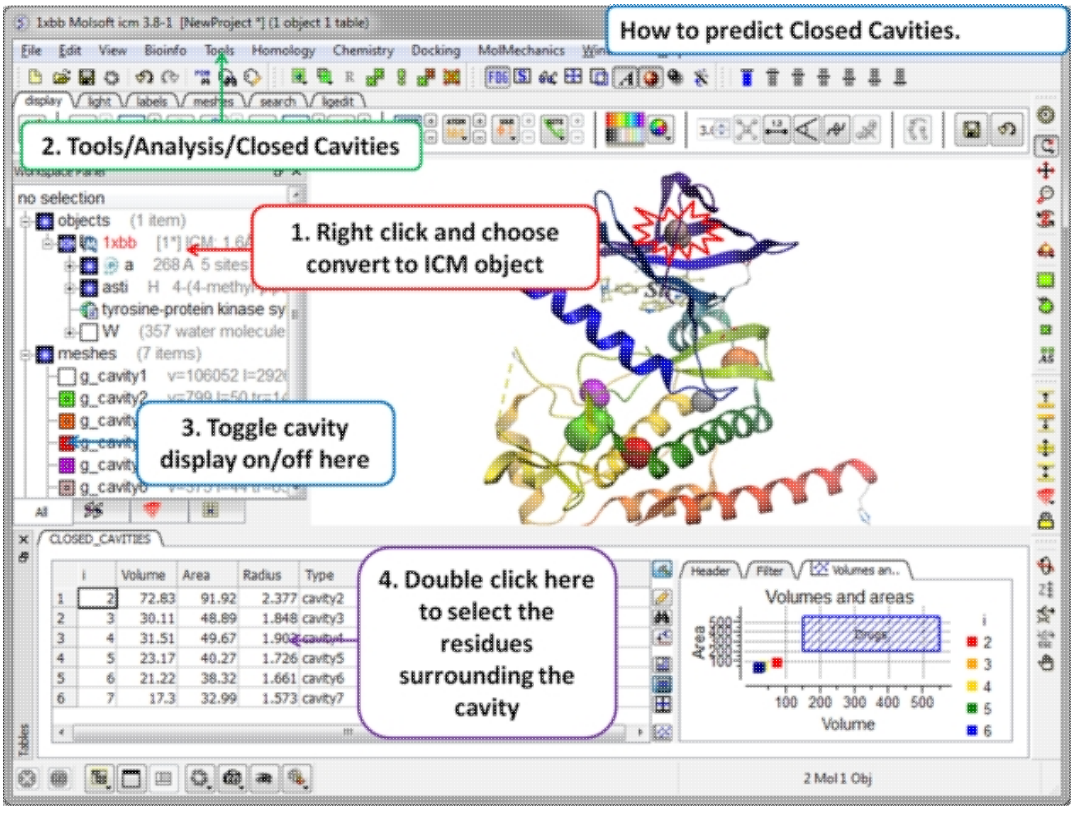
- Read in a protein structure (`File/Open` or `PDB Search`).
- `Select` the region you wish to analyse.
- Tools/Analysis/Contact Areas
- The xstick display in the region will be scaled according to the atom/residue contact area. For example, residues making large contacts with a ligand will be displayed in thicker xstick representation (and colored yellow) than those making less significant contacts.
- A table as shown below will be displayed.The table lists the contact area, exposed area, percentage of contact area compared to exposed, the nearest atom of a residue and the distance.



4.5.4 Identify Closed Cavities

This tool will identify cavities within a molecule which are completely closed,. If you are looking for buried and open pockets then use icmPocketFinder.

- Read in a protein structure (`File/Open` or `PDB Search`).
- Convert the protein structure to an `ICM object`.
- Tools/Analysis/Closed Cavities
- Use the drop down arrow to locate the molecule you are interested in.
- Enter the minimum volume of the cavities you wish to identify.
- Click OK
- The closed cavities will be displayed in the meshes section of the ICM Workspace and a table of the cavities will be displayed. Double click on a row in the table to jump to a particular closed cavity and select the residues surrounding it.



What is the difference between Closed Cavity and ICMPocketFinder? Closed pocket (cavityFinder) is purely geometrical/topological - it is a part of molecular surface that is completely disconnected from the exterior surface. It means that a probe sphere of 1.4A radius (representing a water molecule) can not pass in or out of the cavity (considering protein as completely rigid of course). icmPocketFinder identifies pockets that are likely to contain ligands (not specifically open or closed pockets). Pockets are defined based on physical interaction rather than geometric criterion. Blobs of 'pocket density' generated by icmPocketFinder represent continuous regions of space where there is significant favorable van der Waals interaction with the receptor.

4.5.5 Surface Area

This option calculates solvent accessible area of each selection in multiple objects and stores it in a table. If a molecule is specified in a multi-molecular object, the surface area of an isolated molecule is calculated and other molecules are ignored. The area is reported in square Anstroms and the probe radius is assumed to be the value set in the variable waterRadius.

Output: the macro creates table AREA . The empty comment field is added for user's future use. If the table exists, new rows are appended.

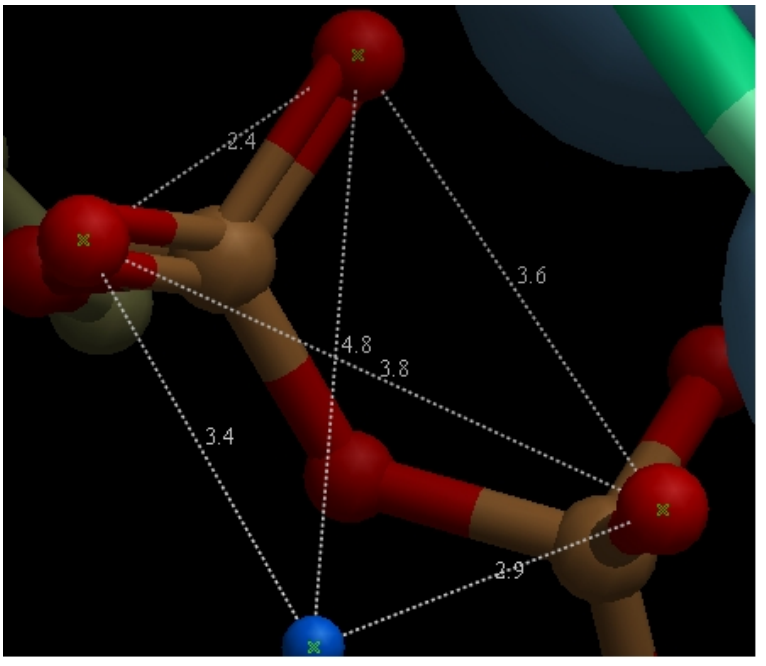
To calculate a surface area:

- Read in a protein structure (`File/Open` or `PDB Search`).
- `Select` the region you wish to analyse.
- Tools/Analysis/Surface Area
- A table will be displayed listing the residues in the selection along with the corresponding total surface area.

4.5.6 Measure Distances

There are two approaches to calculating and displaying distances between atoms. You can either use the options in the `Labels` tab or use Tools/Analysis/Distance.

To display **all to all** distances:



- Select the atoms between which you would like to find the distance. (See `selection toolbar`)
- Tools/Analysis/Distance
- Select all to all

To display **intermolecular** distances

- Select the atoms between which you would like to find the distance. (See `selection toolbar`)
- Tools/Analysis/Distance
- Select **intermolecular**

To display the distances between the same atoms in two objects.

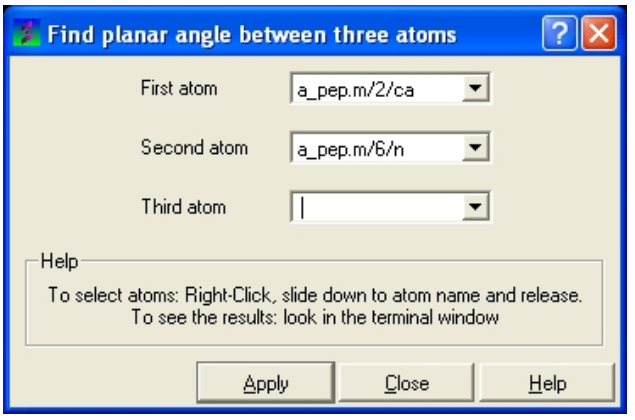
- Select the atoms between which you would like to find the distance. (See `selection toolbar`)
- Tools/Analysis/Distance
- Select **same atoms in two objects**

NOTE: Distances can be displayed and undisplayed in the 3D labels section of the ICM Worskapce. You can change the color of a distance label by right clicking on it in the ICM Workspace. You can alse export the distance to a table.

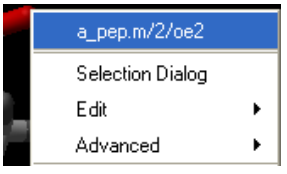
4.5.7 Planar Angle

If you wish to find the planar angle between three atoms:

- Select **Tools/Analysis/PlanarAngle**



- Right click on the each of the three atoms which you wish to use, and select their name. The spaces next to **First atom**, **Second atom**, and **Third atom** should now contain the name of your atoms.



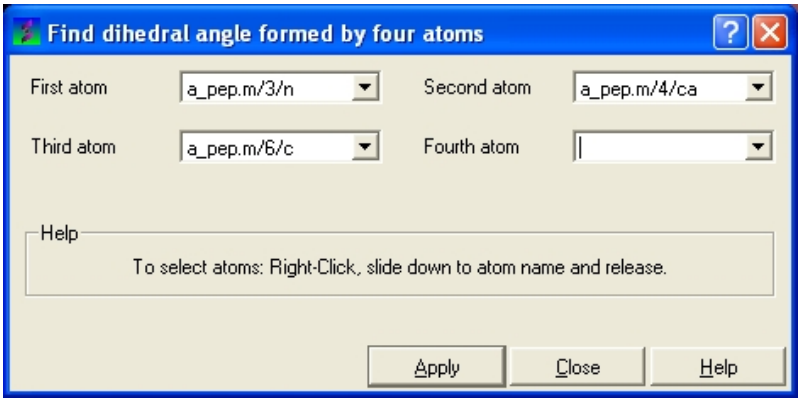
- Click **Apply** to display the angle measure in the terminal window.

```
Angle ( a_pep.m/6/hh21 a_pep.m/2/oe2 a_pep.m/3/o ) = 74.72 deg.
```

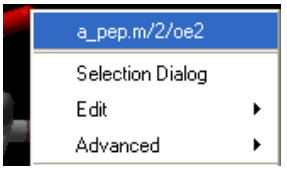
4.5.8 Dihedral Angle

In order to find the angle dihedral angle between two sets of atoms:

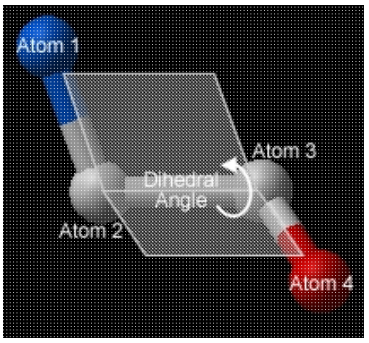
- Select **Tools/Analysis/Dihedral Angles.**



- Right click on each of the four atoms which you wish to use, and select the name of the atoms. The spaces next to **Atom 1**, **Atom 2**, **Atom 3**, and **Atom 4** should now contain the names of your atoms.



- To find the correct angle, select your atoms according to the following diagram:



- Click **Apply** to display your dihedral angle measure in the terminal window.

4.5.9 Ramachandran Plot Interactive

To make an interactive ramachandran plot:

- Read in a protein structure (`File/Open` or `PDB Search`).
- Select the structure you wish to build the plot for. You can do this by double clicking on the name of the structure in the ICM Workspace (a selection is highlighted blue in the ICM Workspace and green crosses in the graphical display) or you can use the right-click button and drag it over the whole structure in the graphical display.
- Tools/Analysis/Ramachandran Plot Interactive
- The interactive ramachandran plot will be displayed in table called **RAMA.**
- You can view the **Omega**, **Phi/Psi** (Gly) or Phi/Psi angles by clicking on the tabs at the top of the plot. Each point is linked to the data in the table **RAMA** and also to the graphical display. Soby clickin on a point in the plot will highlight the corresponding angles in the table and also center on this region in the 3D display.

4.5.10 Export Ramachandran Plot

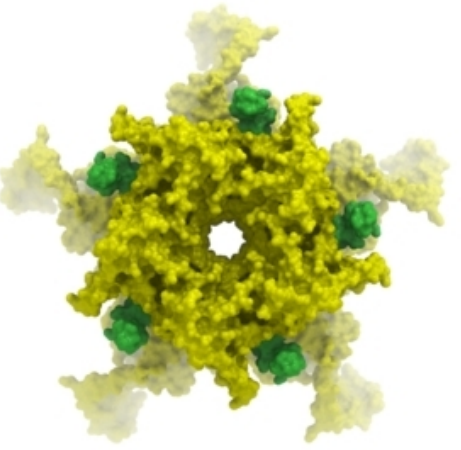
- Read in a protein structure (`File/Open` or `PDB Search`).
- Select the structure you wish to build the plot for. You can do this by double clicking on the name of the structure in the ICM Workspace (a selection is highlighted blue in the ICM Workspace and green crosses in the graphical display) or you can use the right-click button anddrag it over the whole structure in the graphical display.
- **Tools/Analysis/Ramachandran Plot Export**

A postscript viewer needs to be downloaded onto your machine in order to view the plot. This can be downloaded from `http://www.cs.wisc.edu/~ghost/.` Once this software is downloaded you need to tell ICM where it is located by typing the pathname into File/Preferences.

NOTE: You can always export the plot as an image directly in ICM without exporting. You can do this by right clicking on the plot and select **save as image**. Another approach could be to export the RAMA table to Excel and use the plotting tools there. You can do this by right clicking on the table name tab and selecting "Export to Excel" or save as ".csv".

5 Molecular Graphics

In this chapter we describe how to make beautiful graphical representations of molecules and manipulate them in the 3D graphics window. This includes how to change color, light, represenations, clipping planes, and how to use built in graphics effects. We also teach how to label and annotate molecules displayed in the graphical user interface.



Chapter Contents:

5.1 Molecule Representation

Available in the following product(s): ICM-Browser | ICM-Browser-Pro | ICM-Pro

To change the molecule display representation:

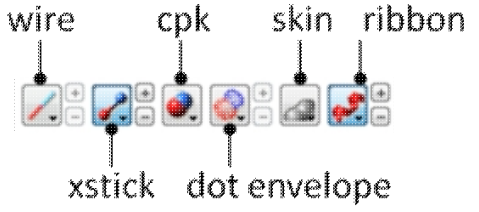
- Select the atoms, residues, molecules, or objects you wish to change in the graphical display or in the ICM Workspace.
- Then use the molecule representation (e.g. wire, ribbon) options in the Display Tab.

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

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:

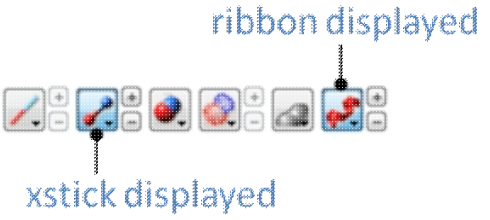
- Click on the representation button you desire in the **display** tab.



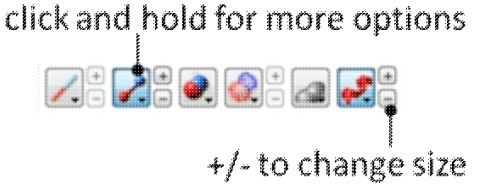
To remove a displayed representation or to toggle between display and undisplay:

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

Identify which representations are displayed: The button display will change appearance (shaded blue) when selected. This makes it easier to identify which representations are currently being displayed.

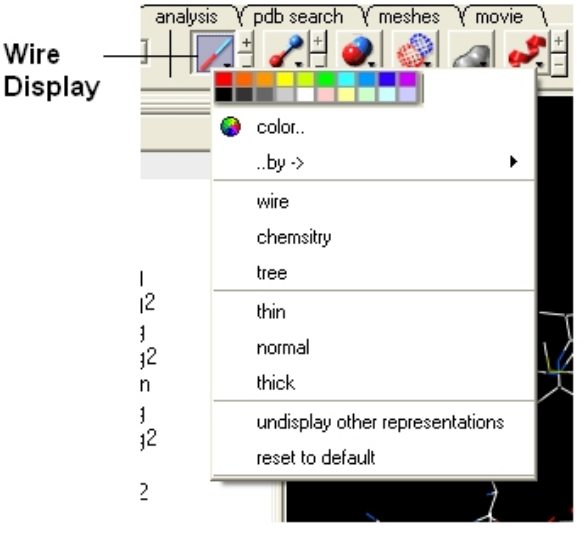


Change the display and size of the representations Many characteristics of the graphical representation such as color can be changed by clicking and **holding** on the button. The size can be changed by clicking the plus(+) and minus(-) buttons next to them.



5.1.1 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:

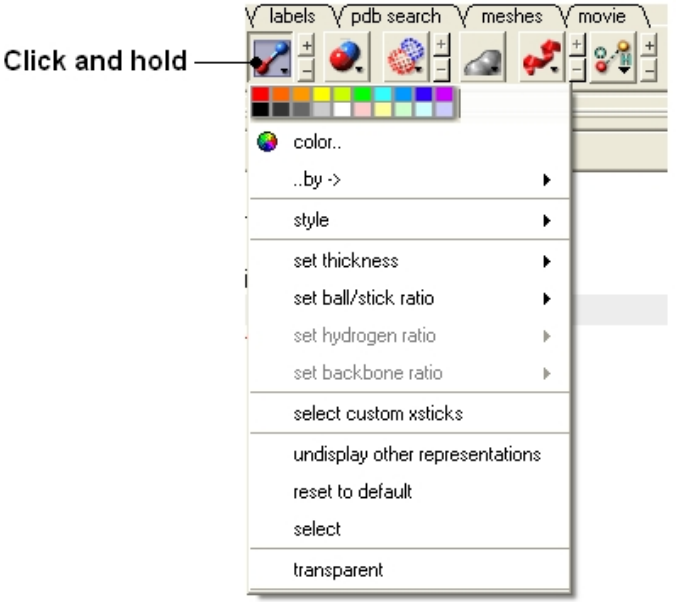
- Click and hold on the **wire representation** button and then click on undisplay other representations.

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.

5.1.2 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 and choose either **plain**, **chemistry**, **Chem Plus**, or **Chem Plus Aromatic**.

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 ratio**.

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.

5.1.3 Ribbon Representation

Click and hold on the ribbon representation button and a menu will be displayed.

To change the style of the Ribbon representation:

- Click and hold on the **ribbon representation button** and then click on a style option: **smooth**, **wide**, **wide smooth**, **cylinders**, **protein worm** .

To assign secondary structure:

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**.

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**.

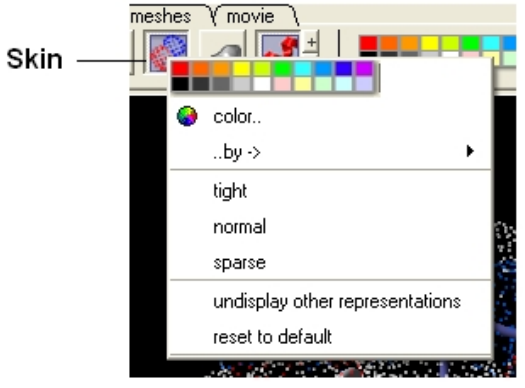
NOTE: Always use the **ICM** assign sec.** structure tool in the ribbon right click menu to get accurate secondary structure assignment. This is particularly important when studying helices which may have non-cannonical elements within them such as 3/10 or pi. To view non-cannonical helix segments use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

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

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

5.1.4 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 infliction select atoms nearby and right click select Advanced->RandomizeAtoms

5.1.5 CPK Representation

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

To undisplay representations other than CPK:

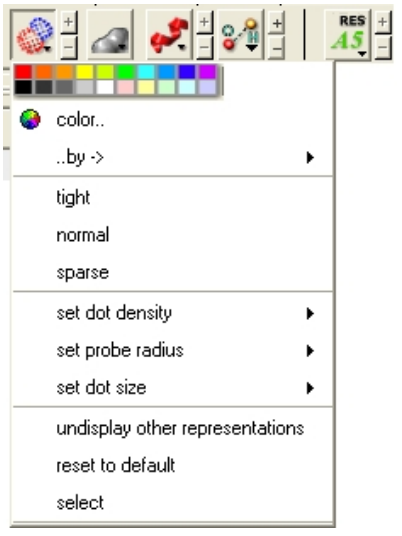
- Click and hold on the **CPK representation button** and then click on **undisplay other representations**.

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**.

5.1.6 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.

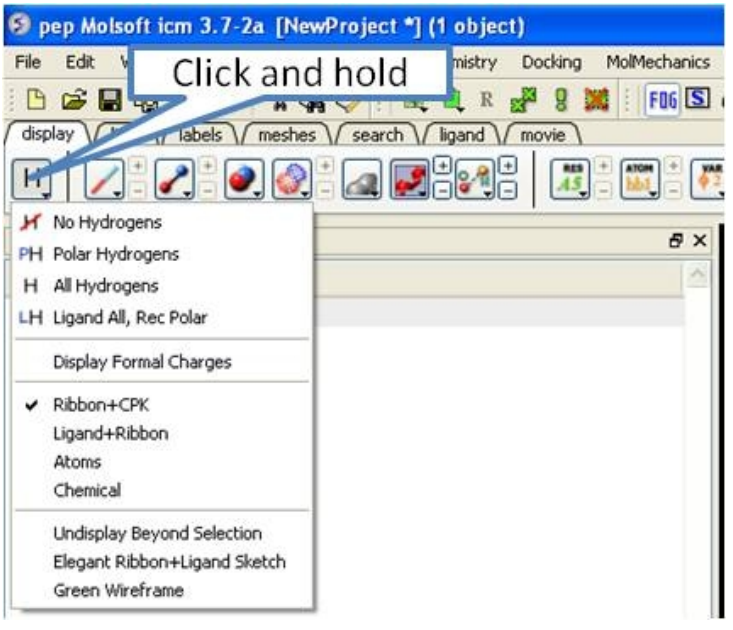
If you make a mistake or you are not happy with the way your structure is displayed with the surface representation:

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

5.1.7 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 hyrogen display options.

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

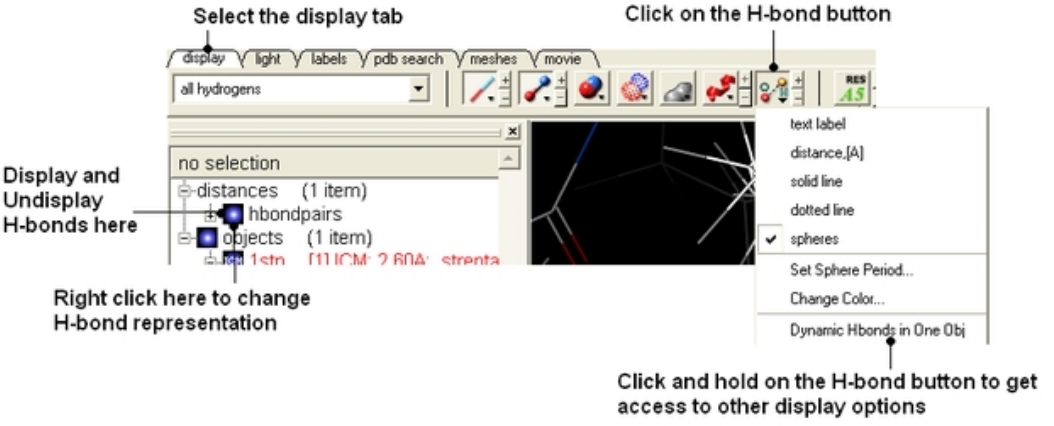


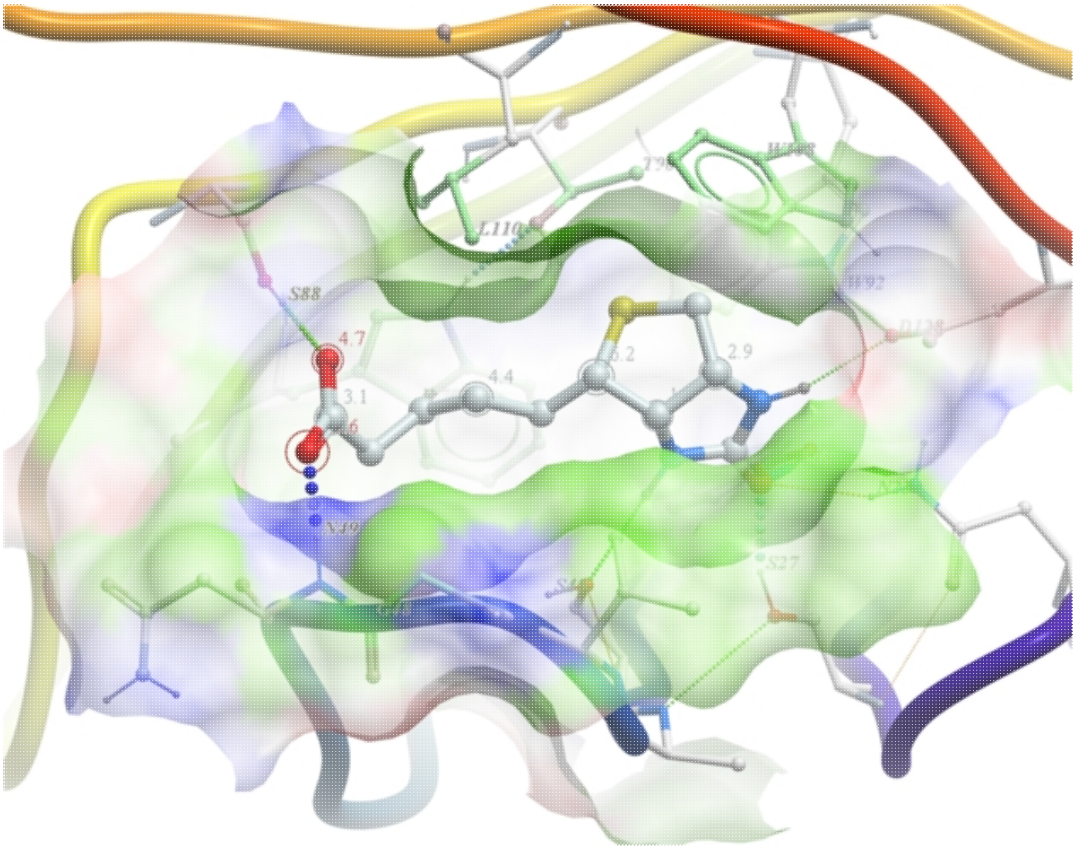
5.1.8 Display Hydrogen Bond

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:

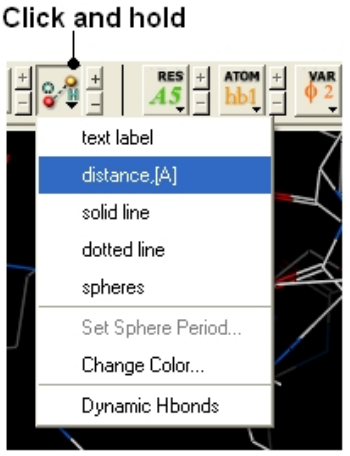
- Convert to an ICM Object
- Make a selection - if you are trying to display the H-bonds between a ligand and the receptor make sure the ligand is part of the selection.
- Click the Display Tab.
- Click on the **Toggle H-bonds** icon in the **display** tab.





- 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.

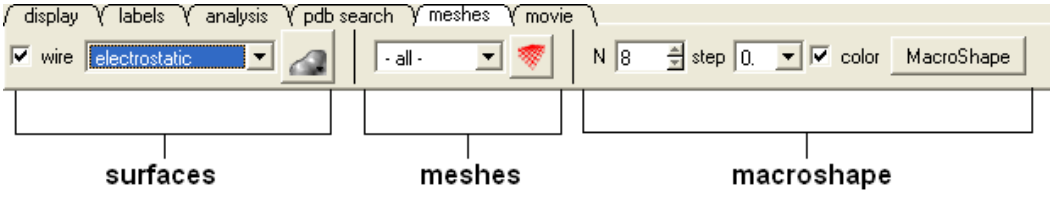
5.1.9 Display Formal Charges

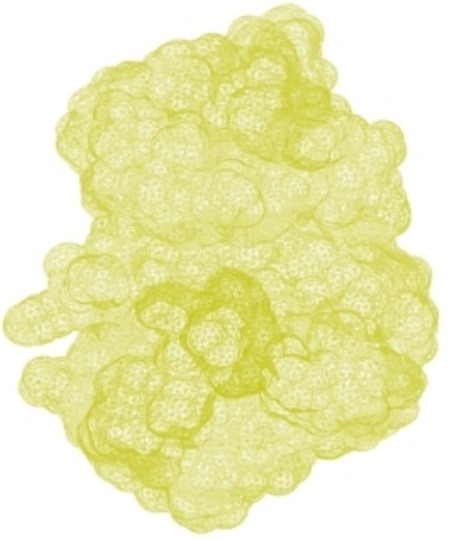
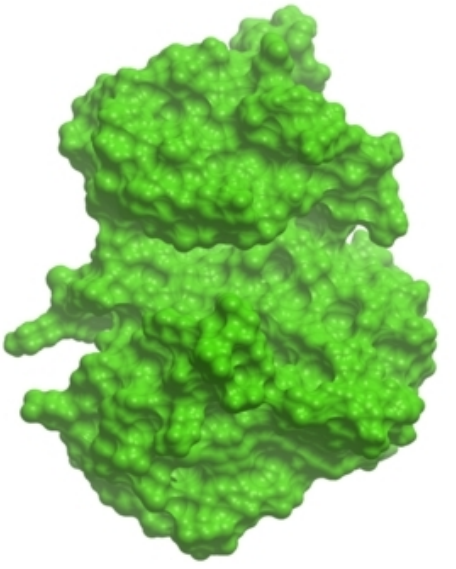
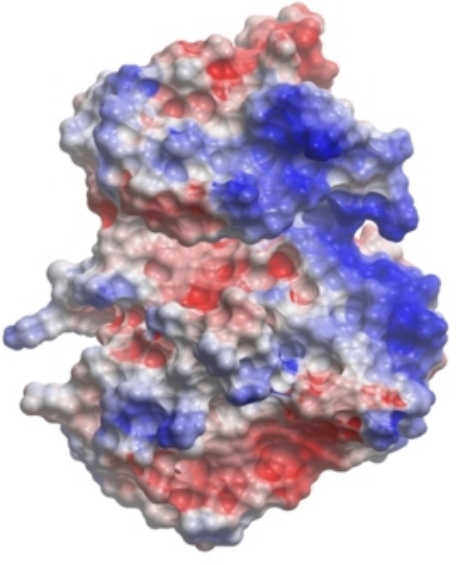
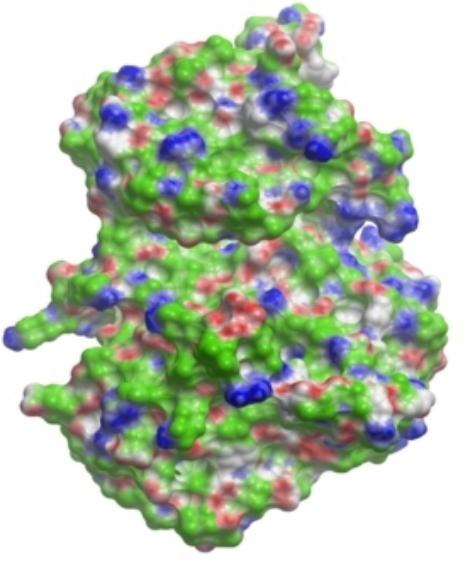
You can display formal charges by clicking and holding on the **"Change Hydrogen Display"** button in the **Display tab**.

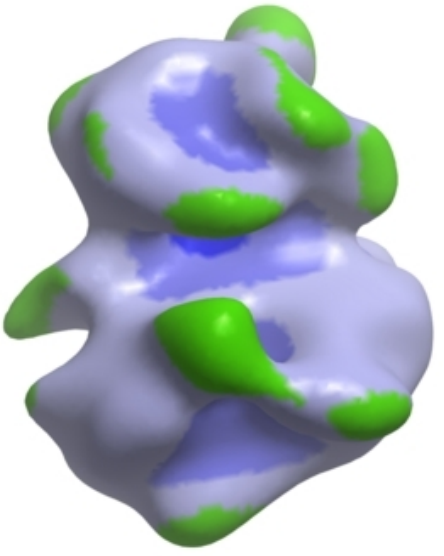
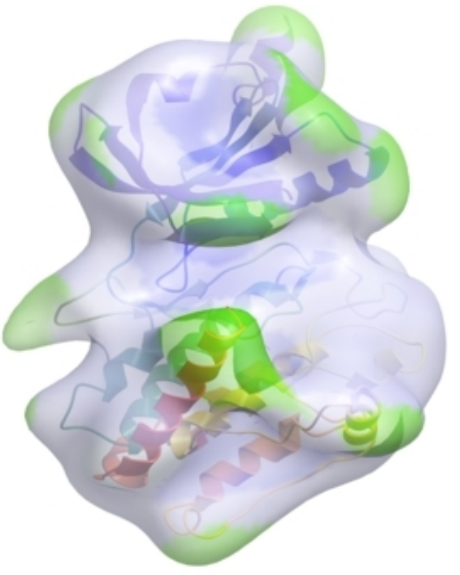
5.2 Meshes - Surface - Grobs

Available in the following product(s): `ICM-Browser-Pro` | `ICM-Pro`

Click on the tab button entitled **'meshes'** and more graphics tools for surfaces are available. In ICM surfaces are sometimes referred to as meshes or graphical objects (Grobs).



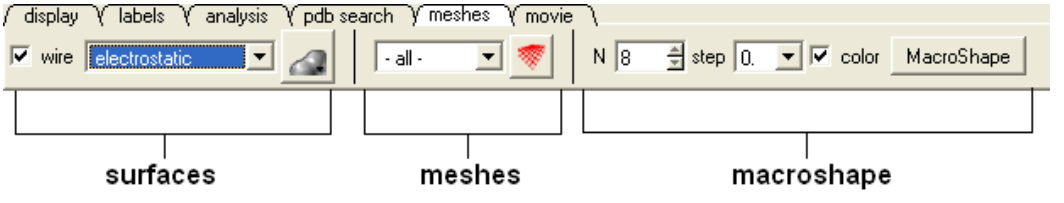
	
Surface	Plain Solid
	
Electrostatic Surface	Binding Property Surface

	
Macroshape Solid	Macroshape Transparent

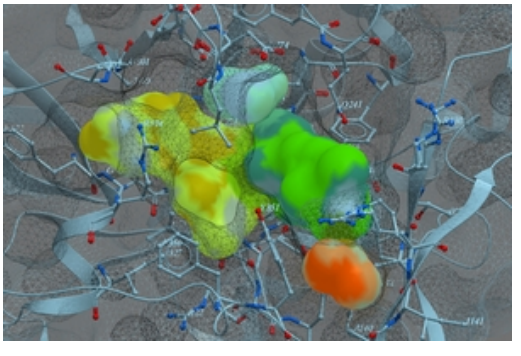
5.2.1 Surfaces

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.
- Click on the drop down arrow menu shown below and select which surface you wish to generate.
- Click on the generate surface button next to the drop down arrow.



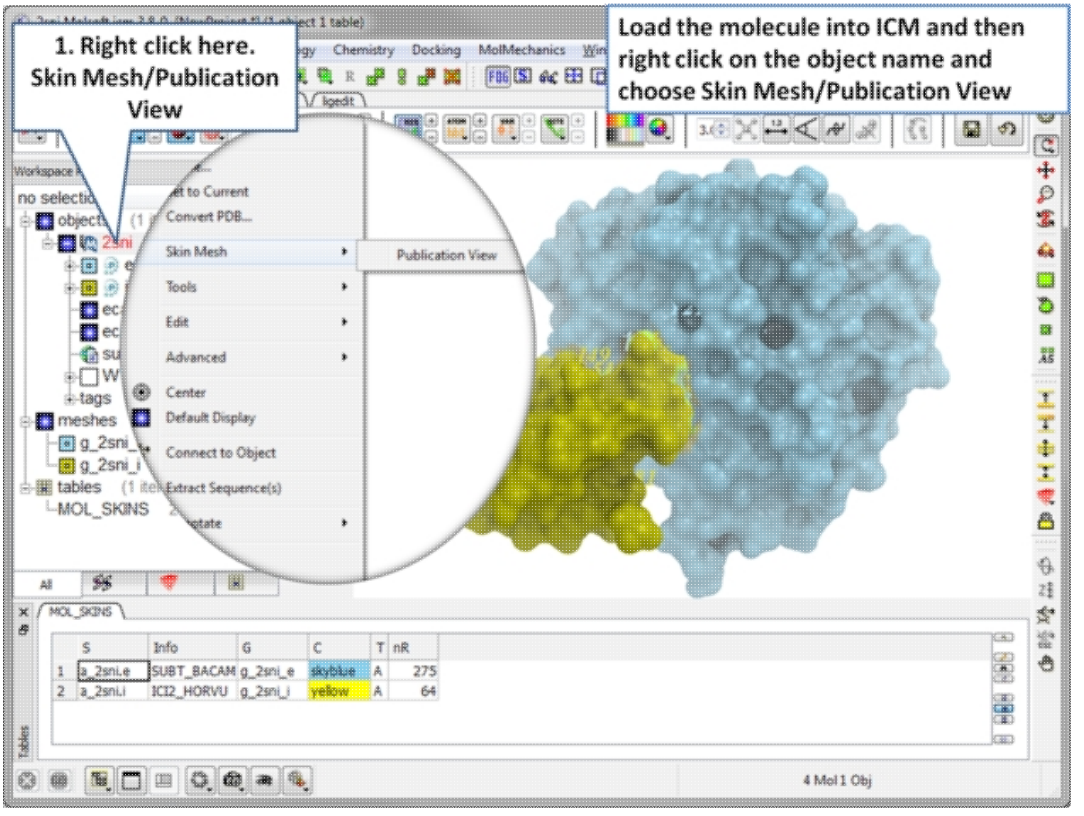
5.2.2 MolSkin



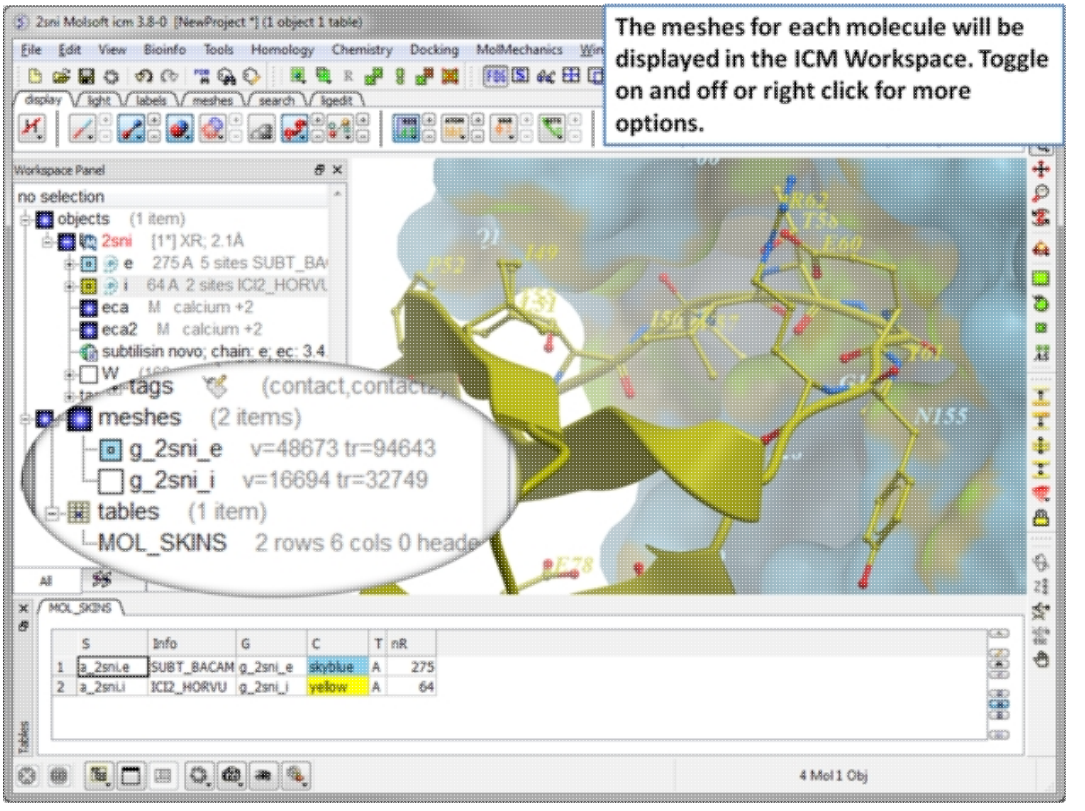
MolSkin is a new macro that instantly makes publication quality graphics and it gives each molecule a color and colors contact patches. It undertakes the following:

- molecular surfaces are generated with those assigned colors and occlusion shaded
- carbons of each molecule are colored by its own consistent color
- labels, ribbons, are colored accordingly
- surfaces are gradually cross-colored by each other to mark the contact patches
- the labels are brought to the surfaces

To use MolSkin:



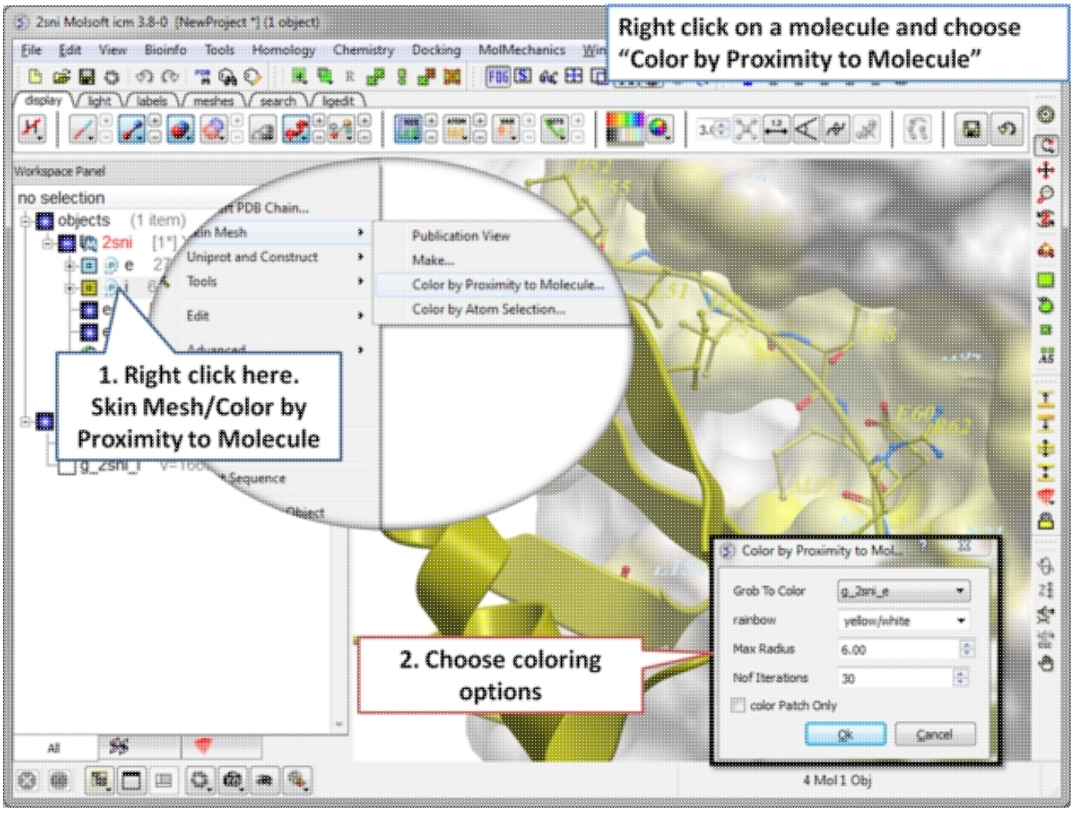
`Read` into ICM a PDB file. Next, right click on the object name and choose Skin Mesh/Publication View .



The surfaces will be displayed in the meshes section of the ICM Workspace.

5.2.3 Color Surface by Proximity

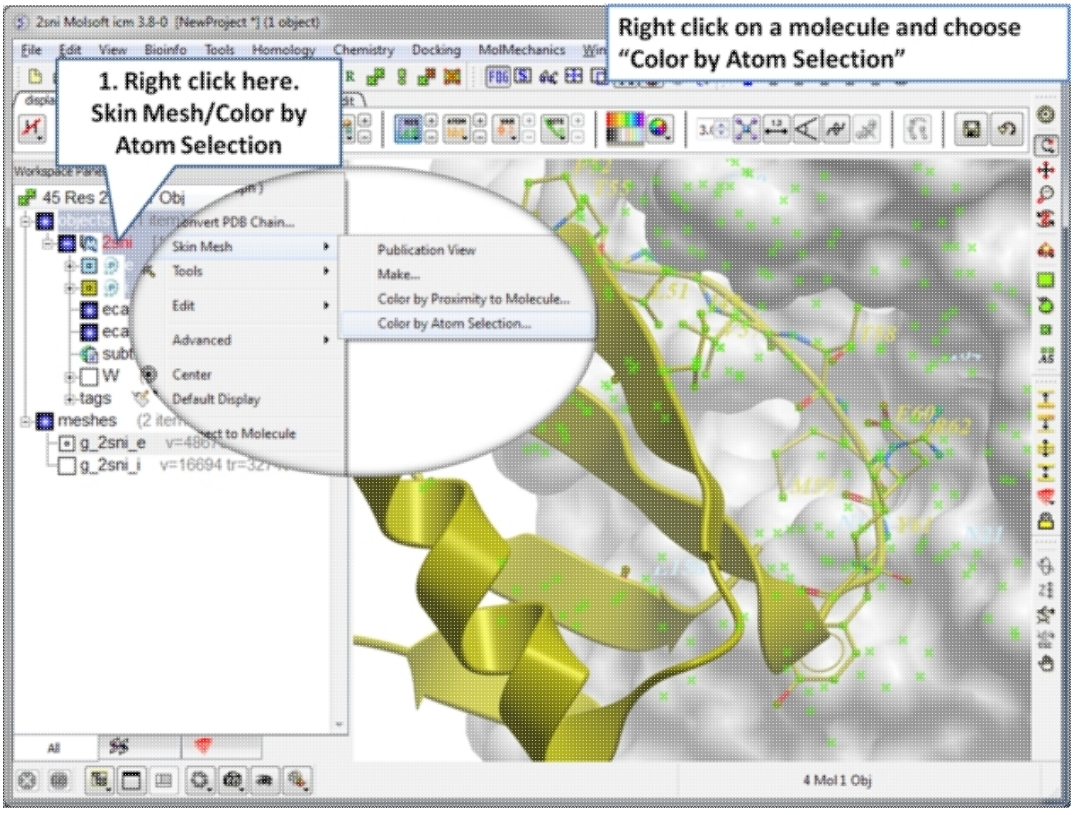
To color a surface by proximity to neighboring molecules:



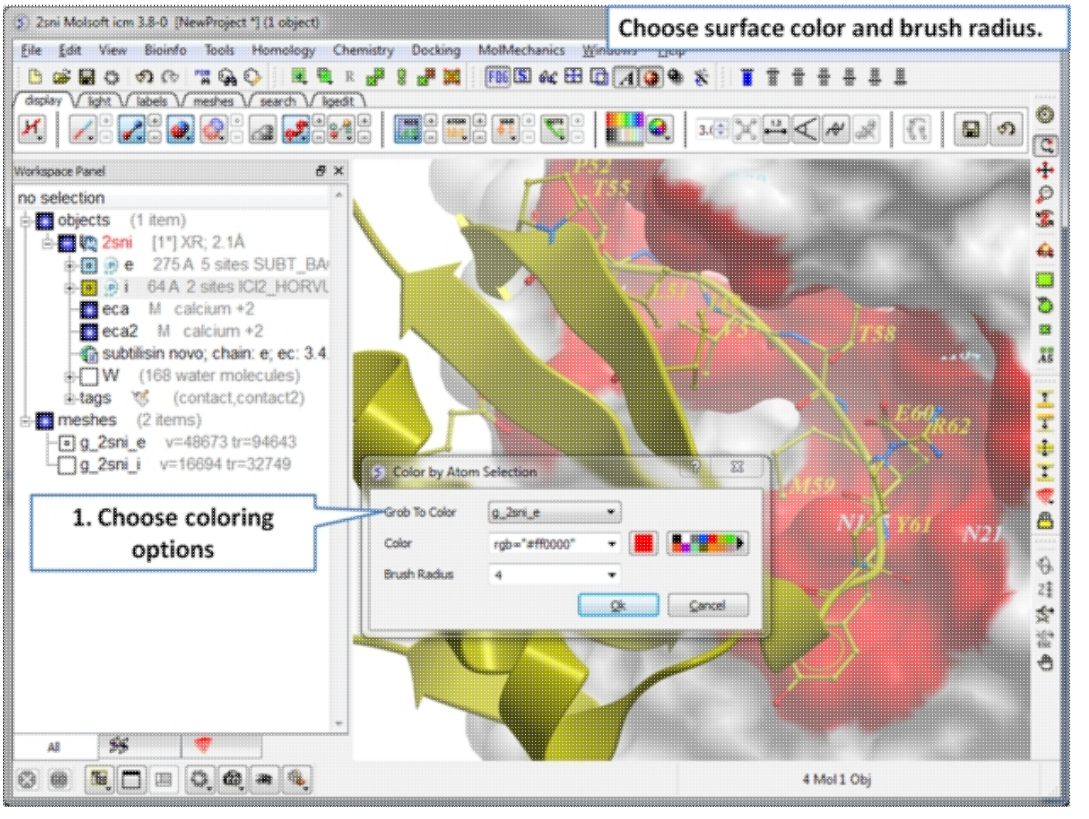
Create a `surface` then right click on the molecule and choose Skin Mesh/Color by Proximity to Molecule".

5.2.4 Color Surface by Selection

To color a surface by a selection:



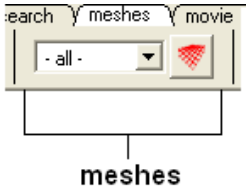
Create a `surface` and then make a `selection`. Right click on the molecule and choose Skin Mesh/Color by Selection.



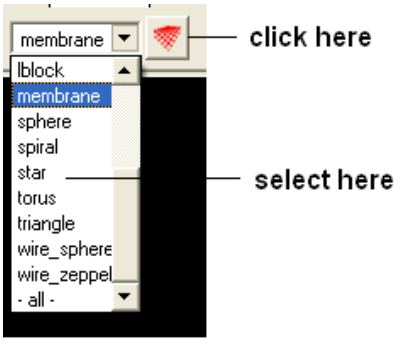
Choose the color and brus radius.

5.2.5 Meshes

A variety of shapes can be constructed automatically using ICM. These shapes are referred to as meshes. The types of shapes you can build are shown in the drop down option in the meshesh tab

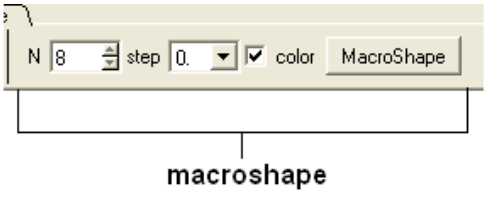


To make a shape select it from the menu by clicking on the down arrow and then click the button next to the menu. The shape will then be displayed in the 3D graphics window.



5.2.6 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

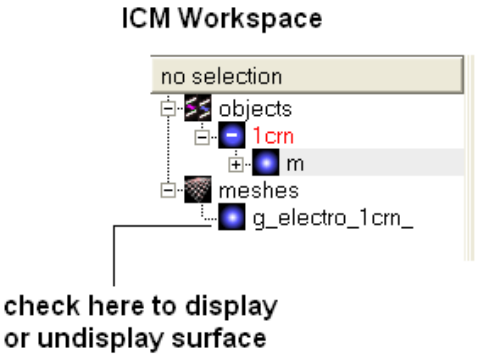
5.2.7 Google 3D Objects (Sketchup)

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

5.2.8 Display or Undisplay Meshes or Surfaces

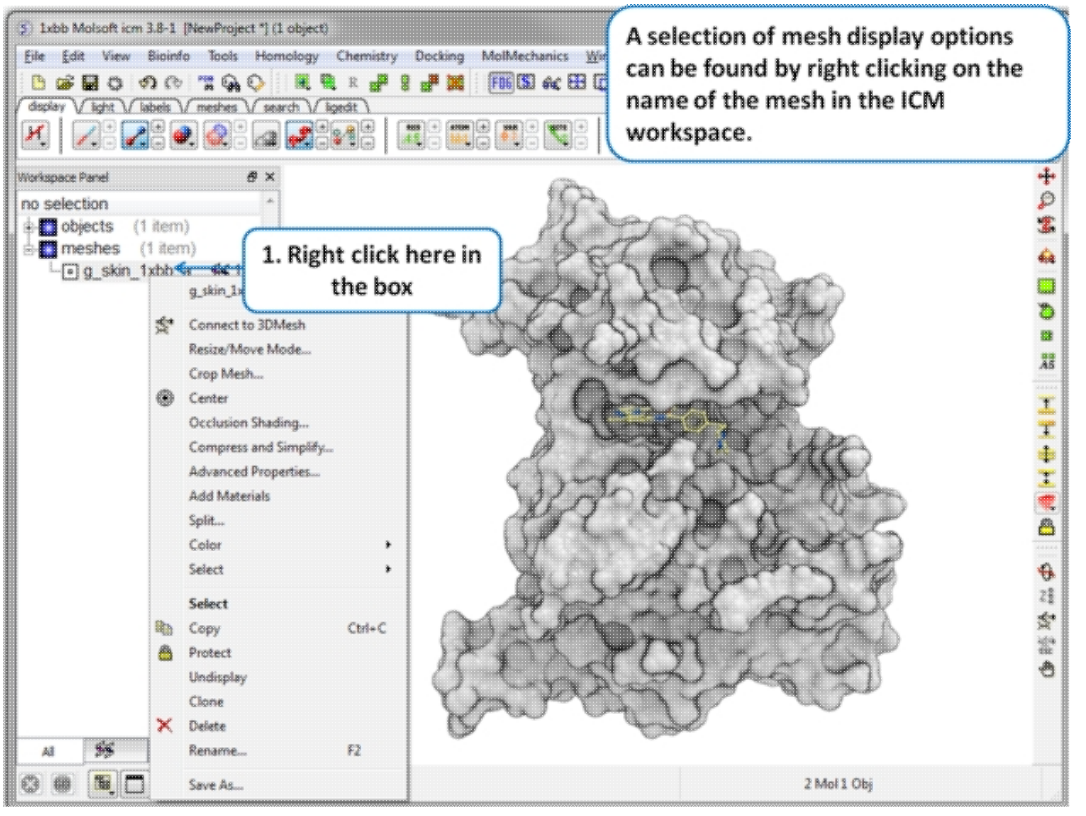
To display or undisplay the surface click in the box in the ICM workspace as shown below:



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

5.2.9 Mesh Options.

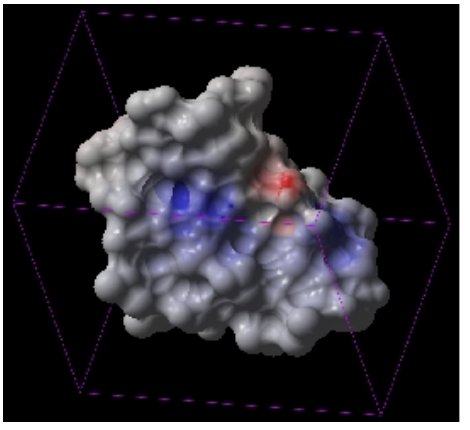
A number of options relating to meshes can be found by right clicking on the mesh in the ICM Workspace. This section describes some of these options.



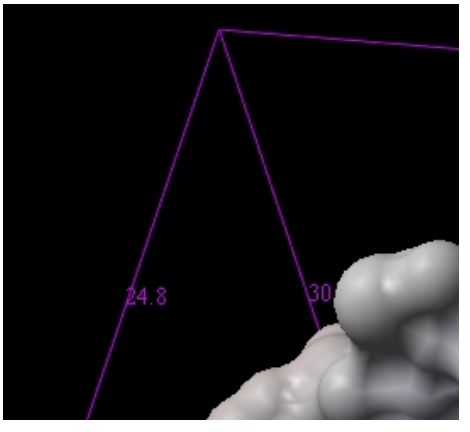
5.2.9.1 Resize Mesh

Once a mesh has been created you can move it and resize it. To do this:

- Locate the mesh in the ICM Workspace and right click on it
- 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.



5.2.9.2 Move Mesh

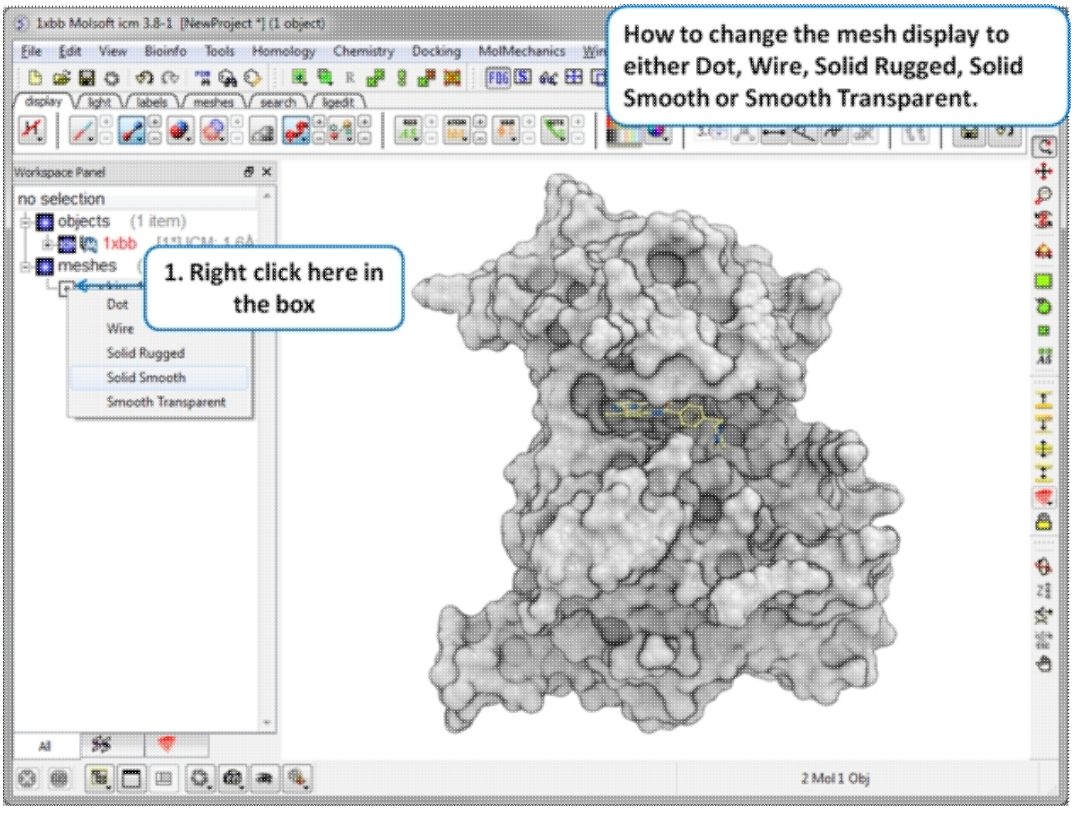
To move a mesh:

- Locate the mesh in the ICM Workspace and right click on it
- Select the **Resize/Move Mode** in the menu.
- Click on the mesh in the graphical display with the **middle** mouse button.

5.2.9.3 Mesh Representation

There are five different display modes:

- Dot
- Wire
- Solid Rugged
- Solid Smooth
- Smooth Transparent.



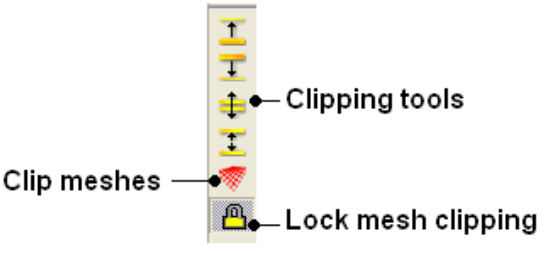
5.2.9.4 Mesh Color and Lighting

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.

5.2.10 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`.

To clip the skin independently of the object as shown in the image above:

- Display object and mesh.
- Click and hold on clip meshes button(red button) and select Reset Clipping to Default and check the option Clipping enabled
- Click on the `front clipping plane button`.
- (Optional) To lock the mesh clipping click on the yellow lock mesh clipping button.

5.2.11 Save Mesh

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

5.2.12 Occlusion Shading

The occulusion 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**. The occlusion shading value can also be changed before generating the mesh in the meshes tab.
- Enter a depth value - default is 0.8. Higher values will generate a more dramatic shading.

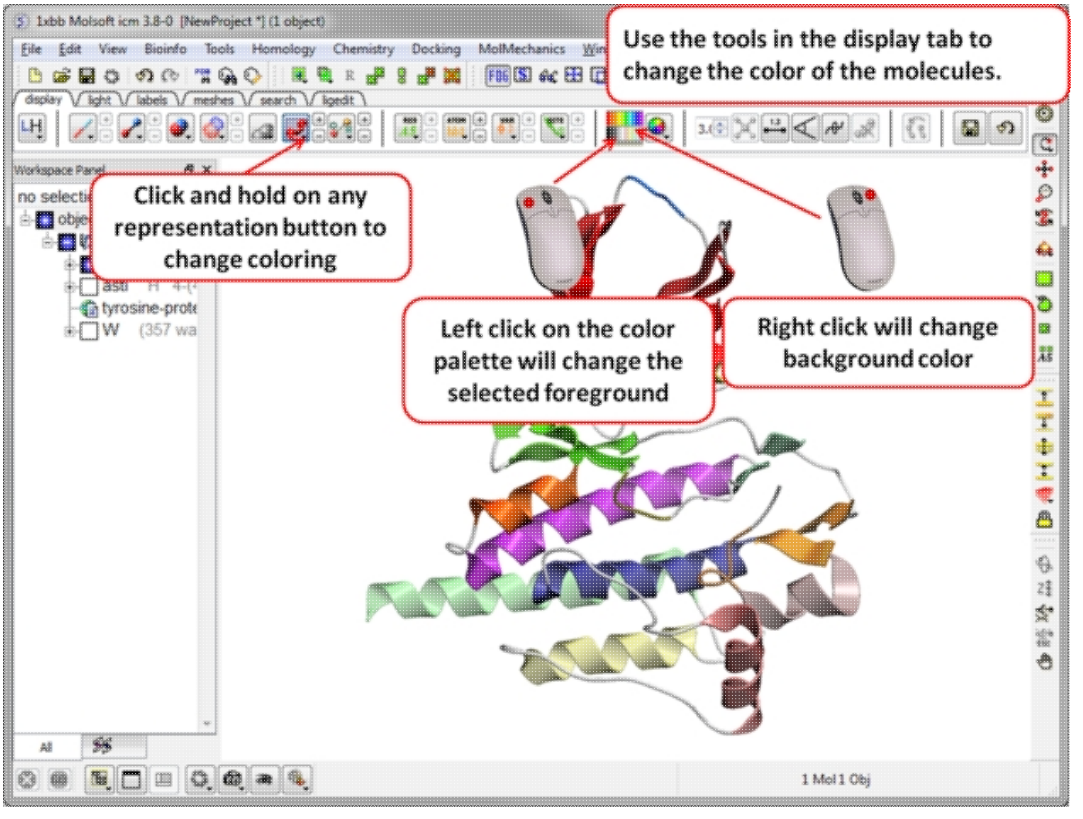
See example `here`.

5.3 Coloring

Available in the following product(s): `ICM-Browser` | `ICM-Browser-Pro` | `ICM-Pro`

To change the coloring of 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`.



5.3.1 Coloring

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

- `Select` the atoms, residues, molecules, or objects you wish to color.
- Click and hold on the structural representation button for the representation you wish to color (e.g. wire, ribbon etc...) in the **Display** tab.
- Select a color by clicking color.

To color by a particular parameter such as atom type, b-factor, secondary structure etc...

- Click and hold on the structural representation button for the representation you wish to color (e.g. wire, ribbon etc...) in the **Display** tab.
- Select ..by-> option

To change the color of everything displayed :

Click on the color palette in the `Display Tab`.

5.3.2 Color Background

To change the color of the 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.

5.3.3 Background Image

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).

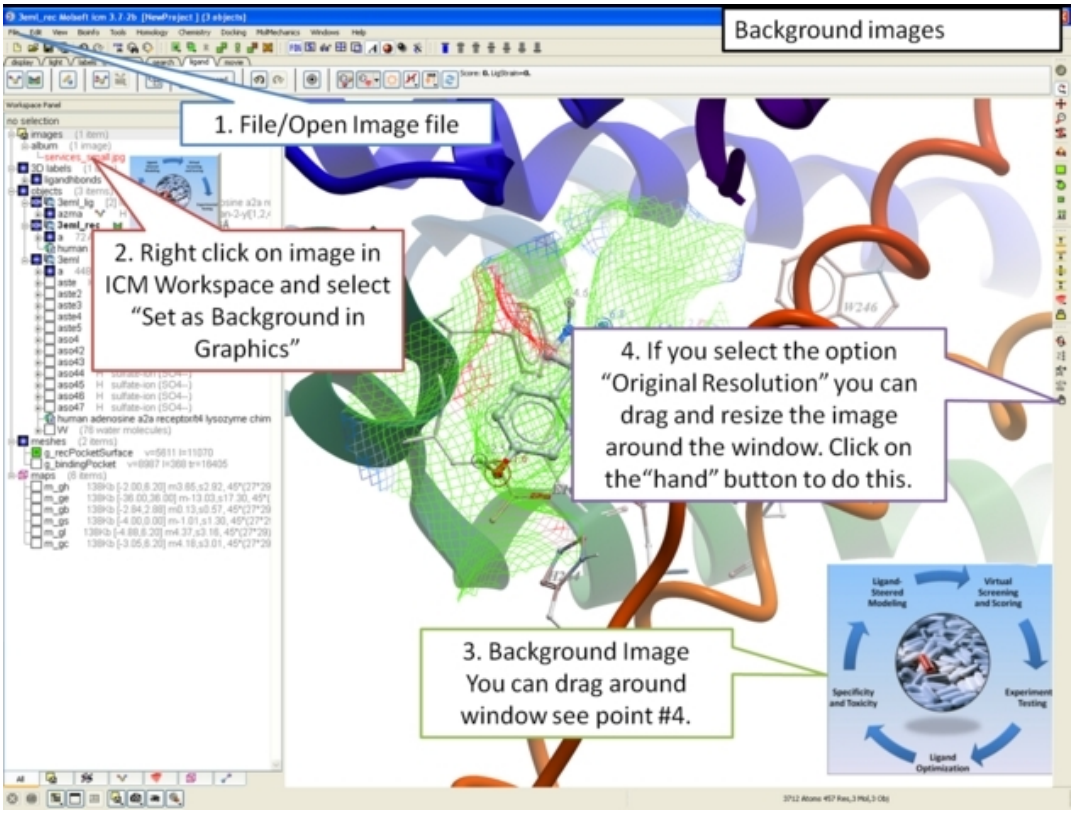
To add a background image from an image file (png or jpeg):

- File/Open Image
- Right click on the image in the ICM Workspace and select "Set as Background in Graphics."
- Choose one of the following: (1) Original Resoution, (2) Original Resolution Centered, or (3) Scale to Fit
- Enter the Scale (%)
- Enter whether you want to keep existing background.

To move and resize a background image: Version 3.7-2b and higher.

- File/Open Image

- Right click on the image in the ICM Workspace and select "Set as Background in Graphics."
- Choose the option **Original Resoution**.
- Click on the drag atom button (looks like a hand).
- Click and drag image.
- Remember to deselect drag atom button.

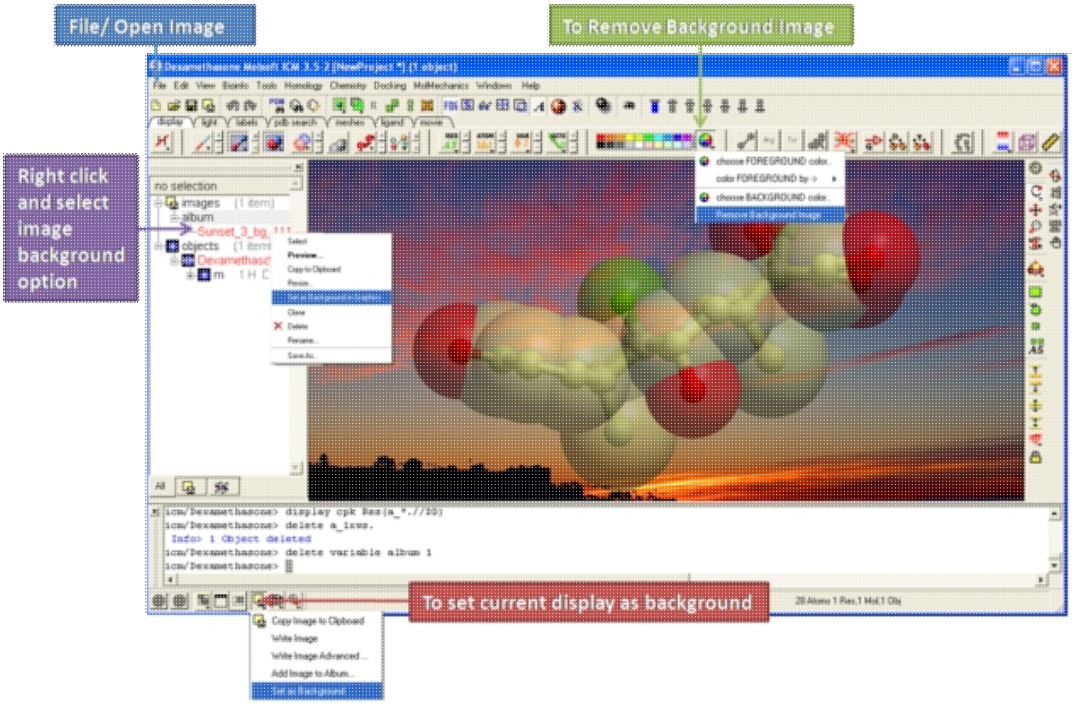


To set current display as background image:

- 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".



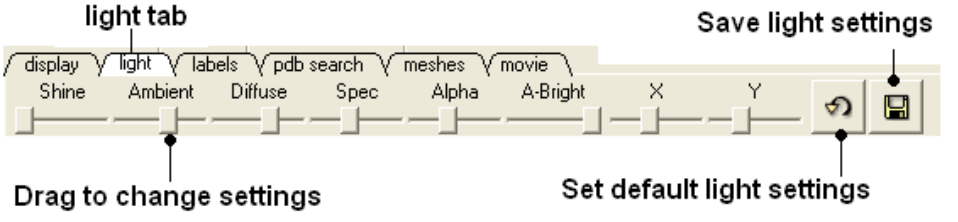
OR

- Right click on the image in the ICM Workspace and select "Set as Background in Graphics."
- Choose the option **Remove From Background**

5.4 Lighting

Available in the following product(s): `ICM-Browser` | `ICM-Browser-Pro` | `ICM-Pro`

These options are in the `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

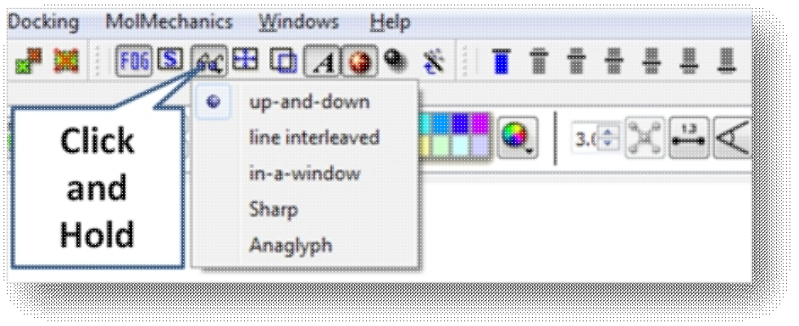
A-Bright - light intensity shinning on grob

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

5.5 3D Stereo

Available in the following product(s): ICM-Browser | ICM-Browser-Pro | ICM-Pro

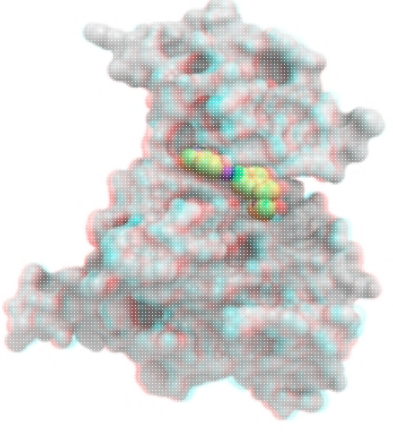
Click and hold on the stereo hardware button (see image below).



There are 5 different options available which are described here http://molsoft.com/man/icm-table.html#GRAPHICS.stereoMode .

1. up-and-down
2. line interleaved
3. in-a-window
4. Sharp
5. Anaglyph

The Anaglyph option is the easiest to used with inexpensive 3D glasses and and without any expensive 3D compatible hardware or monitors. The 3D effect is better with a lighter background.



5.6 Labeling and Annotation

Available in the following product(s): ICM-Browser | ICM-Browser-Pro | ICM-Pro

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".

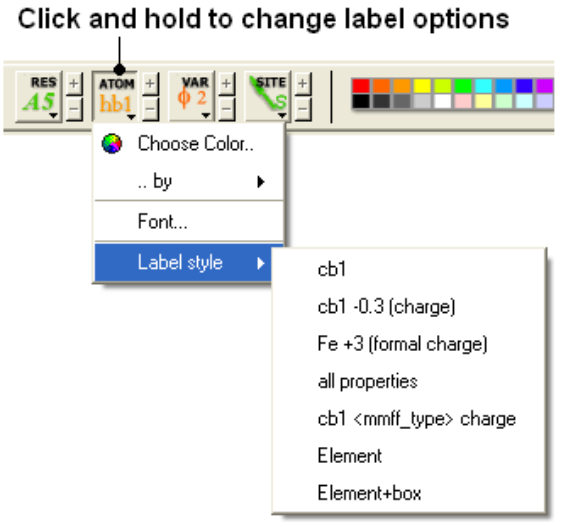
5.6.1 Labeling

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.

5.6.2 Labeling Atoms

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

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



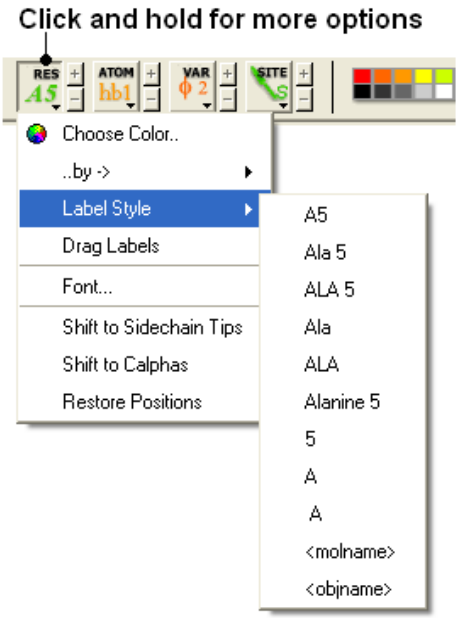
To change the level of label detail:

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

5.6.3 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.



To change the level of label detail:

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

5.6.4 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.

- 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.

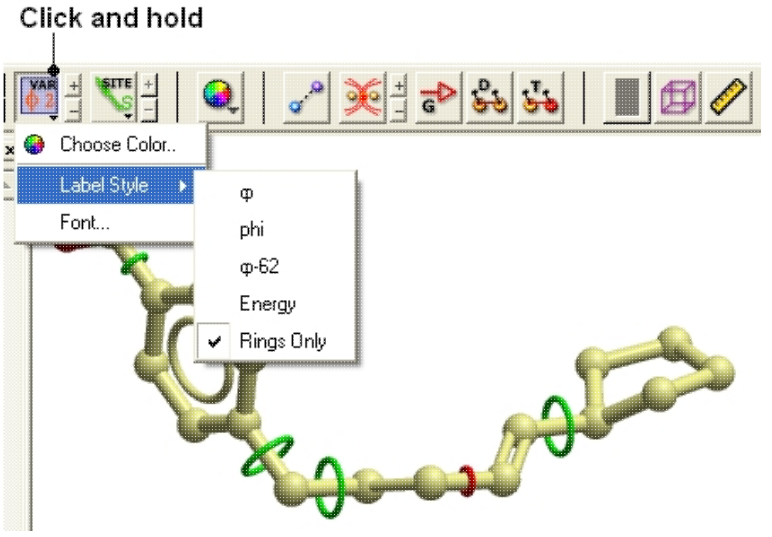
The +/- buttons on the side of the Residue and Atom buttons will shift the label. There are also other **residue label move** options available when you click and hold the residue label button. These options include **Shift to Sidechain Tips**, **Shift to Calphas**, and **Restore Positions**

5.6.5 Label Variables

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

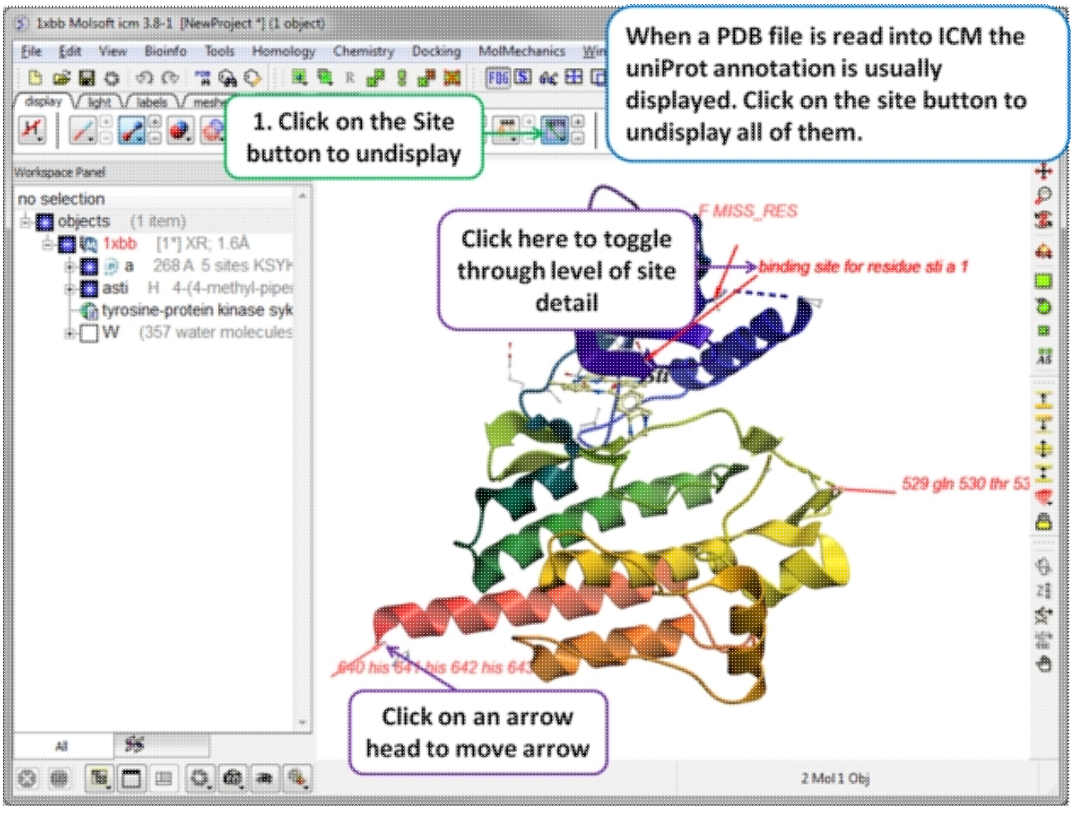
- Convert the molecle to an `ICM object`.
- Select the atoms for which you would like to display the variables (see `display structure` or `selection toolbar`).
- Click on the **toggle variable label** button shown above located in the **display** tab.
- Change the font size by using the +/- buttons.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

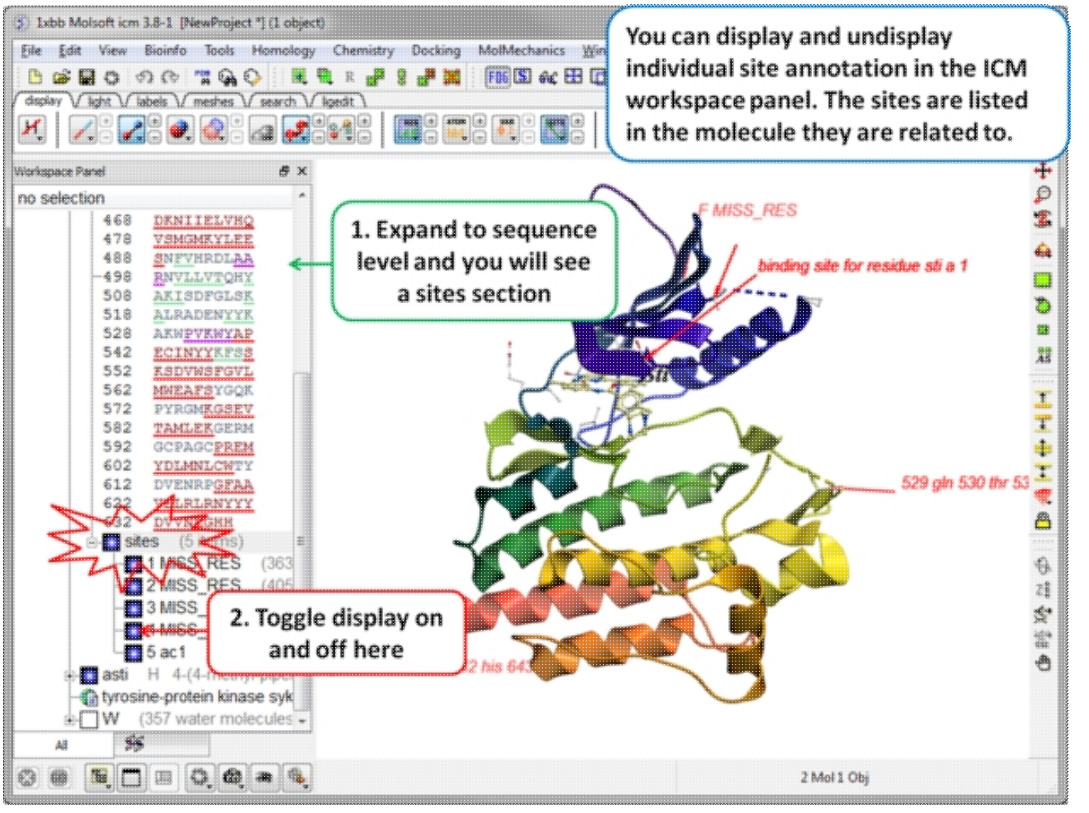


Rings of varying diameter and color are superimiposed on rotatable bonds. Green rings with large diameter are considered less constrained than rings with small green rings. Red rings are highly constrained and non-rotatable. When the **Label Style/Energy** option is selected the first number displayed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

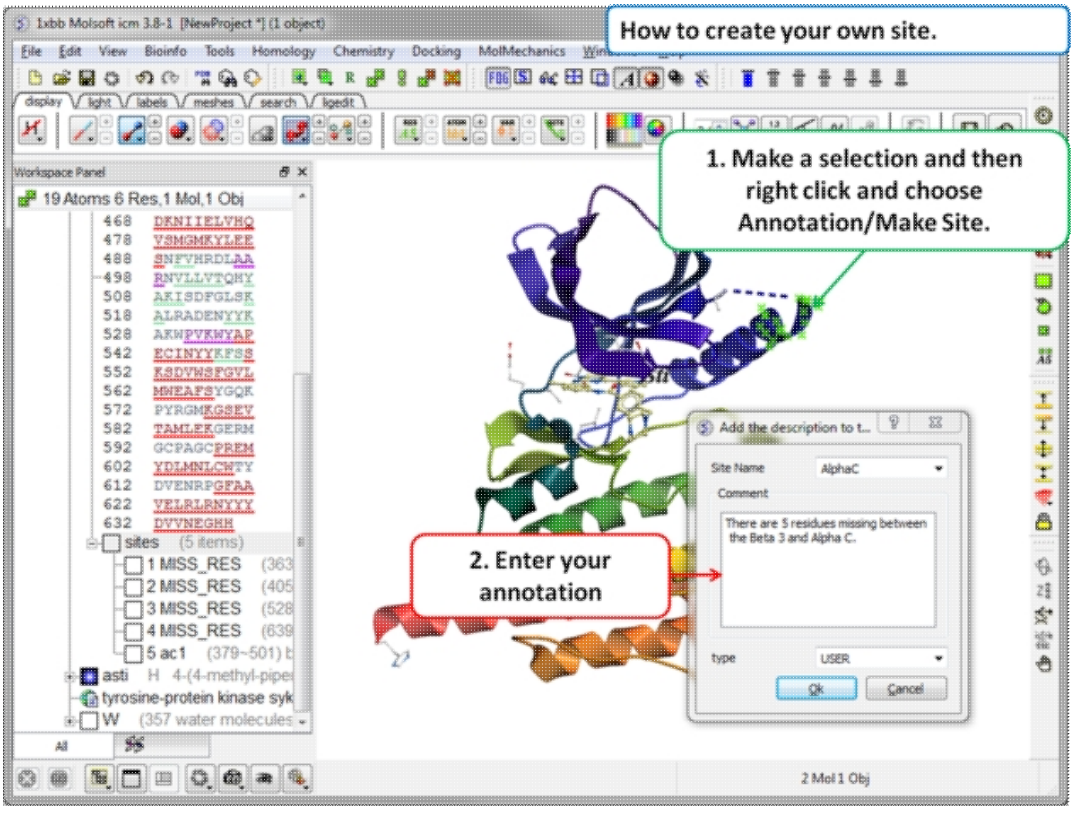
5.6.6 Sites and Annotation



When a PDB file is read into ICM the sequence functional/mutation sites listed in Uniprot are automatically displayed. To undisplay all displayed sites click on the **Sites** button in the `display tab`. Click in the bottom left hand corner of the annotated site to change the level of detail or click on an arrow head to move the location.



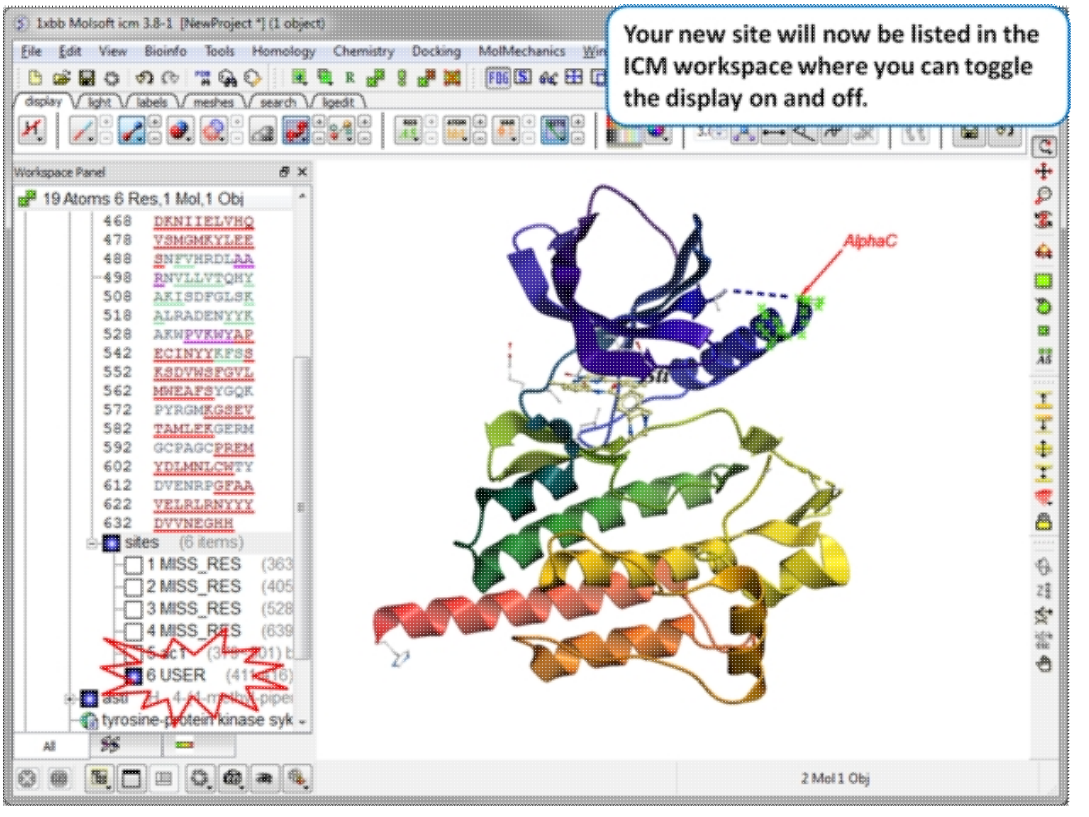
Individual sites can be displayed or undisplayed in the ICM workspace.



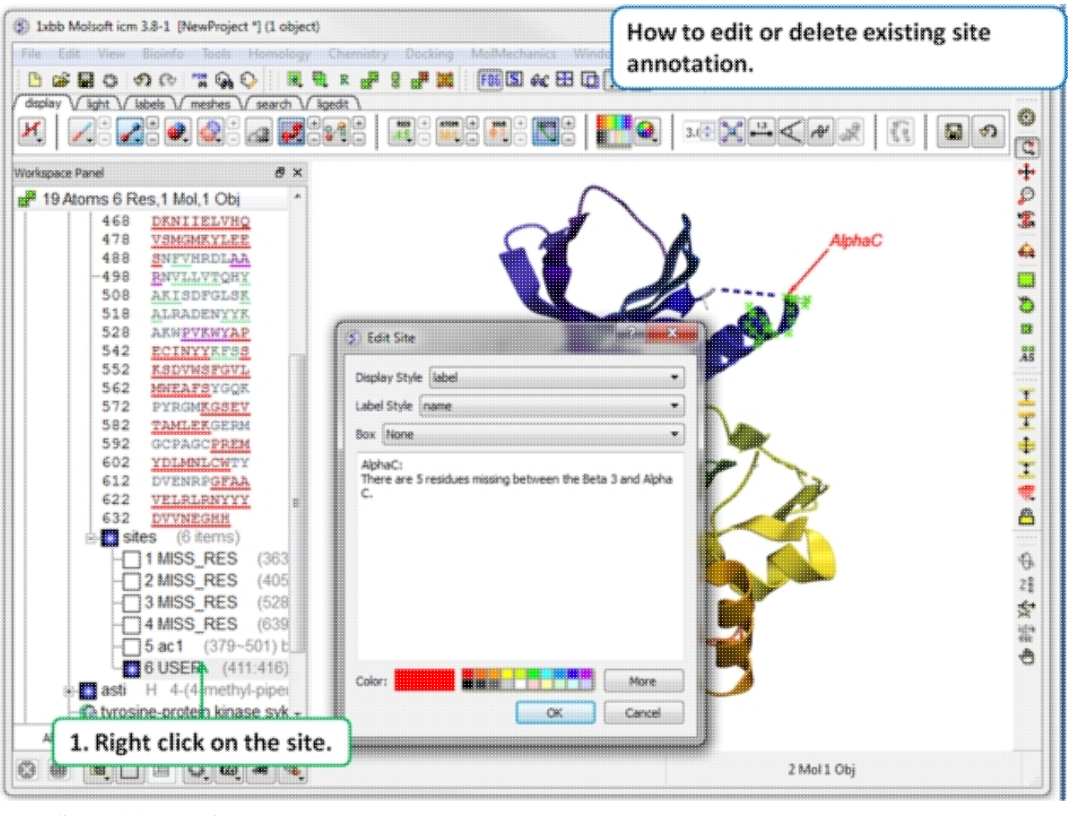
To create your own annotated site:

- `Select` the region you wish to annotate as a Site.
- Right click on the selection.

- Choose the option Annotate/Make Site
- Enter the annotation into the text box and select ok



Your new site will now be listed in the ICM Workspace.



To edit or delete a site:

- Right click on the site in the ICM workspace.

5.6.7 Changing Label Colors

To change the color of any label:

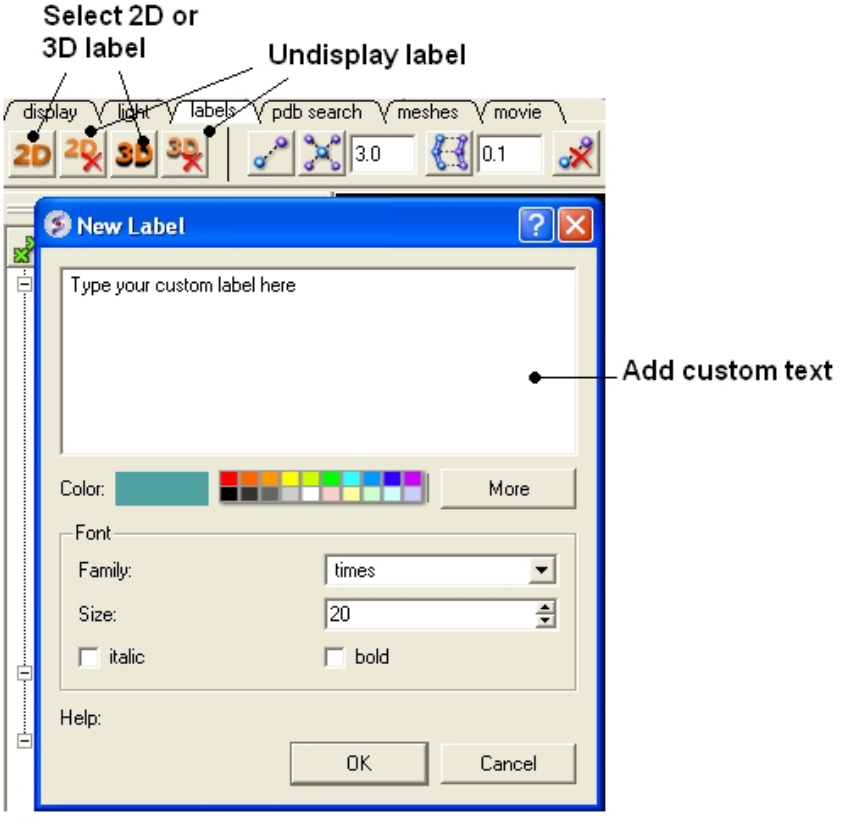
- Click and hold down the required label button and a menu as shown below will be displayed.

- Select **color.**

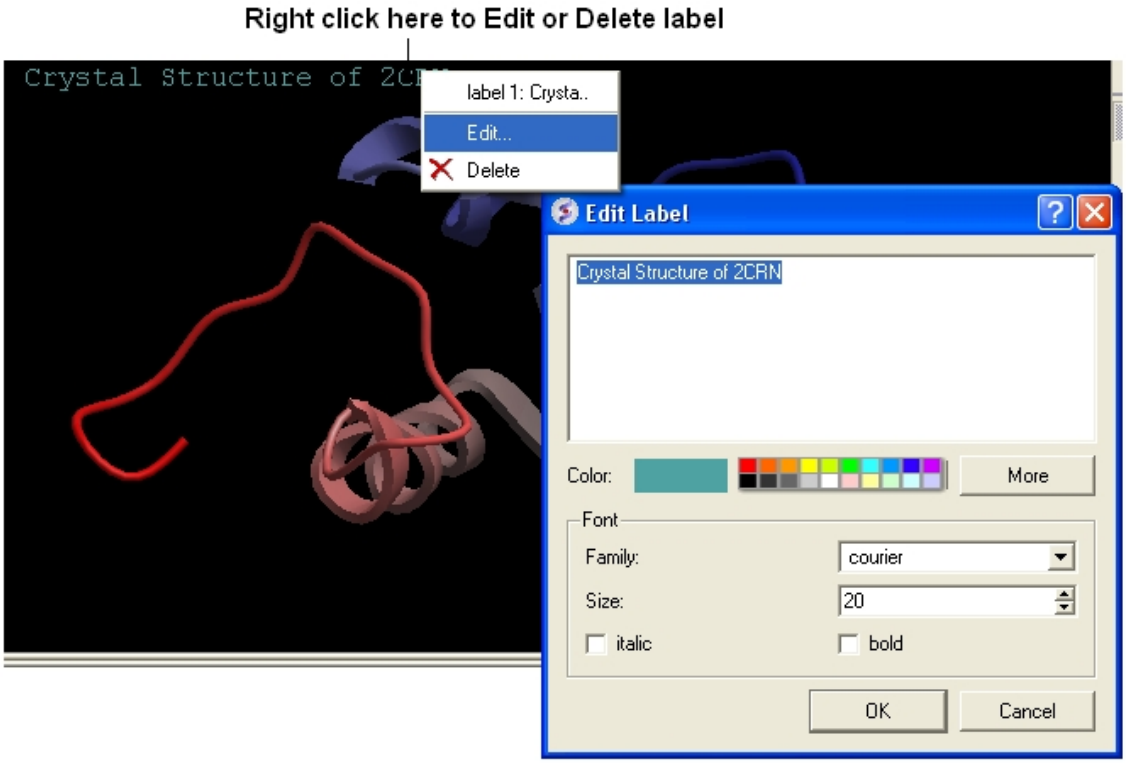
5.6.8 Customized Label 2D or 3D

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.



5.6.9 Undisplay Customized Label

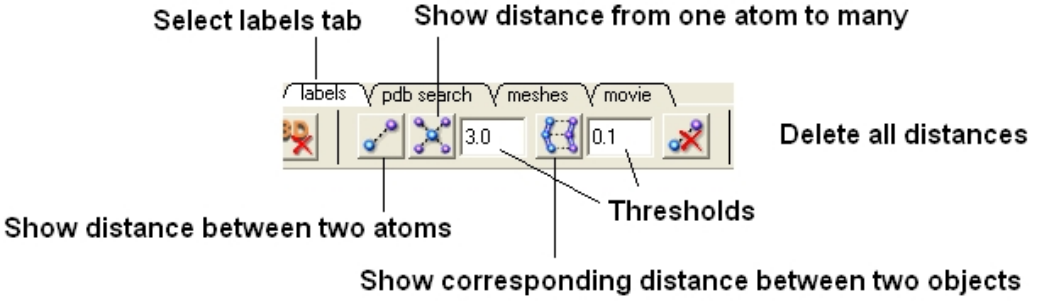
Undisplay Residue, Atom, and Variable Label Any label that is displayed can be undisplayed by selecting the region of the molecule related to the label and clicking on the corresponding label button in the labels tab. For example if you wish to undisplay an atom label - click the atom label button. If a label is displayed the coresponding 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 onthe 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.**

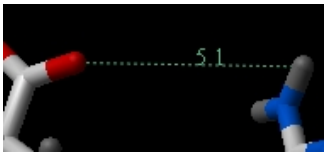
5.6.10 Labeling Distances

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:

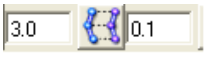
- Click on the labels tab (previously called advanced tab).
- Select the atoms between which you would like to find the distance. (See `selection toolbar`)
- Click on the 'Show Distances Between Two Atoms' Button
- The distance will be displayed in angstroms, in green.



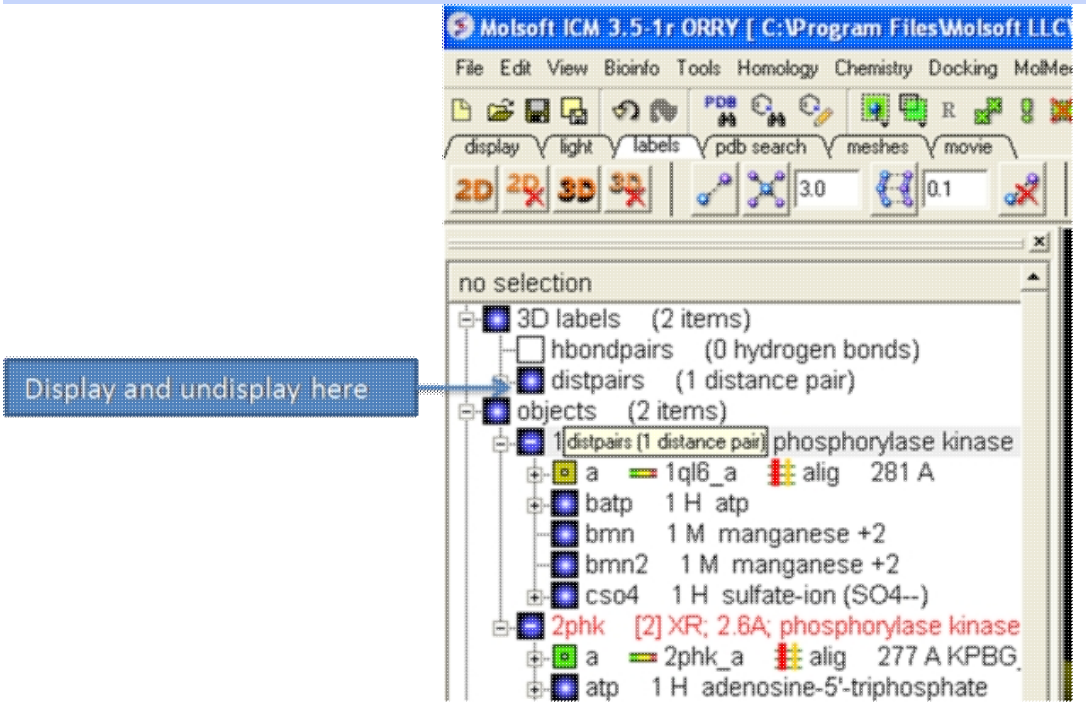
To find the distance from one atom to many:

- 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.



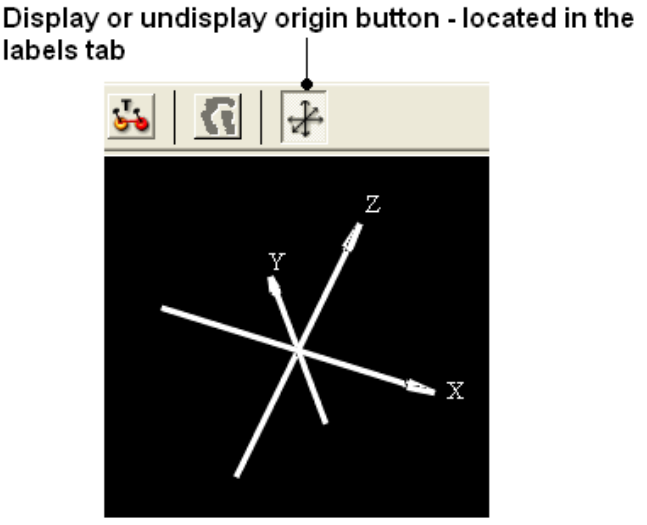
To change the color of the distance label

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

5.6.11 (Un)display Origin

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

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



5.6.12 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.

5.6.13 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.

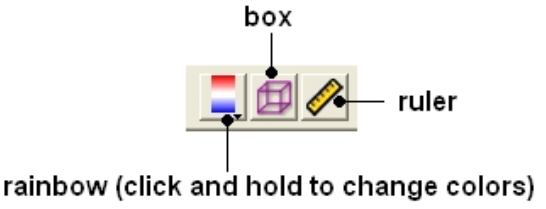
5.6.14 Display Clash

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.

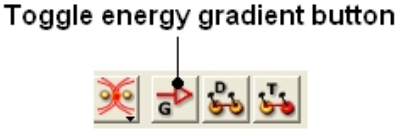
5.6.15 Display Rainbow, Box, Ruler

To (un)display a rainbow scale, box or ruler use the buttons shown below located in the `Labels Tab`.



5.6.16 Display Gradient

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



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

5.7 Display Distances and Angles

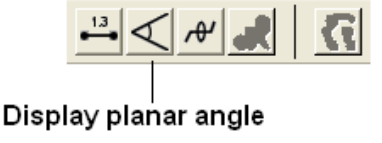
Available in the following product(s): `ICM-Browser` | `ICM-Browser-Pro` | `ICM-Pro`

5.7.1 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**.

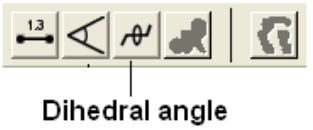
5.7.2 Display Planar Angle

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



5.7.3 Display Dihedral Angle

- Select the **display** tab.
- `Select` four atoms.
- Select the button shown below.



5.7.4 Delete Label

To delete distance or angle labels

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

5.8 Graphics Effects

Available in the following product(s): `ICM-Browser` | `ICM-Browser-Pro` | `ICM-Pro`

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

5.8.1 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.

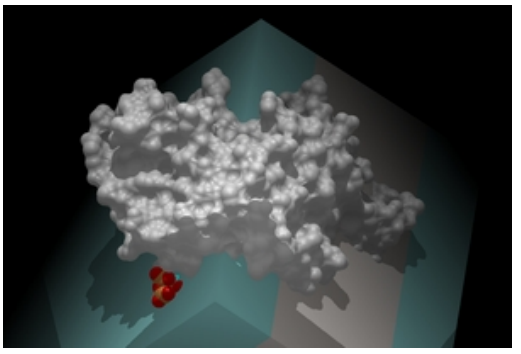
- View/Fog

5.8.2 Shadows

- View/Shadows

OR

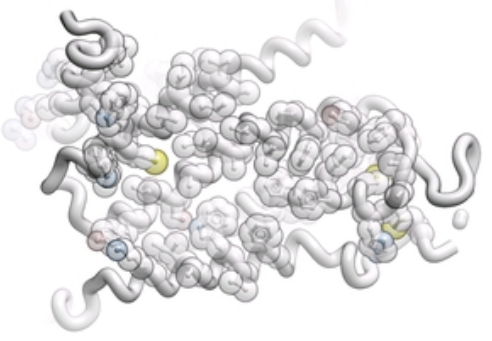
select the shadow button shown below.



5.8.3 Sketch Accents

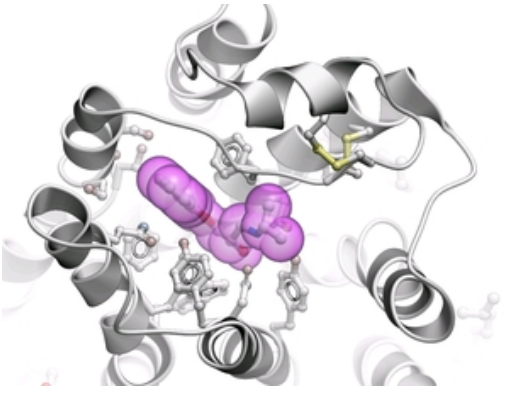
To make images as shown below use:

- View/Sketch Accents



5.8.4 Elegant Ribbon & Ligand Sketch

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

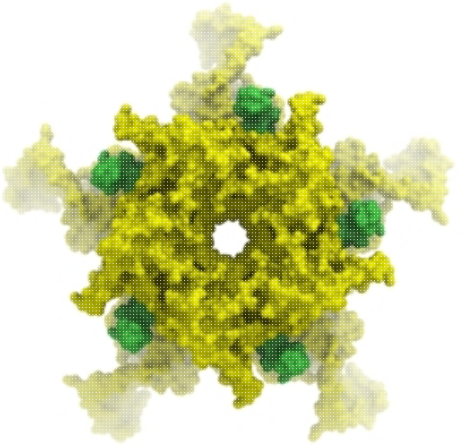


5.8.5 Occlusion Shading

Occlusion shading is for surfaces and meshes to give a perception of depth.

To add occlusion shading:

- Right click on the mesh in the ICM Workspace and select Occlusion Shading. The occlusion shading value can also be changed before generating the mesh in the meshes tab.
- Enter a depth value - default is 0.8. Higher values will generate a more dramatic shading.



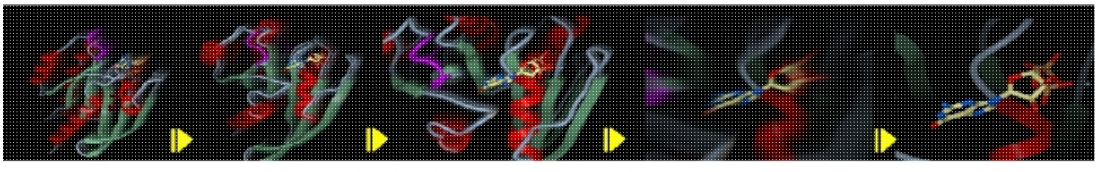
5.8.6 Perspective

Toggle perspective Ctrl_P this will add perspective to your structure, enhancing depth in the graphical display.

- View/Perspective

5.8.7 Animate View

Learn how to build fully interactive and interruptable animations.

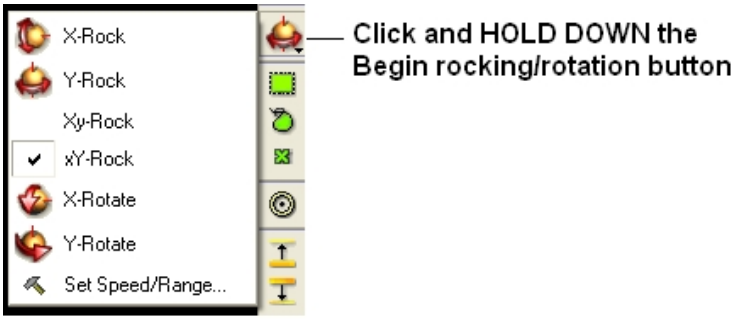


Smooth Animated Transitions

5.8.7.1 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.

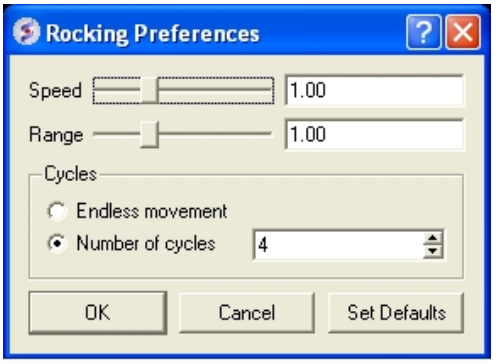


NOTE: Default rocking representation can be changed in the `File/Preferences/Gui` menu.

5.8.7.2 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 defaut values can be changed in `File/Preferences/Gui`.

NOTE: Default rocking speed can be changed in the `File/Preferences/Gui` menu.

5.8.7.3 Interrupt Animation

An ICM Animation or Transition is fully interactive and is interrupted by a single click of the mouse.

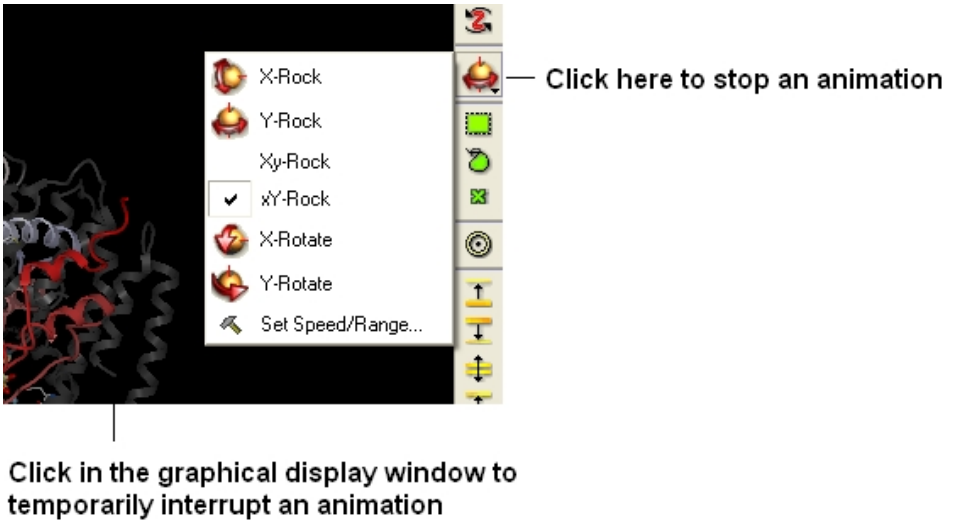
To stop or change an animation or transition:

- 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.



5.8.7.4 Saving an Animation

An animation can be saved in an ICM project:

`File/Save Project`

Or

as a `slide`.

5.9 Graphics Shortcuts

Available in the following product(s): `ICM-Browser` | `ICM-Browser-Pro` | `ICM-Pro`

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

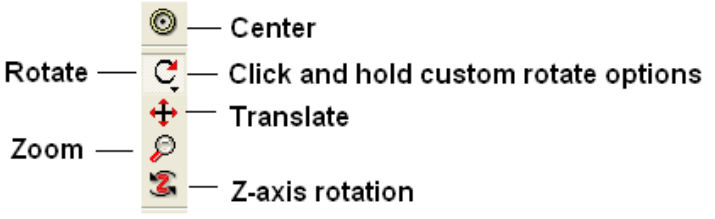
Many useful graphics tips are summarized `here`.

NOTE: Key mouse controls are summarized in the command line manual here
`http://www.molsoft.com/man/graphics-controls.html`

5.10 Molecule Move Buttons

Available in the following product(s): ICM-Browser | ICM-Browser-Pro | ICM-Pro

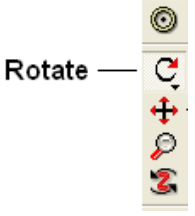
To move your structure it must first be displayed in the graphics window (for instructions on how to display a structure see the Display Tab). All of the following options are displayed in the Move Tools toolbar (shown below).



5.10.1 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:

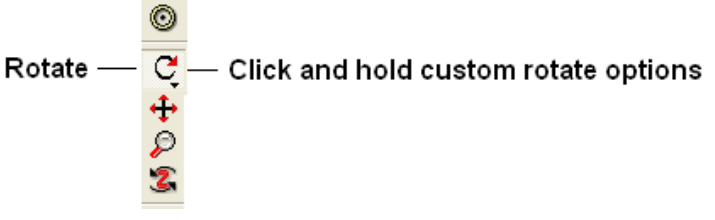
- Click on the **rotation** icon on the toolbar.



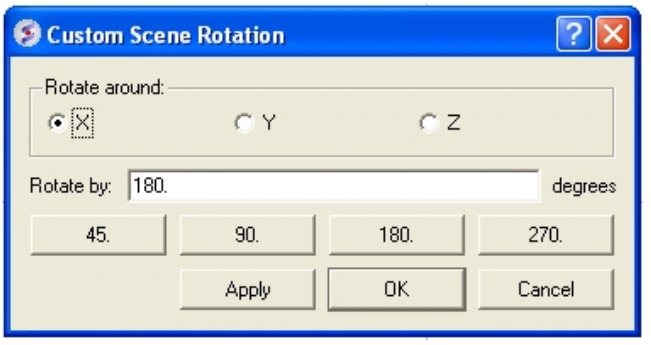
- Click and drag on your structure in the display window until it is in the desired position.

5.10.2 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.

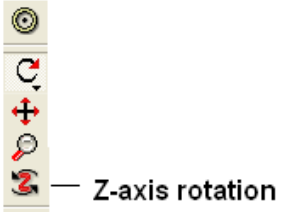


To continuously rotate the picture:

- 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.

5.10.3 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.

5.10.4 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.

5.10.5 Center

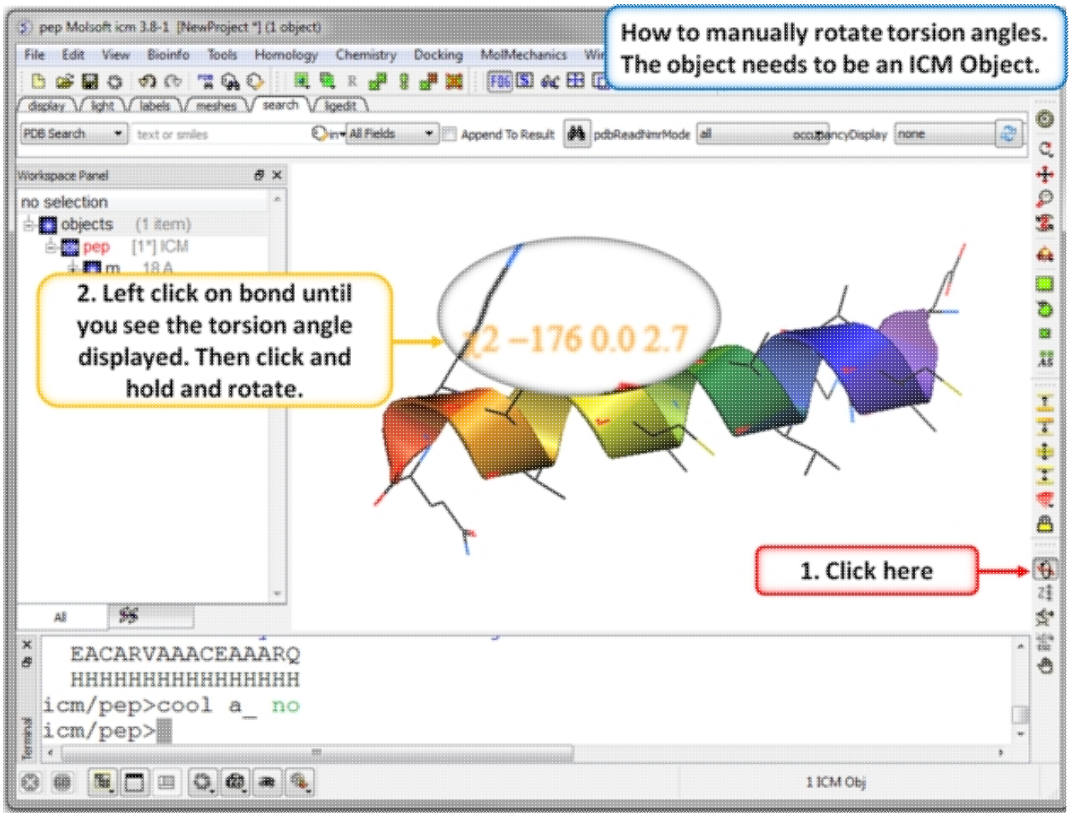
To restore your picture to the center of the graphical display window or to center on a selection:

- 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.

5.10.6 Torsion Angles

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

- `Convert` your pdb structure into an ICM object.
- Click on the **change torsion angles** icon on the toolbar (see image below).
- Click on the bond until you see the torsion angle displayed in yellow (see image below). Click and hold on the bond around which you wish to rotate a residue. The changing torsion angle will be displayed in orange.



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

To alter torsions by entering specific angle values:

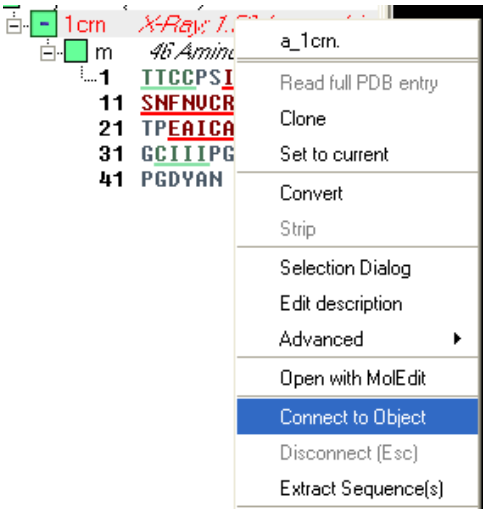
- You can edit torsions by specifically defining the exact angle as described here.

5.10.7 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.



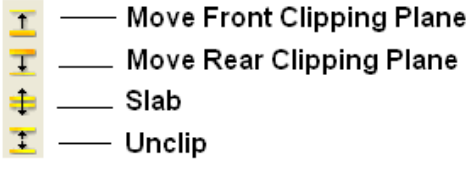
- The object is now controlled separately from the rest of your objects by your mouse.
- Disconnect your object by once again right clicking on the name of the object in the ICM Workspace and selecting disconnect in the drop down menu or **Press the ESCAPE key**.

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

Note: use the Escape button to disconnect

5.11 Clipping Tools

Available in the following product(s): `ICM-Browser` | `ICM-Browser-Pro` | `ICM-Pro`



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.

5.11.1 Mesh Clipping

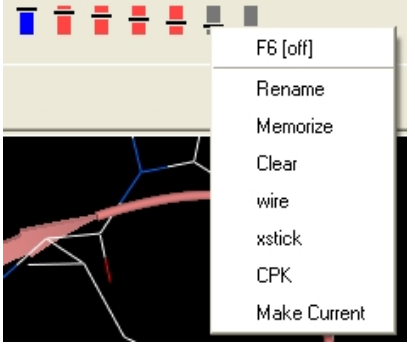
Clipping tools can be used to adjust the frames of the mesh independently of other objects. This is described `here`.

5.12 Graphic Layers

> Available in the following product(s): `ICM-Browser` | `ICM-Browser-Pro` | `ICM-Pro`

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.

5.13 High Quality Publication Images

> Available in the following product(s): `ICM-Browser` | `ICM-Browser-Pro` | `ICM-Pro`

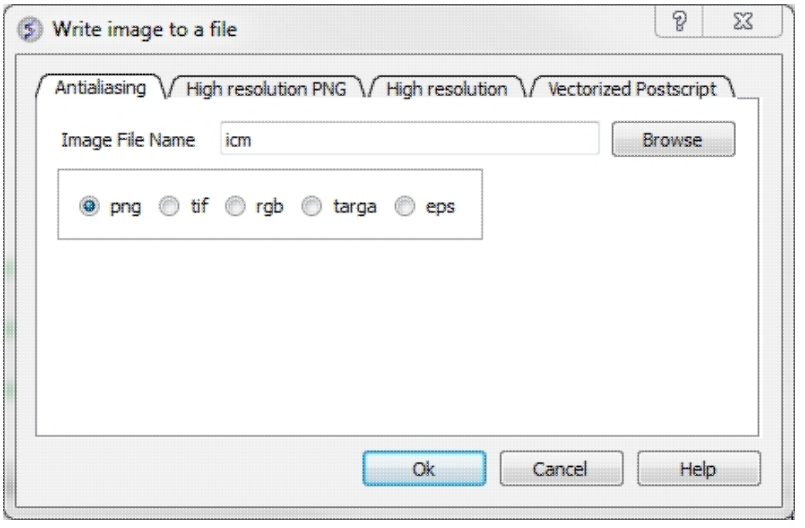
5.13.1 High Quality Image

To make high quality publication images:

The first step is to improve the quality of the image using the **High Quality Image** and **Antialias** buttons shown below.

To save and write an image:

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

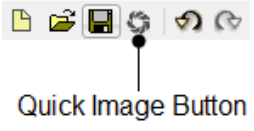


- Enter the name for the picture in the **File name** data entry box.
- Select which file format you would like to save the picture in by clicking in the circular selection button next to the file types. The options are .tif; .png; .rgb; .targa .eps.
- To specify which resolution you wish the picture 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.

5.13.2 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.

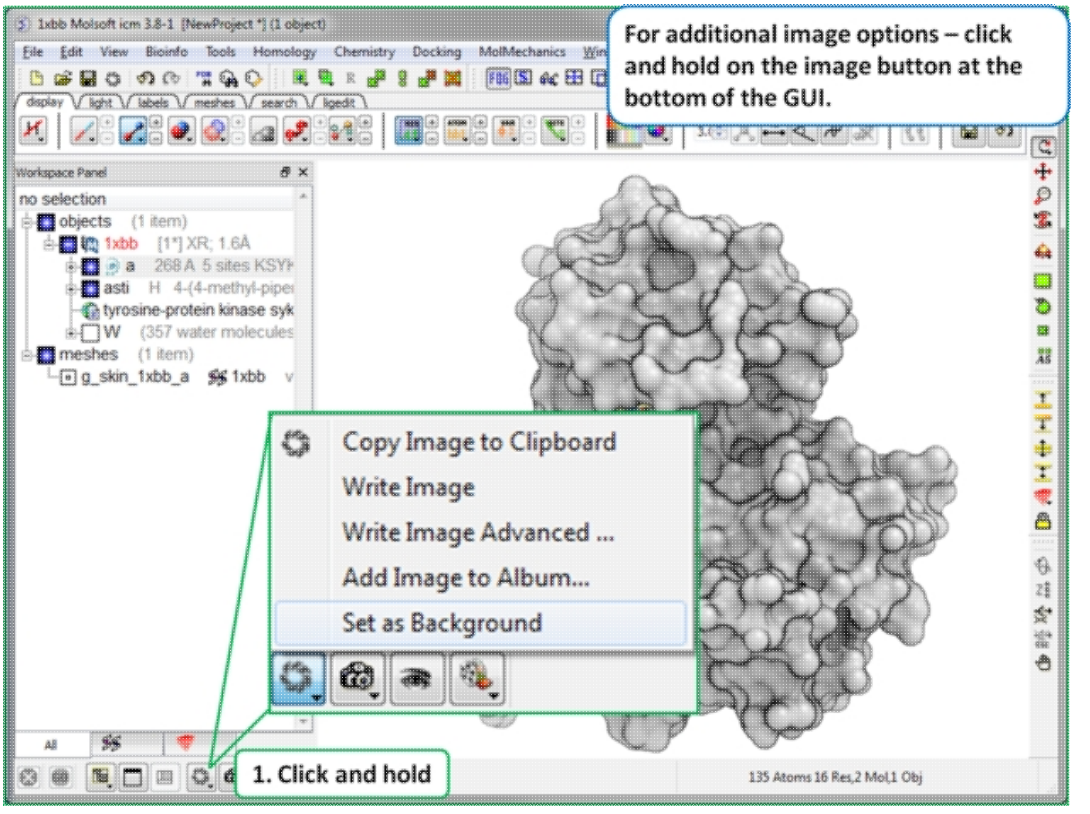
This option is also available via a button as shown below:



5.13.3 Image Options

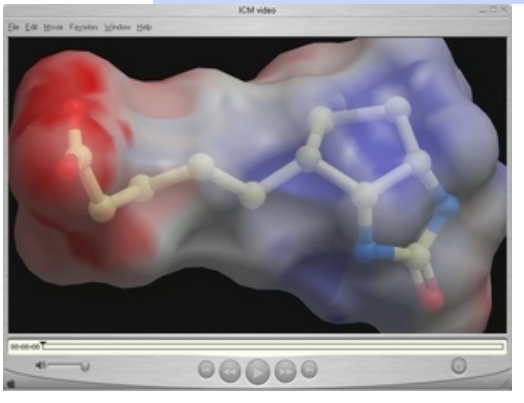
Click and hold on the **image** button at the bottom of the GUI to:

- Copy image to clipboard (single click on the button also does this).
- Resize image (Write Image Advanced)
- Transparent Background Write Image Advanced)
- Store an image in ICM (Write Image Advanced)
- If you are making an `ICM document` you may want to store images inside ICM (Add Image to Album).



5.14 Movie Making

Available in the following product(s): `ICM-Browser-Pro` | `ICM-Pro`



A movie is an excellent way of communicating 3D structural data. The resulting movie can easily be transfered into other applications such as Microsoft Powerpoint.

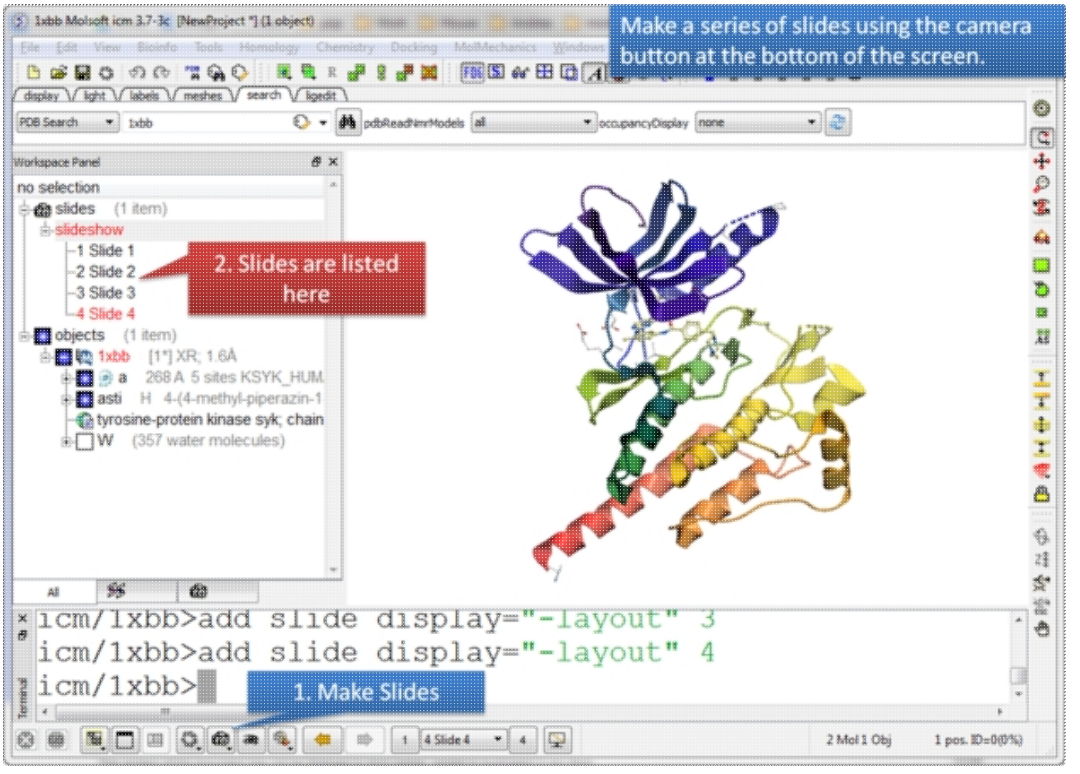
There are two ways to make a movie:

- Make a movie directly from a series of `slides`.
- Make a movie directly from `screenshots`.

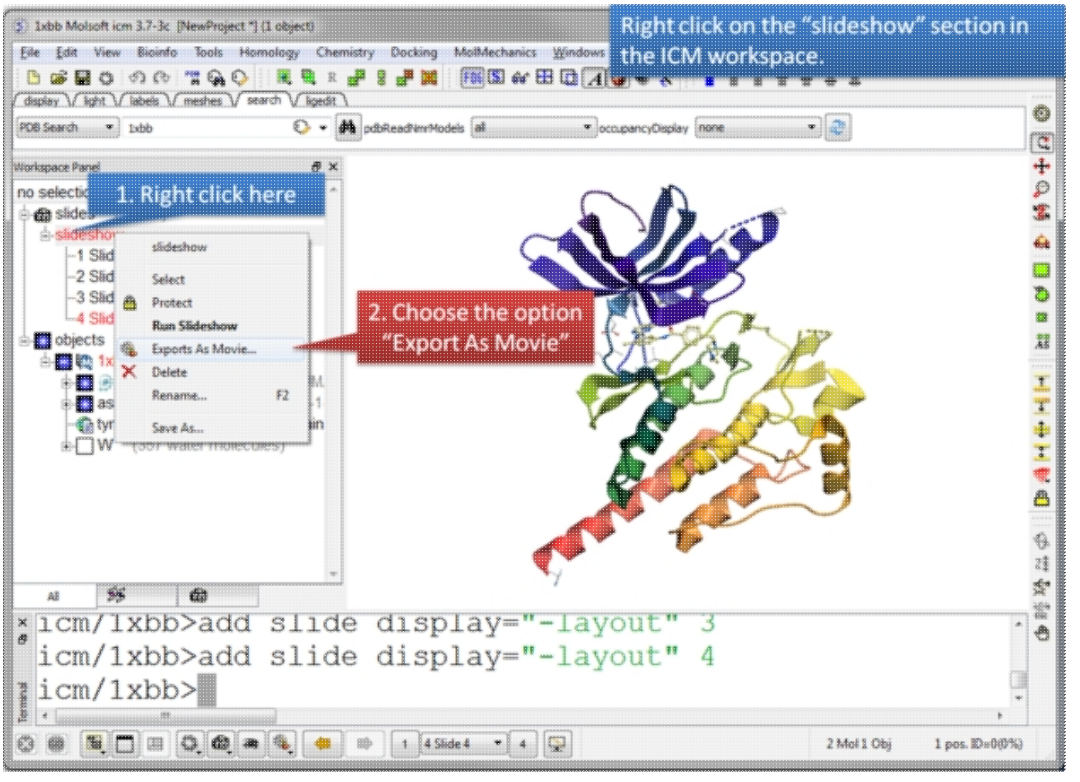
An alternative to a movie is a fully interactive 3D document embedded in Windows PowerPoint or a Web Browser, this can be undertaken using slides and the `ActiveICM` plugin.

5.14.1 Making a Movie from a Set of Slides

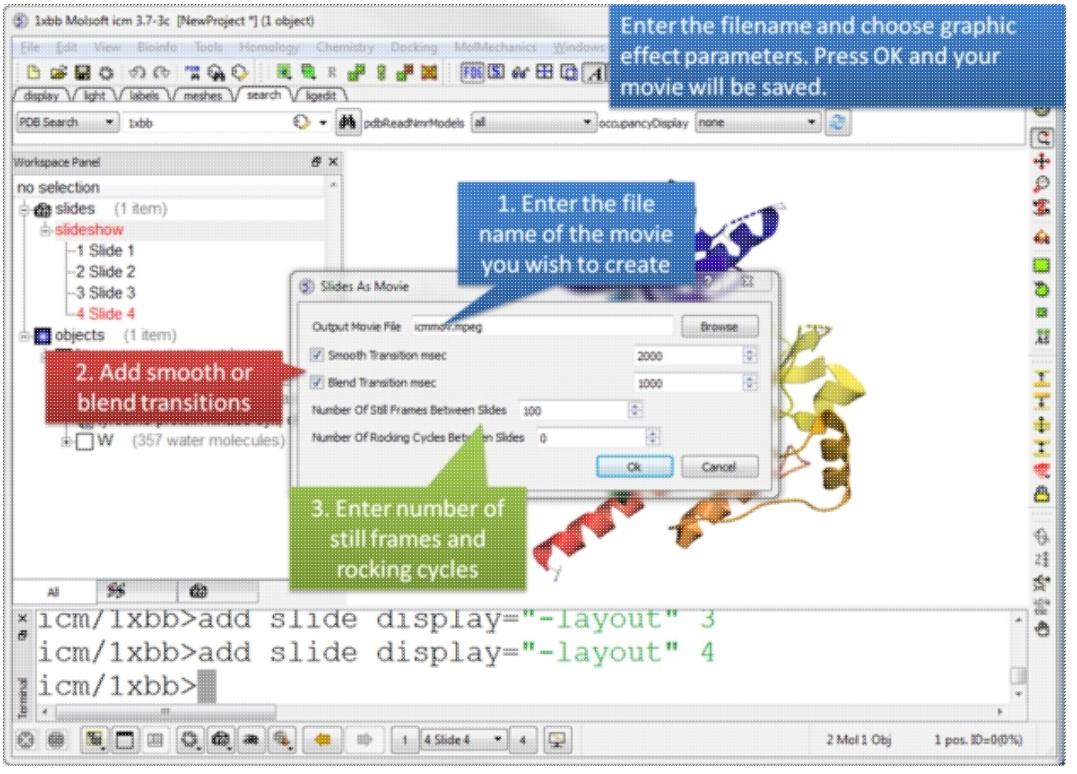
To make a movie from a set of slides:



Make a series of `slides` using the camera button.

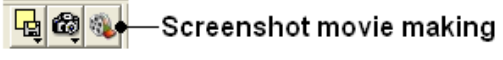


Right click on the slideshow in the ICM Workspace and choose the option "Export as Movie".



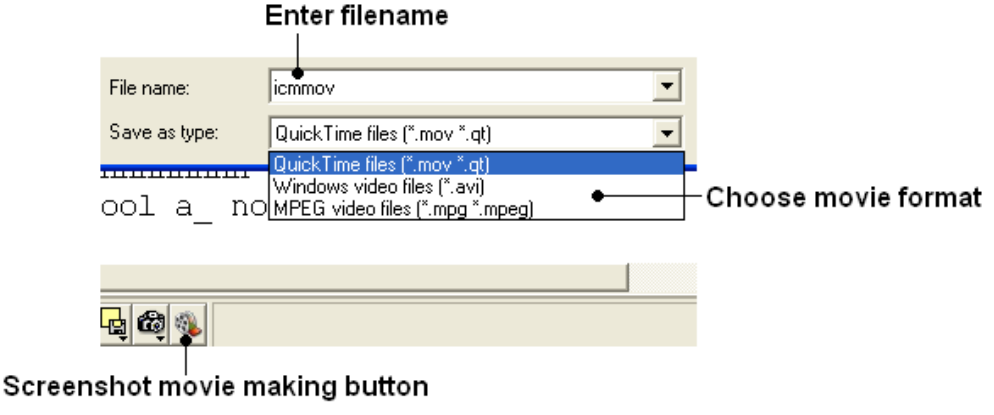
Enter the filename for your movie and set the movie effect parameters. Press OK and the movie will be written to a file.

5.14.2 Screenshot Movie



To make a **Screen-grabbing Movie** follow these steps:

- Resize the graphical display to the screen size/resolution you need. You may also want to select the `high quality` image button and antialiasing to improve the quality of the movie or add visual effects such as `shadows`.
- To begin making a movie click on the movie making button at the bottom of the graphical user interface (as shown below).
- Enter a file name for your movie and select the movie format (.mov, .avi, mpeg).



NOTE: If you want to make a movie to include in a PowerPoint presentation you need to save the movie in AVI format.

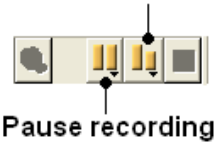
- To begin recording the screenshot movie click on the red **Record video** button. Anything displayed in the graphical display will be recorded, for example you can record `animations and transitions`. Specifying the `number of cycles` in the animation (rocking, rotation) is an ideal tool for screen-shot movie making. If you have a fast computer you can use **Realtime screen grabbing** which can be selected by clicking and holding the **Record video** button. The real time option can also be set in `File/Preferences/Gui` menu.

Record video button

- The length of the movie in minutes, seconds and milliseconds is displayed in the top right hand corner of the graphical display.

- You can pause the movie and fade out by clicking on the button shown below. The number of frames for the fading out option can be controled using the option in `File/Preferences/Gui`

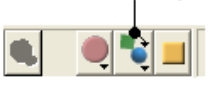
Pause and fade out



Pause recording

- You can record a smooth transition from a previous frame by clicking on the button shown below.

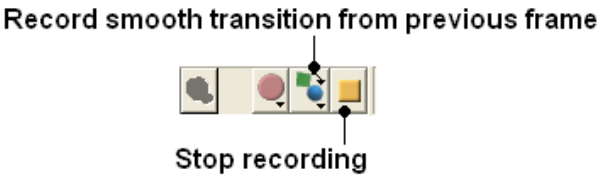
Smooth transition from previous frame



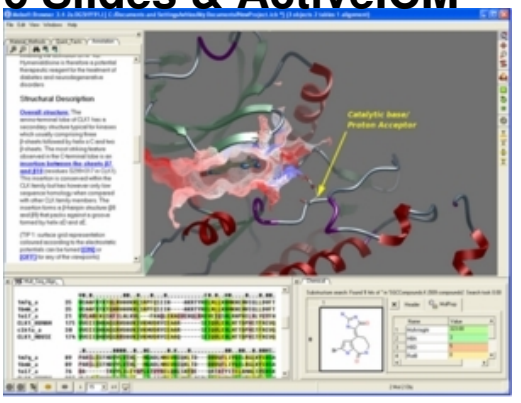
NOTE: Anything you do in the graphical display will be recorded in the movie. For example you can change representations, lighting, add new molecules etc. This can be achieved in a more controled manner using the **pause** and **record smooth transition** button.

- Once you have paused the recording the viewpoint and representation of the molecules can be changed and a smooth transition from the previous frame can be generated by selecting the **Record smooth transition from previous frame** button.

- To stop recording a video press the button shown below.


Record smooth transition from previous frame
Stop recording

6 Slides & ActiveICM



In this chapter you will find a description of the tools available to create files (.icb) containing fully-interactive three-dimensional (3D) molecules and two-dimensional (2D) data. These files can contain multiple interactive views and animations of molecular structures and objects in conjunction with related hyperlinked text, chemical, biological sequence, alignment and data views. The files are small and easily transferable and downloadable. The files can be used for Molecular Presentation and Documents inside the ICM browser or displayed on the web and in PowerPoint using the `ActiveICM` plugin. For examples of ICM Molecular Documents please see MolSoft's ActiveICM product page at www.molsoft.com/activeicm.html

Chapter Contents:

6.1 Making Slides

Available in the following product(s): `ICM-Browser` | `ICM-Browser-Pro` | `ICM-Pro`

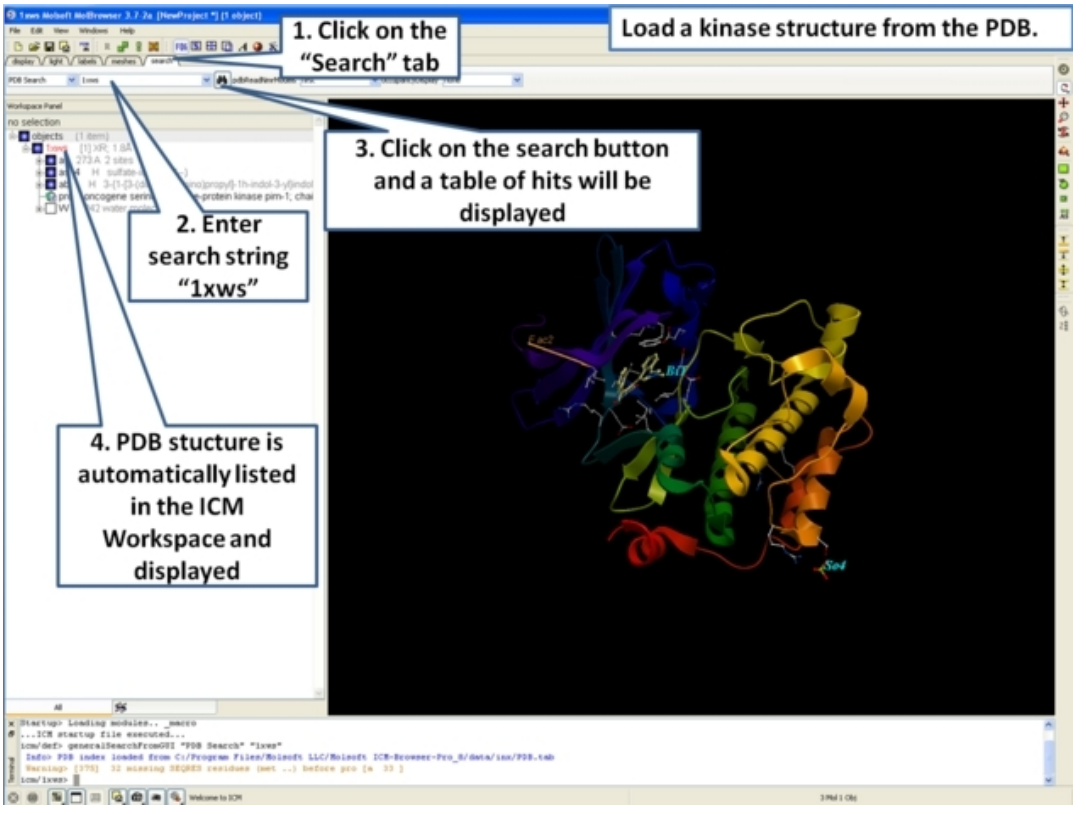
A slide enables you you to store a large number of different 3D visualization along with text and window layout.The following information can be stored in a slide:

- Viewpoint (e.g. rotation, translation, zoom, lighting and depth effects)
- A set of atom-specific graphical representations such as surfaces, which can be represented as smooth, transparent or wireframe, ball-and-stick models, CPK (space-filling) models.
- A set of atom, residue or distance labels on any of the atomic items
- A set of arbitrary 3D textual annotations assigned to a point in space
- A set of arbitrary 2D annotations assigned to specific 2D coordinates on a screen
- Parameters of the parametric `animation`
- Window layout - for when the slides are viewed in the browser.
- Current table(s)
- Sequences and Alignments
- HTML text with hyperlinks
- 2D images
- For each grob (mesh): representation and colors.

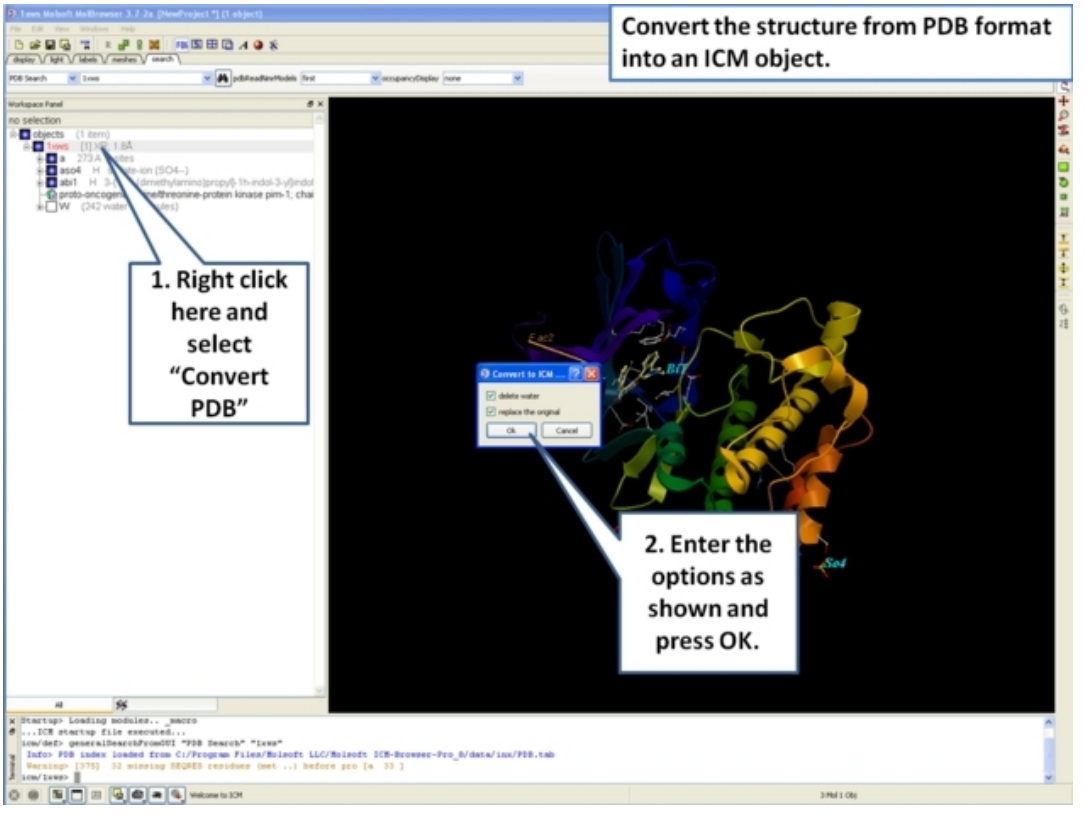
This tutorial takes you through the steps to create a series of fully interactive 3D slides. The slides can then be embedded into the web, or PowerPoint using ActiveICM or viewed in ICM-Browser (or ICM-Pro).

To begin making ICM Molecular Slides:

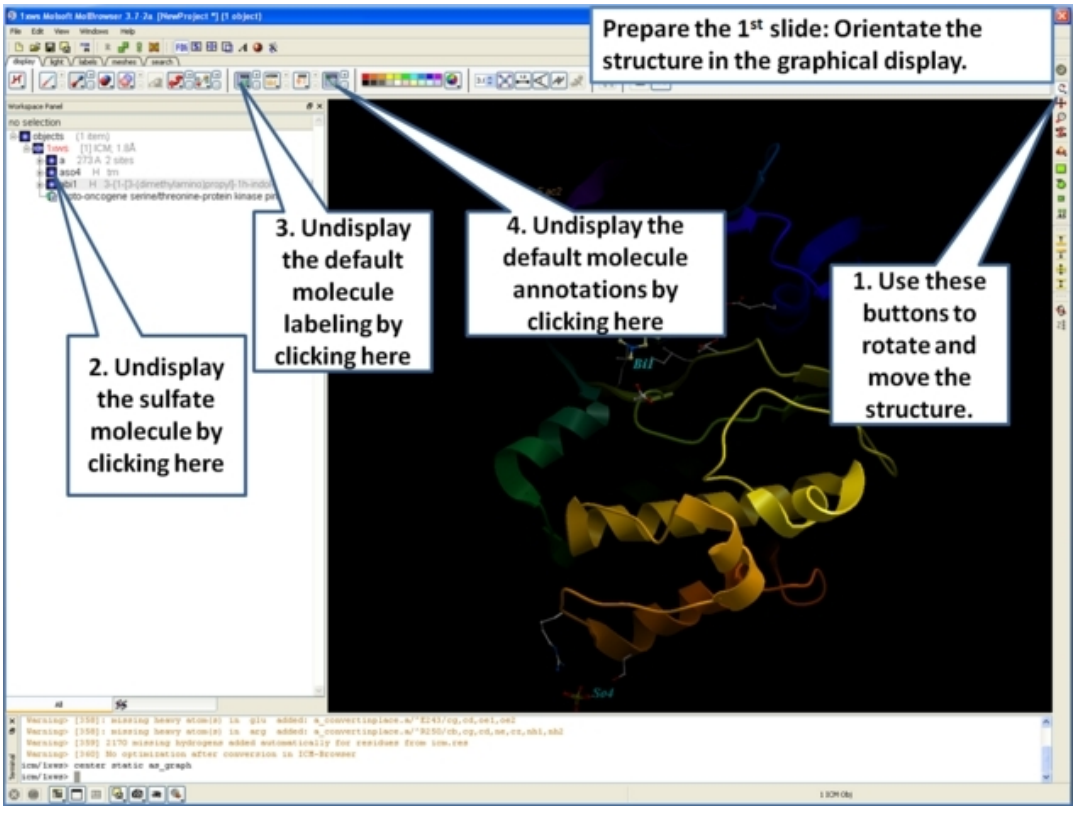
- First load the structure or structures you wish to display in your first slide. Additional structures, labels etc and text can be added at any point during the slide making process. In this example we will load the PDB file 1XWS a PIM1 kinase.



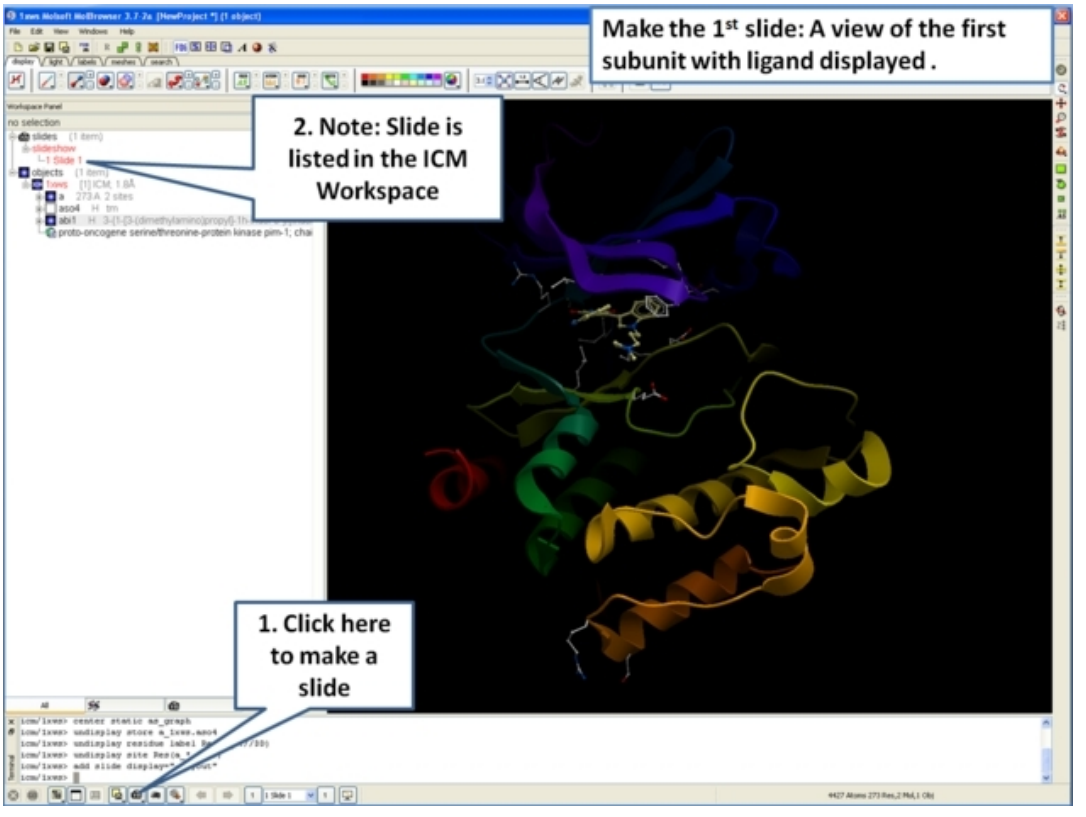
- Next, we will convert the PDB file to an ICM object so we can make slides of the ligand-receptor hydrogen bonds and binding pocket surface.



- 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.

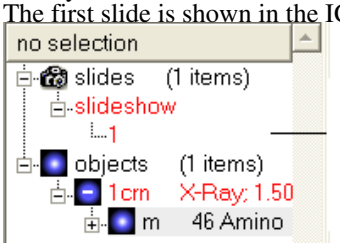


- Next, make the first slide by clicking on the camera button at the bottom of the graphical user interface.



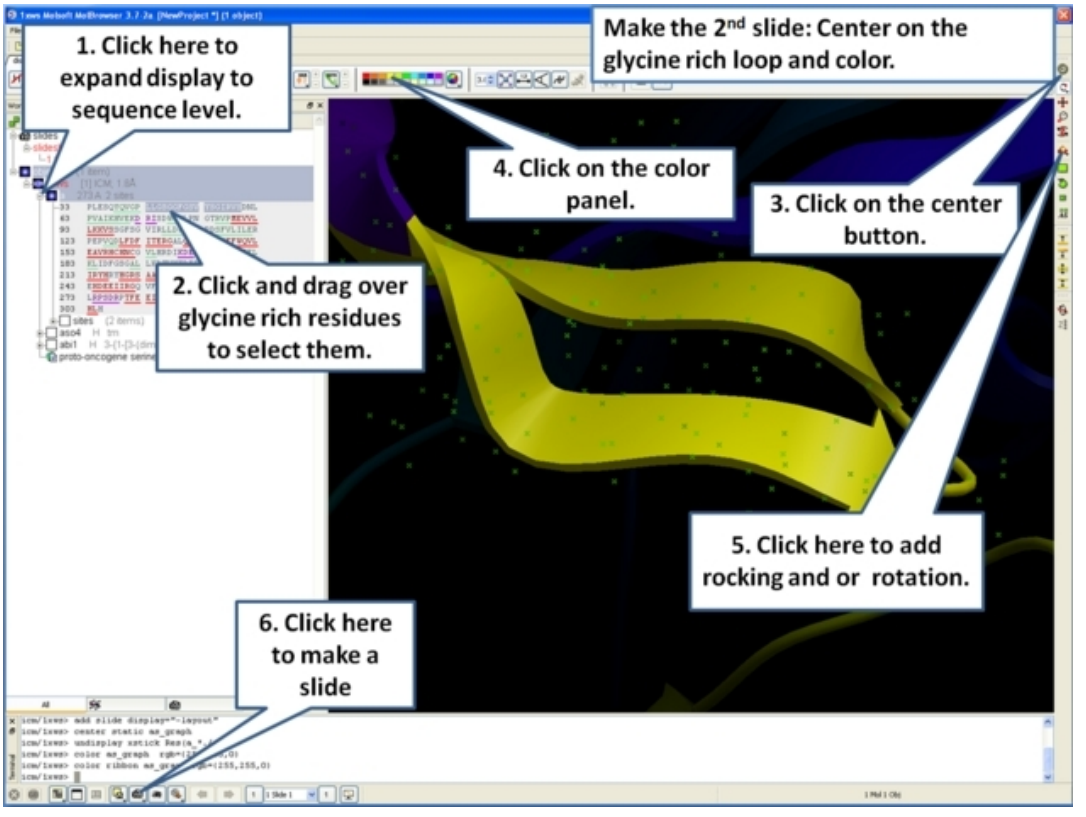
Click to add slide

- 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.

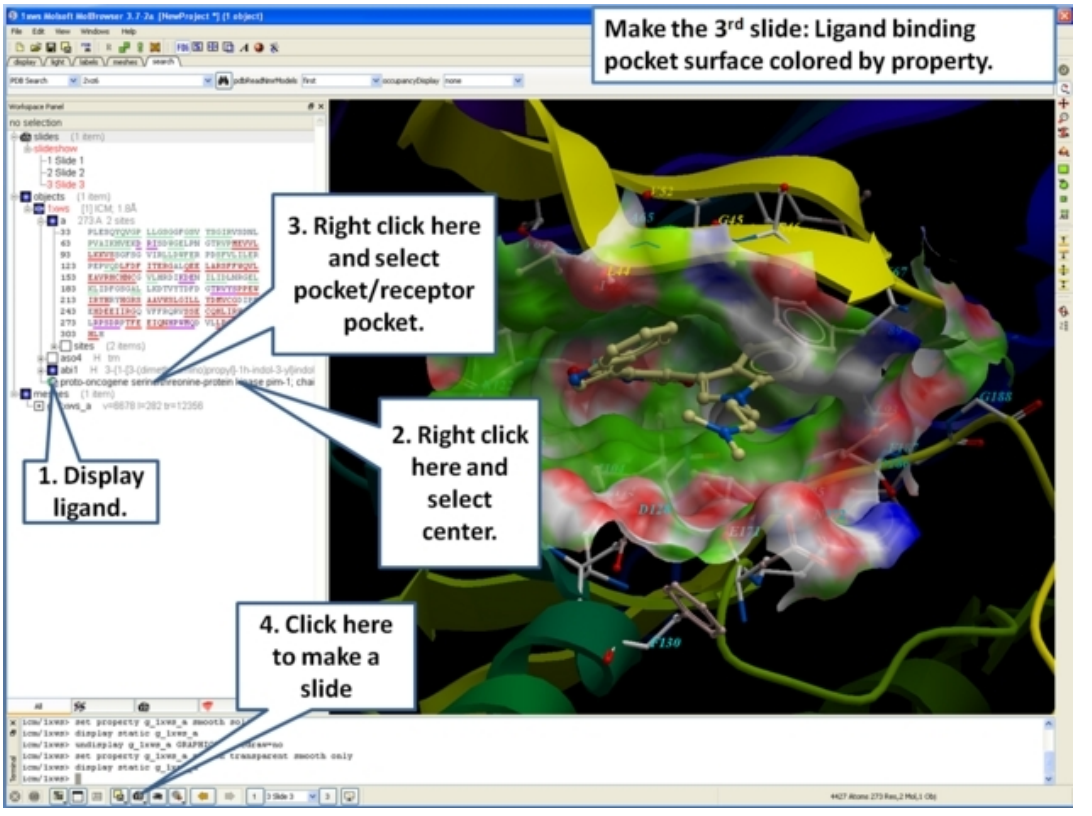


The number and name of the first slide is displayed in the ICM Workspace

- 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...

6.2 Make a Movie from a Set of Slides

Available in the following product(s): `ICM-Browser-Pro` | `ICM-Pro`

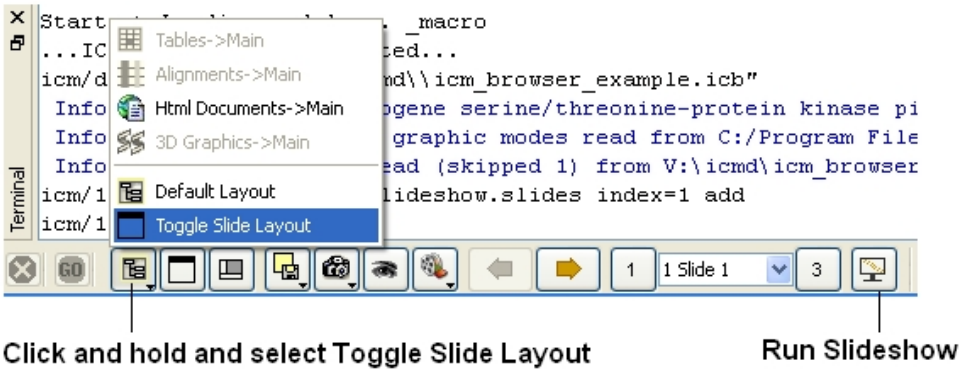
Please see the `movie` chapter on how to make a movie from a set of slides.

6.3 How to View and Navigate Slides

Available in the following product(s): `ICM-Browser` | `ICM-Browser-Pro` | `ICM-Pro`

6.3.1 View 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.

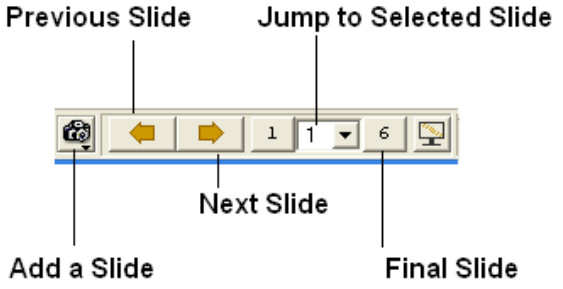
To save a slide show

- File/Save Project

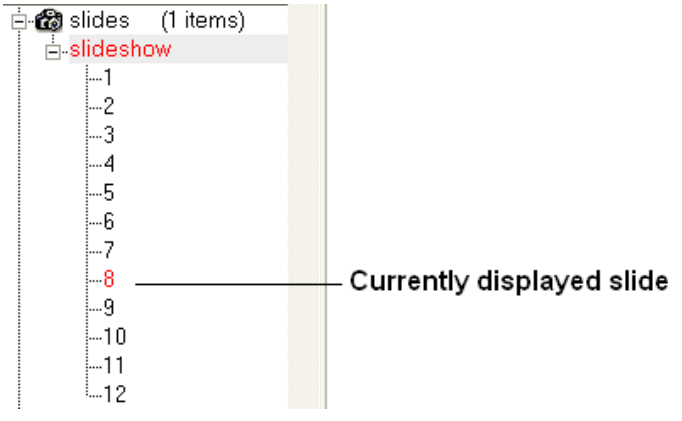
6.3.2 Slide Navigation

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.

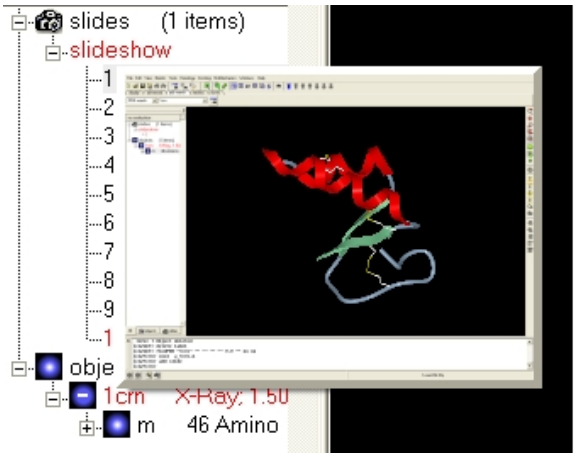


The slide currently displayed is highlighted in red in the ICM Workspace.



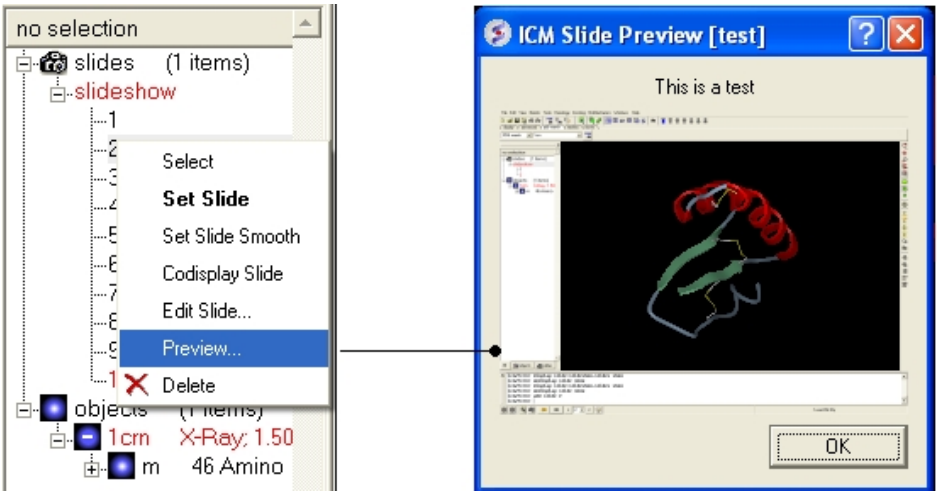
To jump to another slide right click and select "Set Slide".

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.



Hover mouse over slide name in the ICM Workspace and a thumbnail sketch of that slide will be displayed.

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

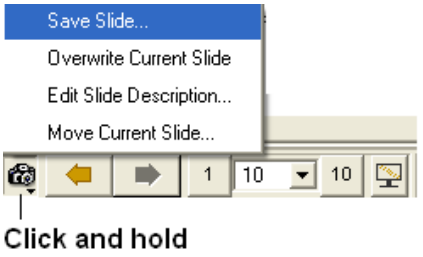
Available in the following product(s): `ICM-Browser` | `ICM-Browser-Pro` | `ICM-Pro`

You can jump to the slide you wish to edit by following the `slide navigation instructions`.

6.4.1 Edit Slide

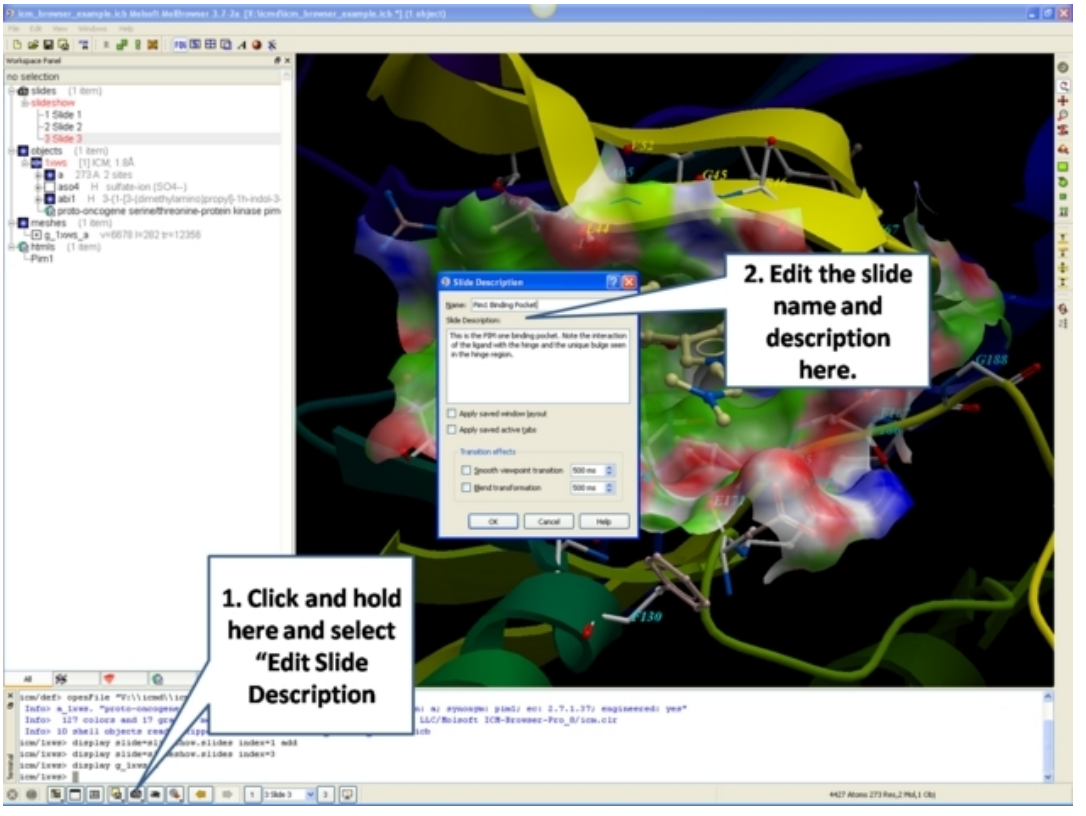
Edit slide contents: To edit the content of a slide the procedure is to add a new slide and then delete the old one or use the "overwrite current slide" option as shown below:

- Click and hold down on the camera button.



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.

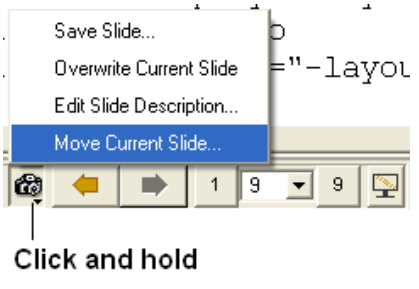
To change the name of a slide

- Right click on the name of the slide in the ICM Workspace and select Edit Slide.

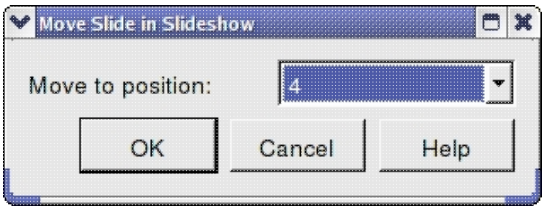
6.4.2 Move Slide

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.



- Select the position in the slide show where you want to move the slide to.



Co-display more than one slide

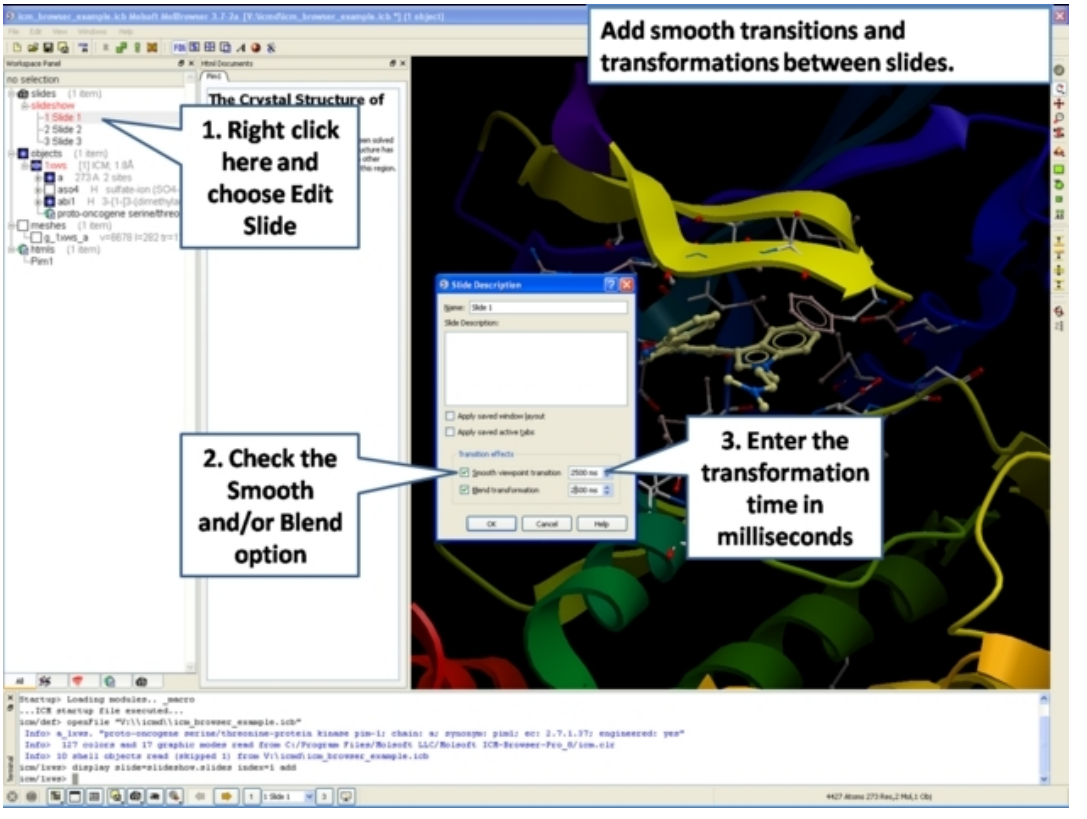
- Right click on the name of the slide in the ICM Workspace you wish to co-display with the curently displayed slide.
- Select the option co-display slide.

6.5 How to Add Smooth Blending and Transition Effects Between Slides

Available in the following product(s): ICM-Browser | ICM-Browser-Pro | ICM-Pro

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.



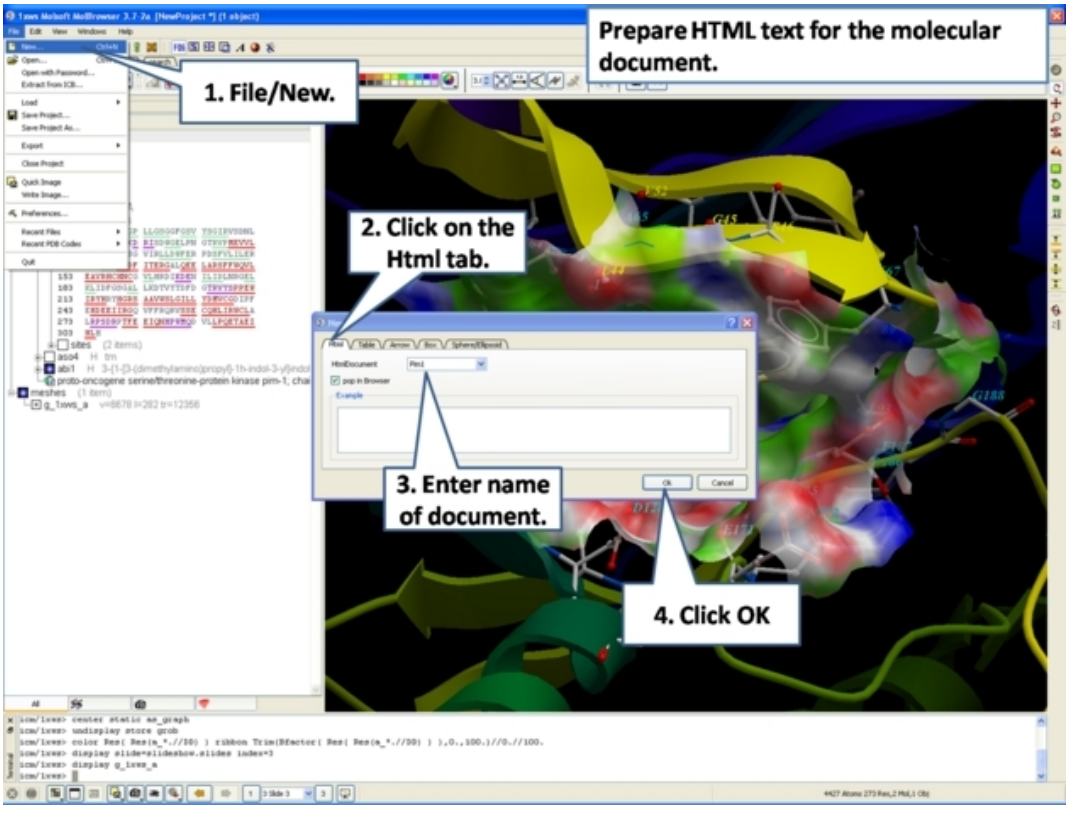
6.6 How to Make Molecular Documents - Link HTML Text to Slides

Available in the following product(s): ICM-Browser | ICM-Browser-Pro | ICM-Pro

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



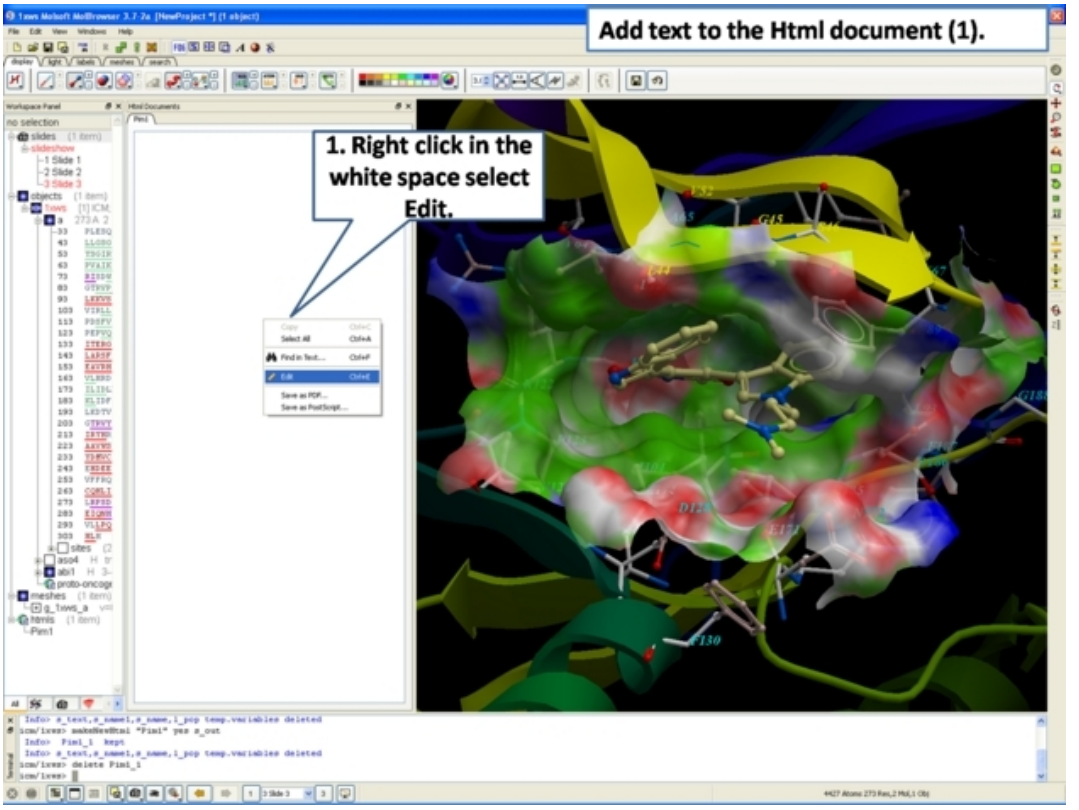
- A HTML text panel will be displayed in the graphical user interface.

NOTE: You can add multiple documents into a single file. The documents will be accessible via tabs at the top of the HTML panel.

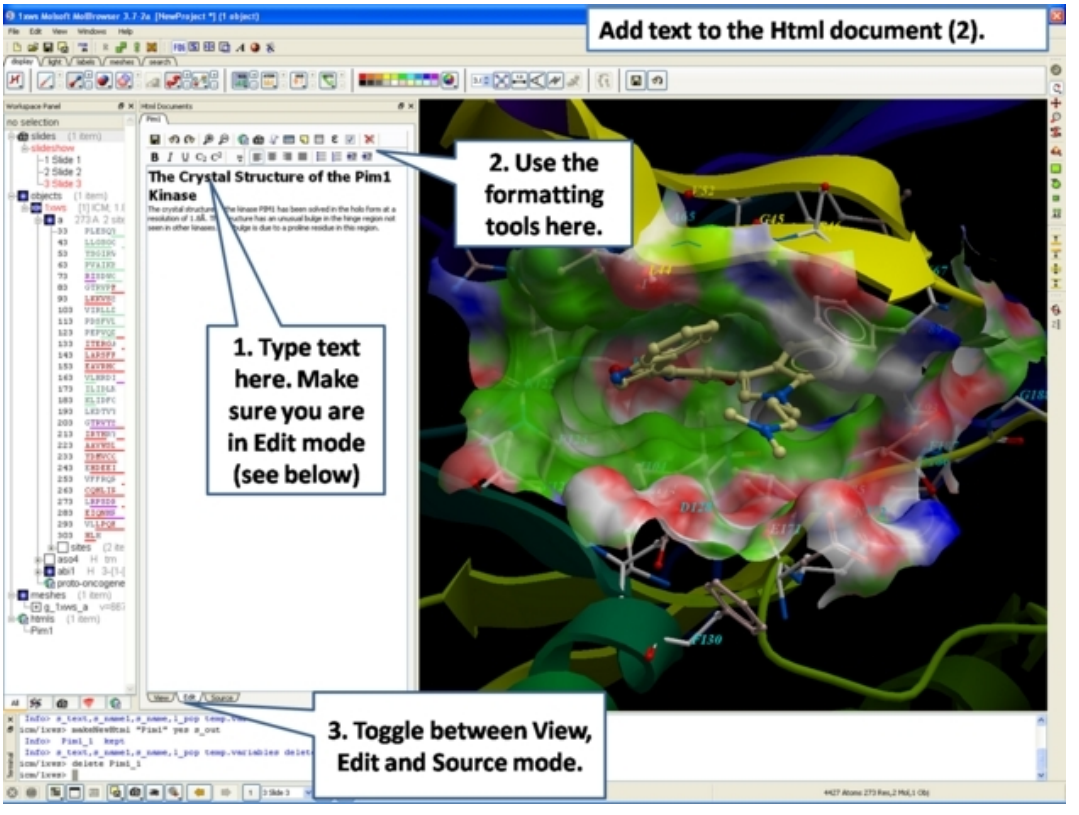
6.6.1 How to Add Text or Edit a Molecular Document

To edit the HTML text in the graphical display

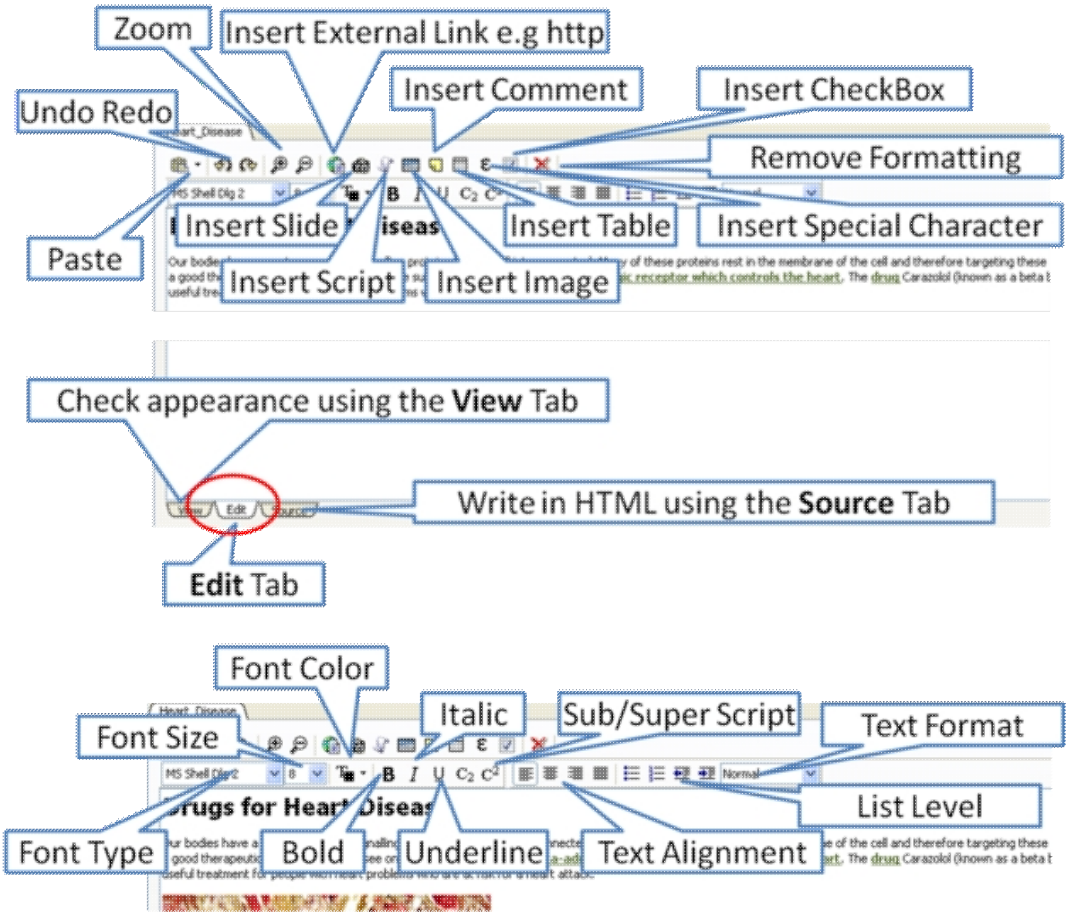
- First `create` an HTML document and the text panel will be displayed in the graphical user interface.
- Right click in the body of the text display panel and select **Edit.**



- 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.

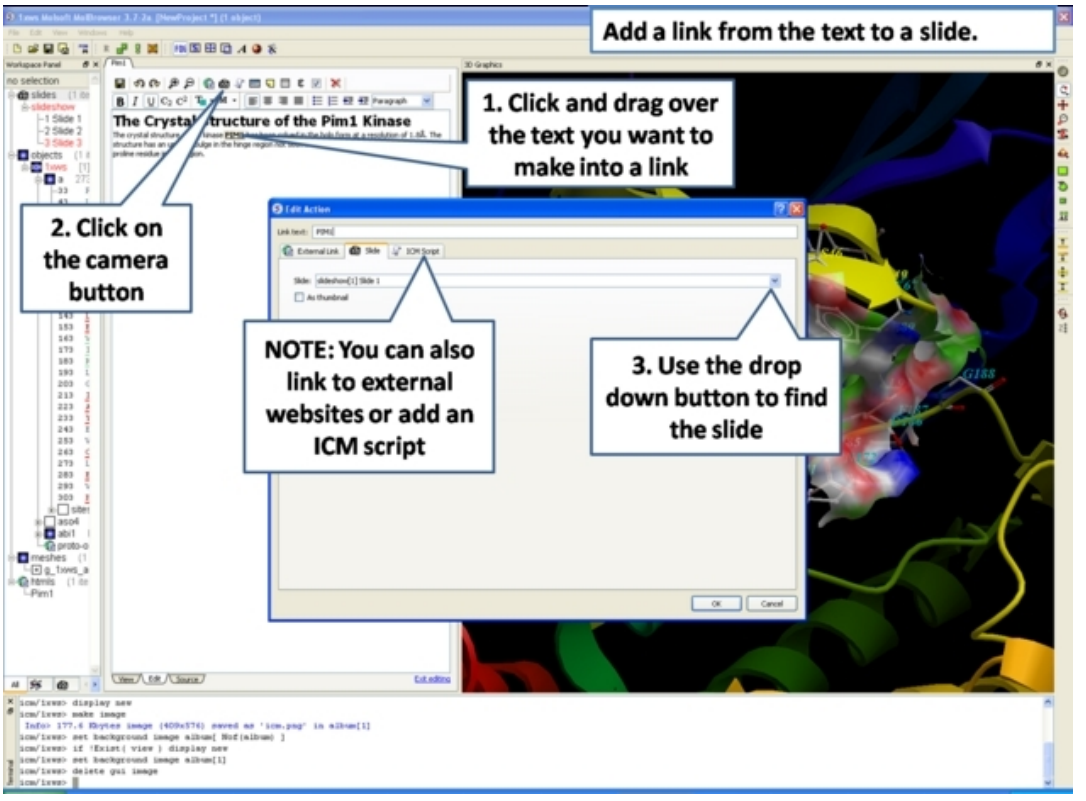


6.6.2 How to Make a Hyperlink Between Text and a Slide

To make a hyperlink between the text and the graphical display (slide)

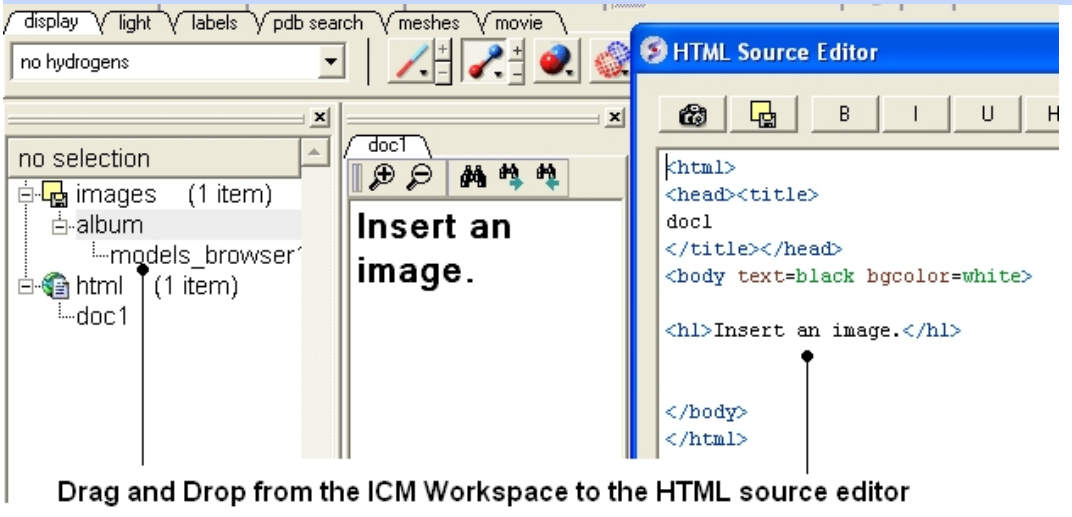
Make a slide or set of slides of the graphical display you wish to link to. See `Making Molecular Slides` for help on this.Once slides have been created:

- 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

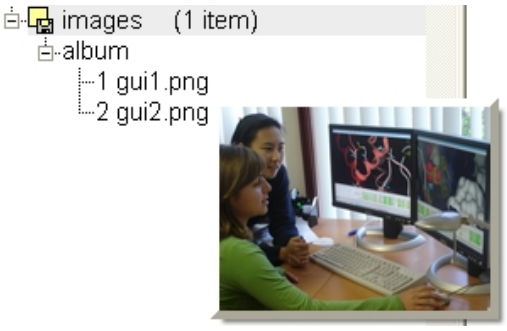
NOTE: The easiest way to add images (PNG or JPEG) into an ICM Document is to use drag and drop. You can drag and drop the image into the ICM Workspace or go to File/Open. Once the image is in the album in the ICM Workspace you can then drag it from the ICM workspace into tthe HTML editor.



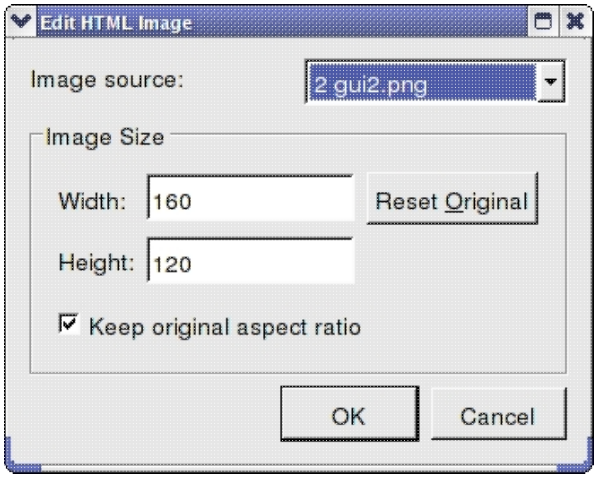
Another way to insert a picture into the HTML text panel

- 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

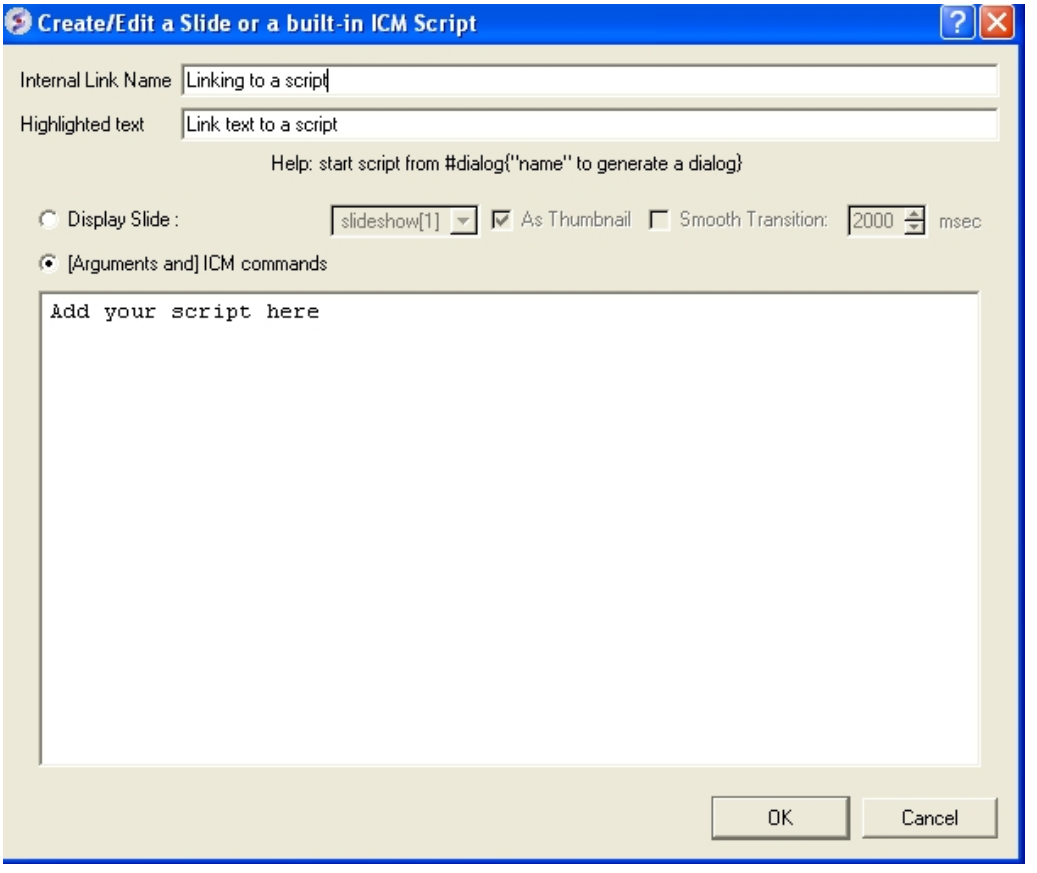
- Create a script File/New/Script
- The script will be displayed in the ICM Workspace.
- Right click in the HTML Text Panel (for instructions on how to create this panel see `create molecular document`) and select edit source and the HTML Source Editor will be displayed.
- Click-Drag and Drop the script 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.



- 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.

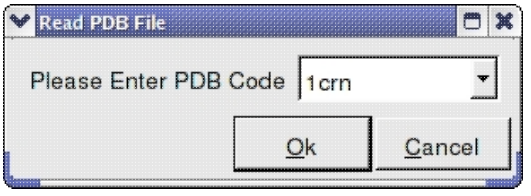
```
<!--icmscript name="script2"
#dialog{"Test"}
# i_number1 (2)
# i_number2 (3)
print $1 + $2
--><a name="script2" href="#_">script2</a>
```

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

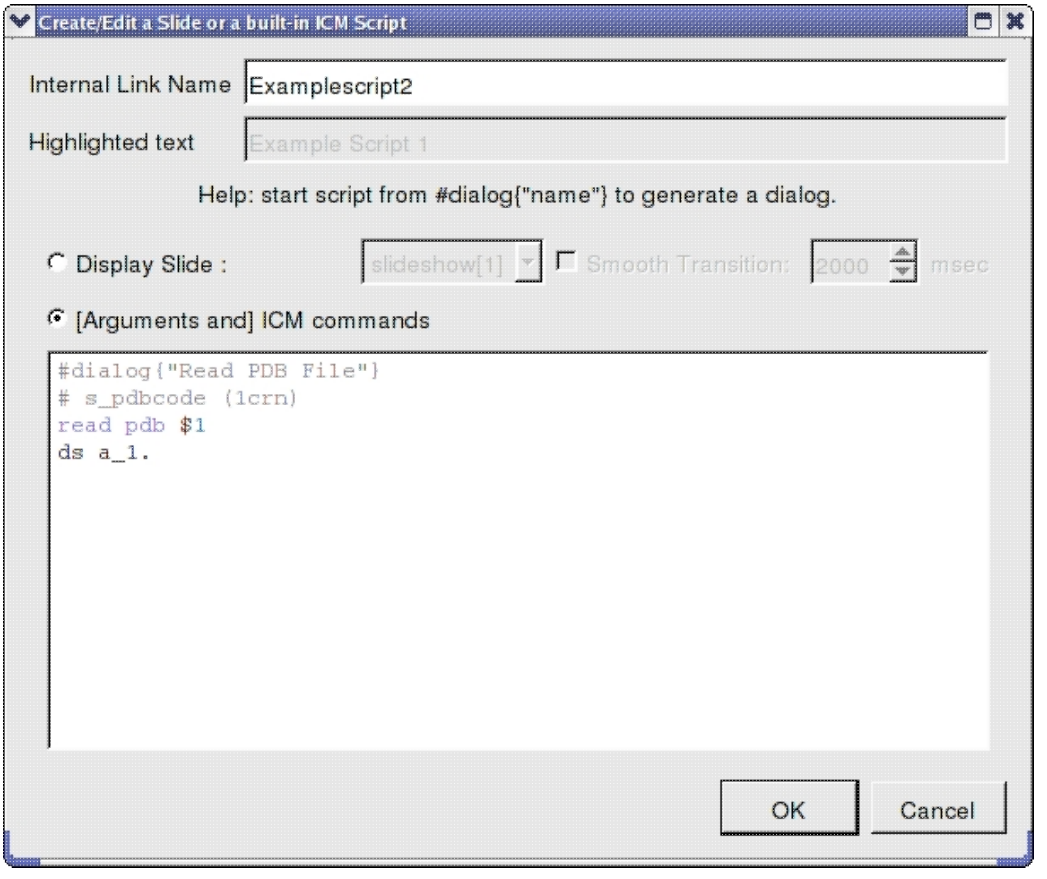
code:

```
#dialog{"Read PDB File"}
# s_pdbcode (1crn)
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.



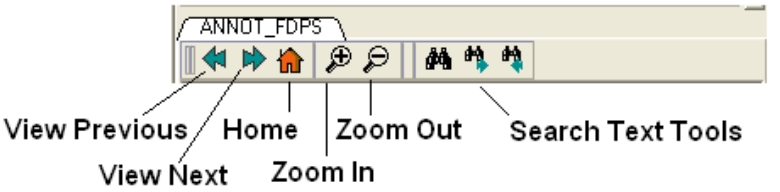
OR.

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.

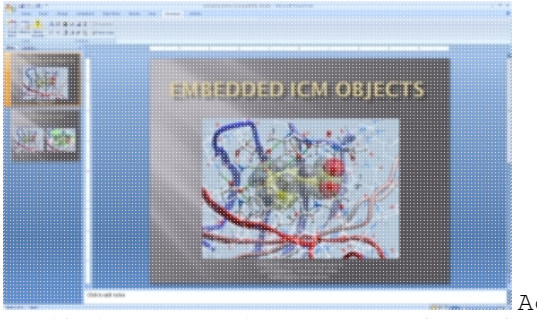


6.6.7 Protect Shell Objects From Deletion

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.

6.7 ActiveICM



`ActiveICM` enables you to view and display ICM graphical `slides` and `animations` interactively inside Windows Microsoft PowerPoint and web browsers such as Internet Exporler and Mozilla Firefox.

Chapter Contents:

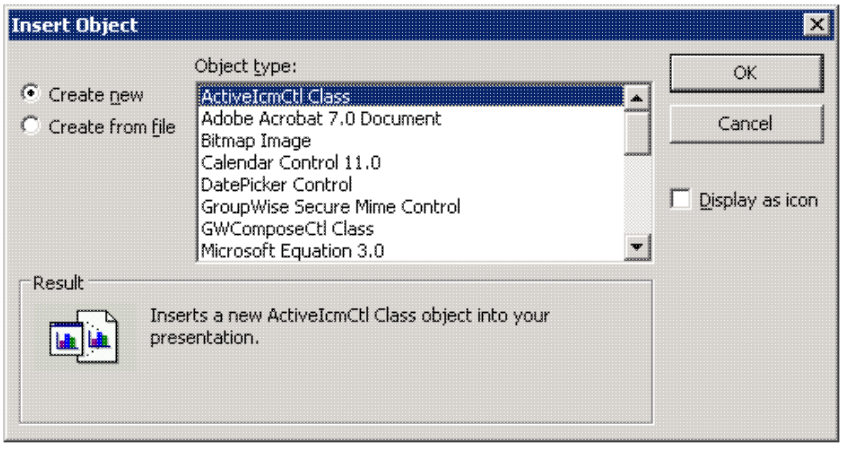
6.8 How to Embed in Microsoft PowerPoint 2003

Setup

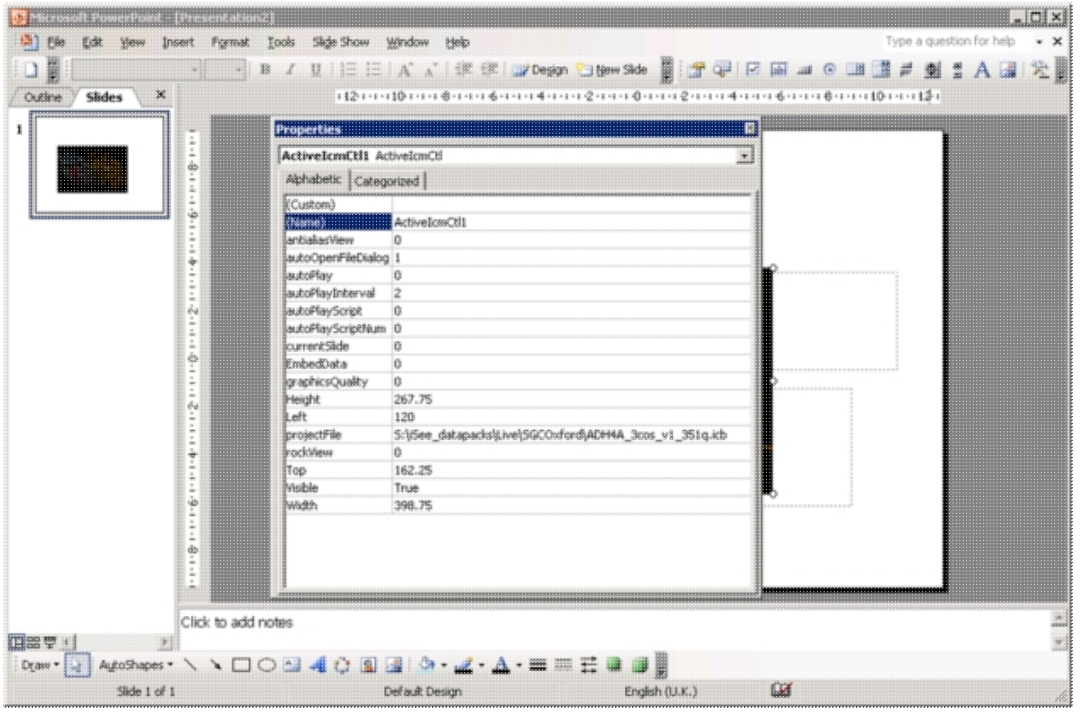
- Download ActiveICM from www.molsoft.com/support
- Save an ICM file (.icb) containing slides. Click `here` to see how to make slides.

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

6.9 How to Embed in Microsoft PowerPoint 2007

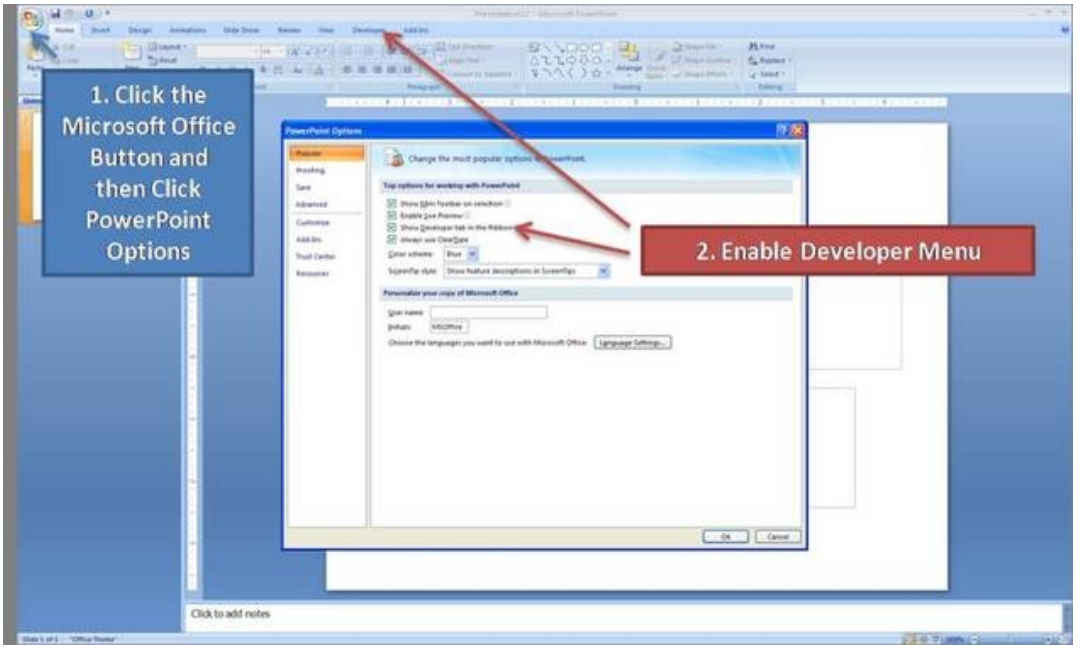
Setup

- Download ActiveICM from 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`.

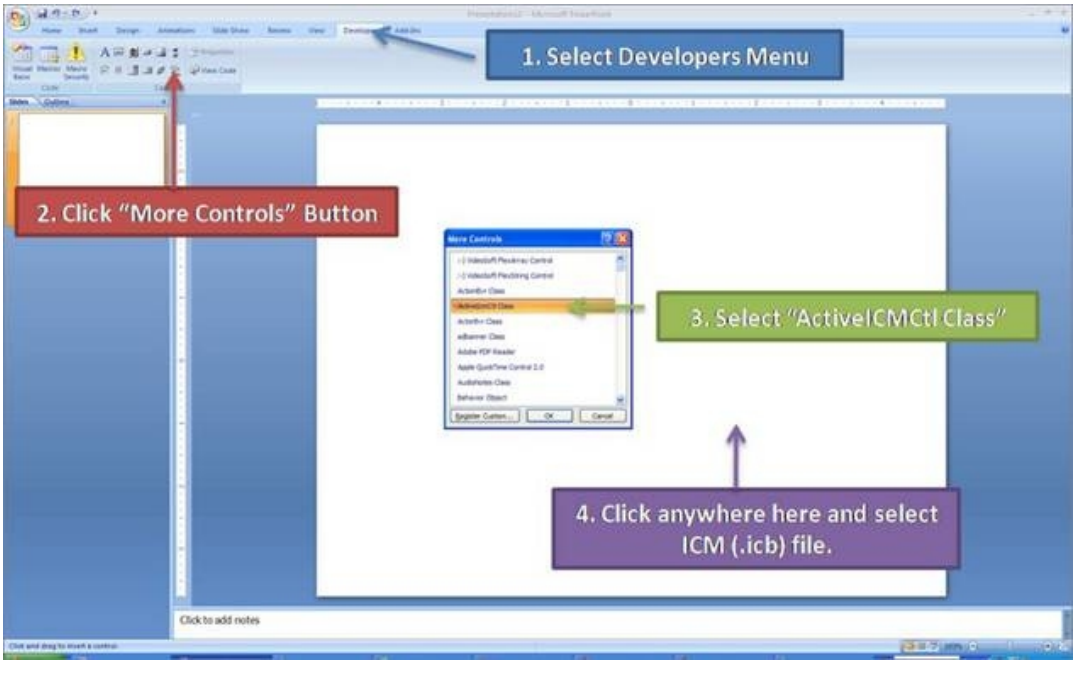
Enable the Developer Menu:

- 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**, selet 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.



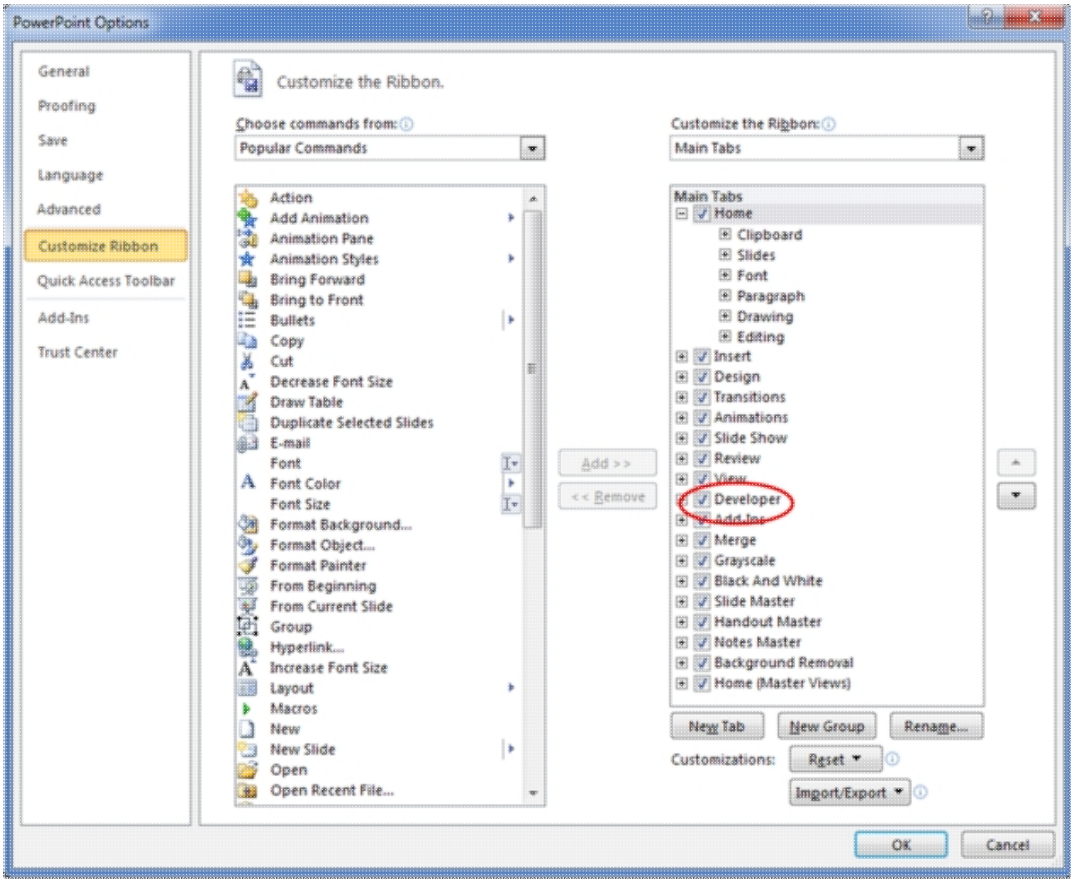
6.10 How to Embed in MicroSoft PowerPoint 2010

Setup

- Download ActiveICM from www.molsoft.com/support . Please always check you are using the latest version.
- Save an ICM file (.icb) containing slides. Click `here` to see how to make slides.

Enable the Developer Menu:

- Click on the File tab, and then click Options menu.
- Select the **Customize Ribbon** option and then check the **Developer** option in the right hand side panel (see image below).
- Click on the **Developer Menu**.
- **IMPORTANT!** Click OK and then you will see the Developer Menu in the Ribbon at the top of 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.



6.11 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..

NOTE. There is an issue with FireFox21 because it disables the ActiveICM plugin. The workaround at the moment is:

- type about:config in the location (address) bar and press the "Enter" key to open the about:config page, just like you open a website by typing the URL in the location bar.
- if you see a warning message then you can confirm that you want to access the about:config page.
- in the Search bar at the top of the about:config page type 'load_appdir_plugins'
- double click on the preference to set value to true
- restart FF

6.12 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 ï¿½ 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

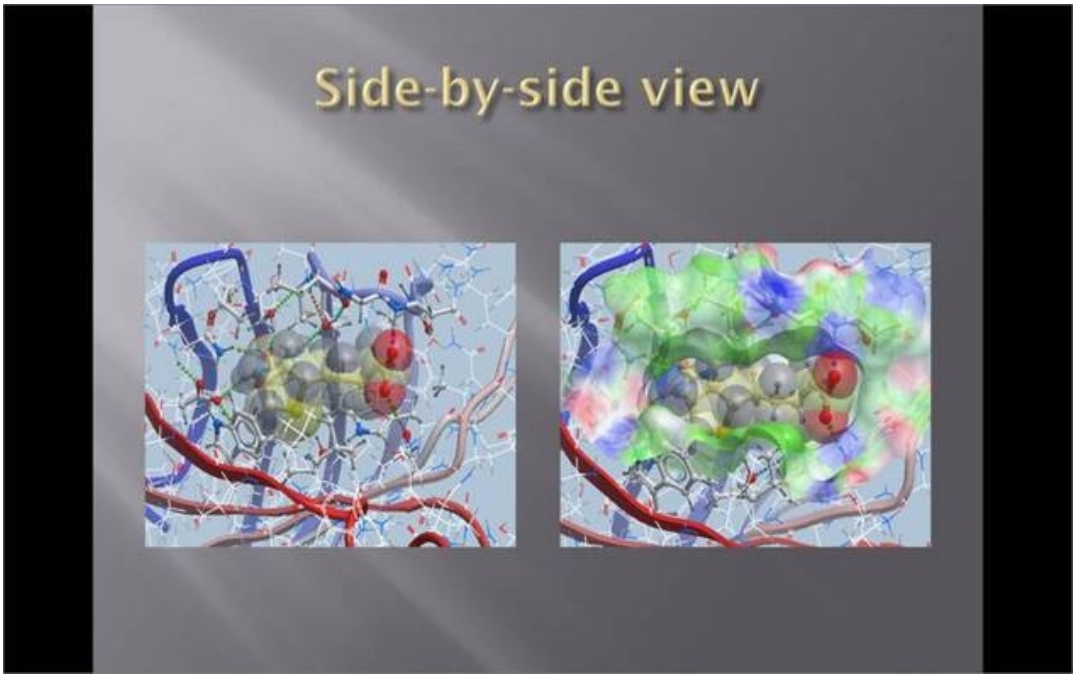
- Use the left and right cursor keys to change slides.

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

You can also add multiple ActiveICM 3D displays in one slide:

- To display mutliple 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.



6.13 How to Change ActiveICM Component Properties

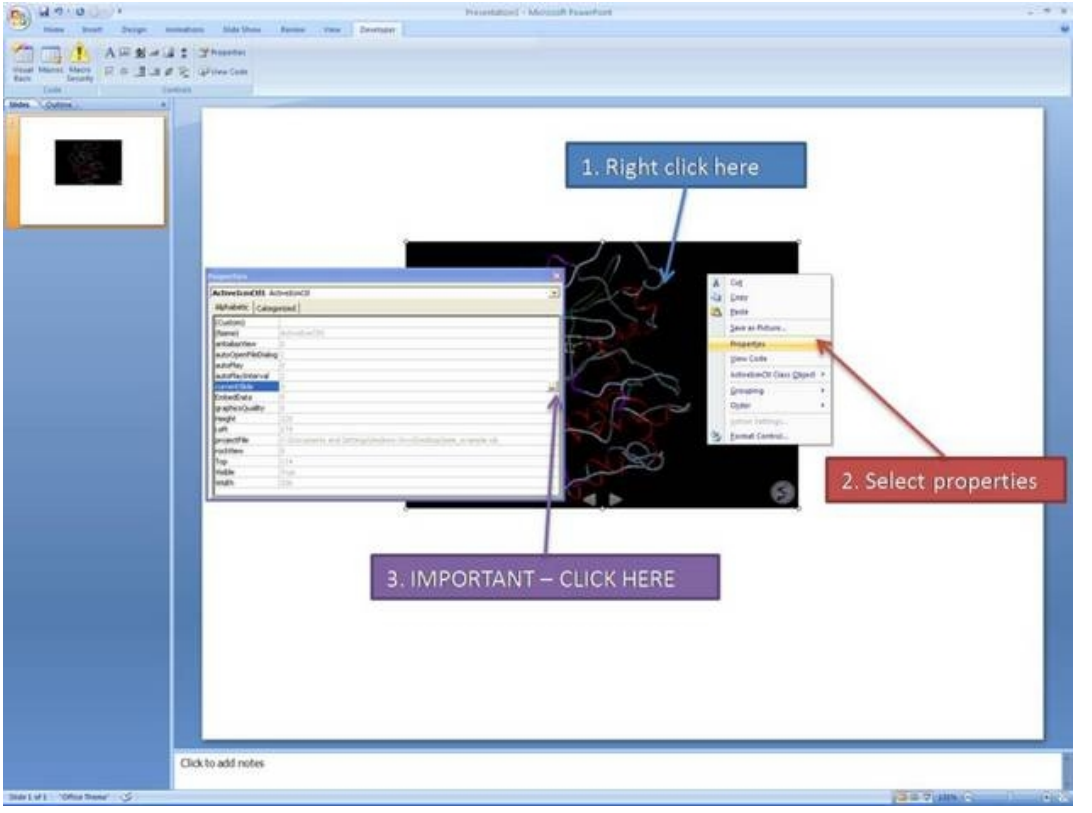
A number of properties of ActiveICM can be changed once embedded in powerpoint. The options include:

- Select the first slide to be displayed.
- Set slide auto play.

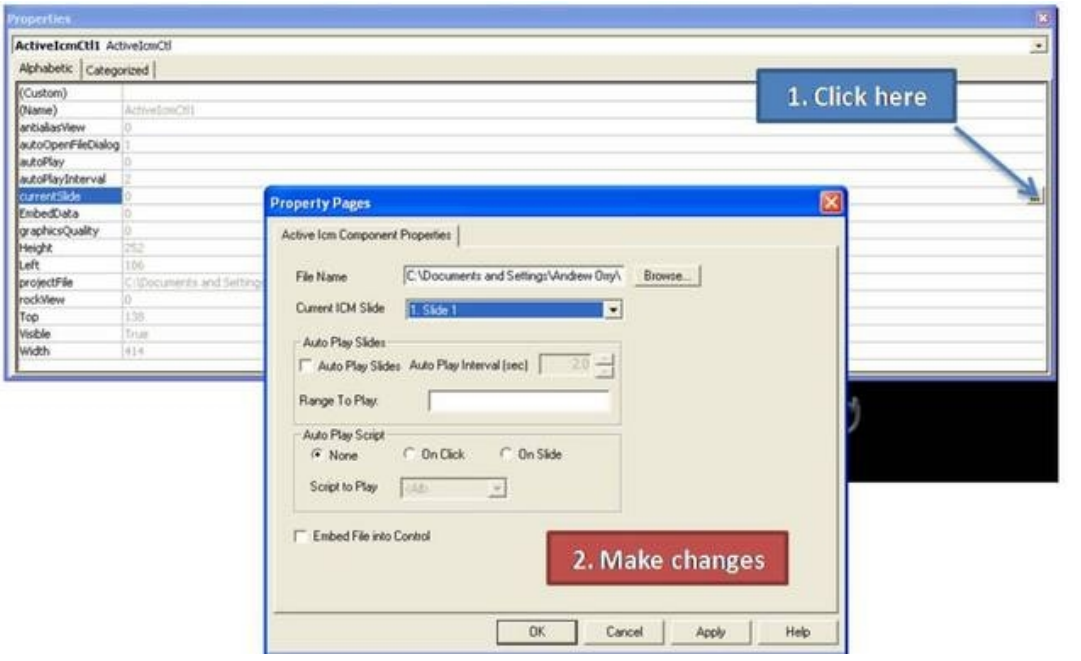
- Set auto play of a script.
- Embed the powerpoint file and the icb file all into one file.

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.

6.14 Advanced use of activeICM: Macros to direct visualisation changes

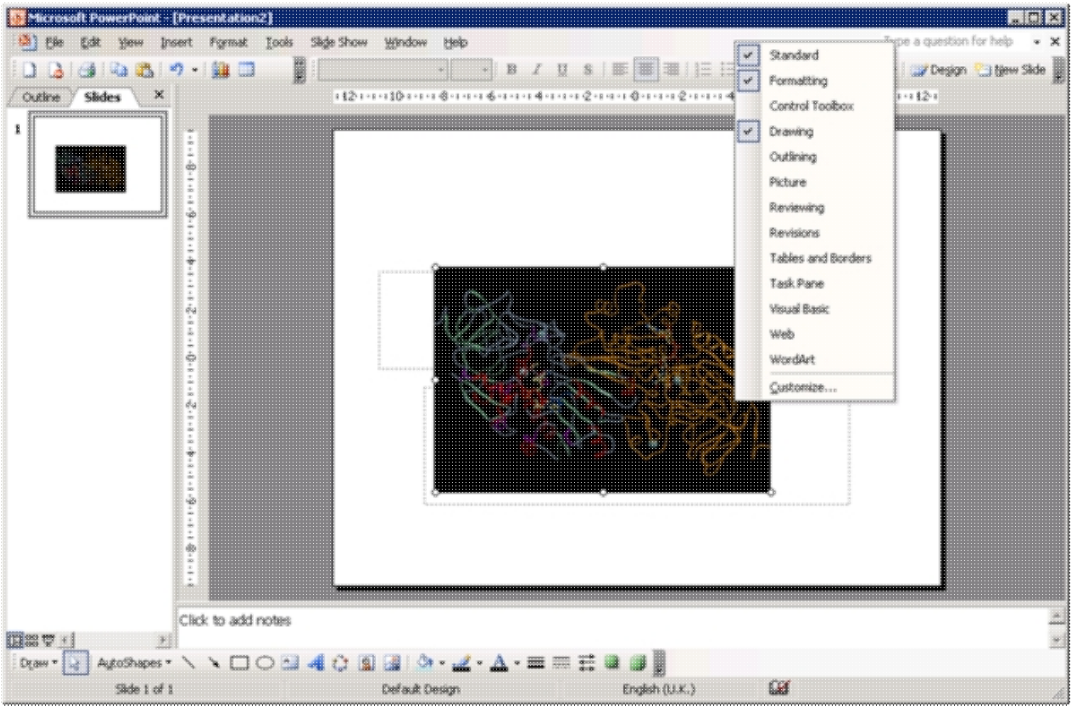
Documentation kindly provided by Dr. Brian Marsden (SGC Oxford `http://www.sgc.ox.ac.uk/people/brian/`)

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

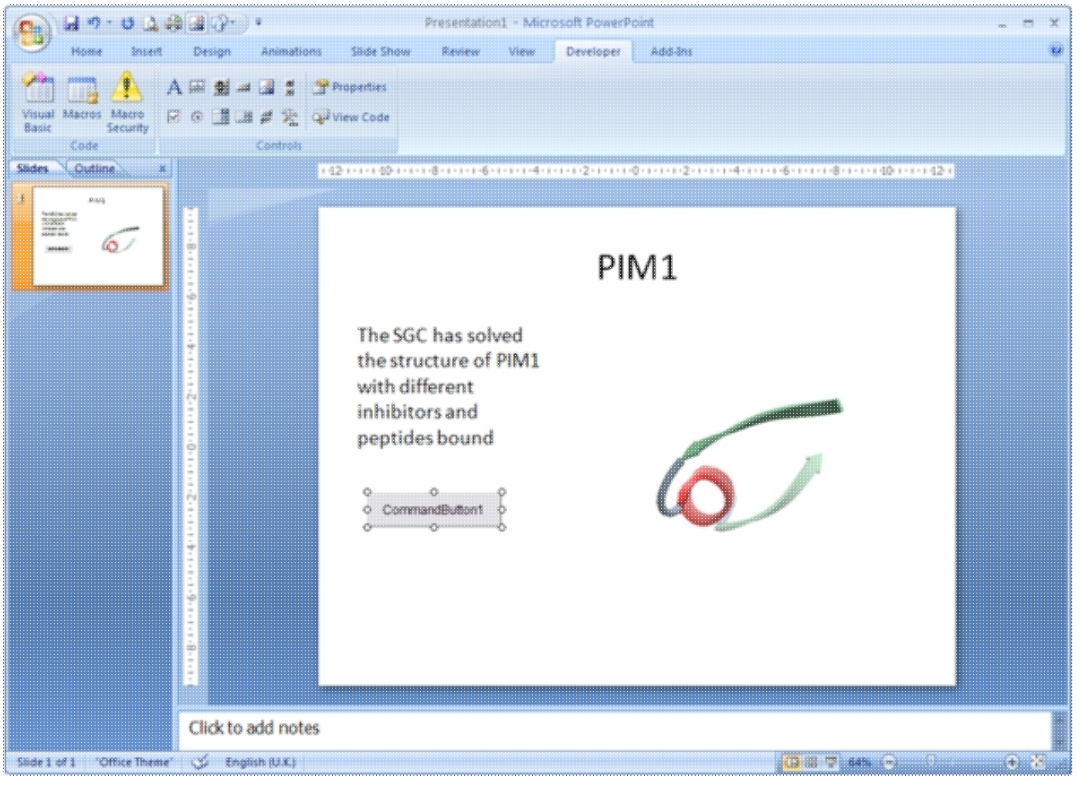
- In edit mode, make sure the control toolbox toolbar is shown by right-clicking the blank area at the top of the top bar and ensuring **Control Toolbox** is ticked.



- 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:

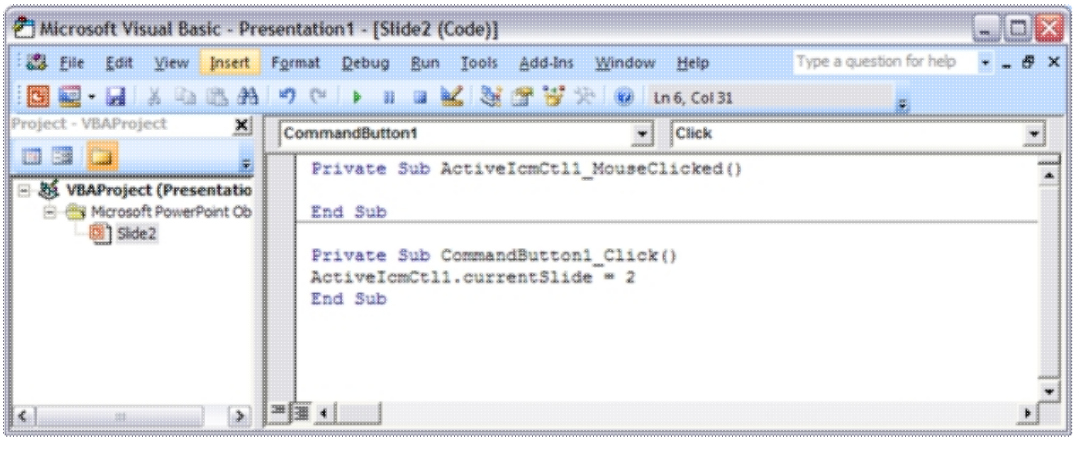
- In edit mode, click on an icon in the Developer menu or ribbon which corresponds to the sort of button you wish to use. Then click and drag in the PowerPoint slide to generate the button.



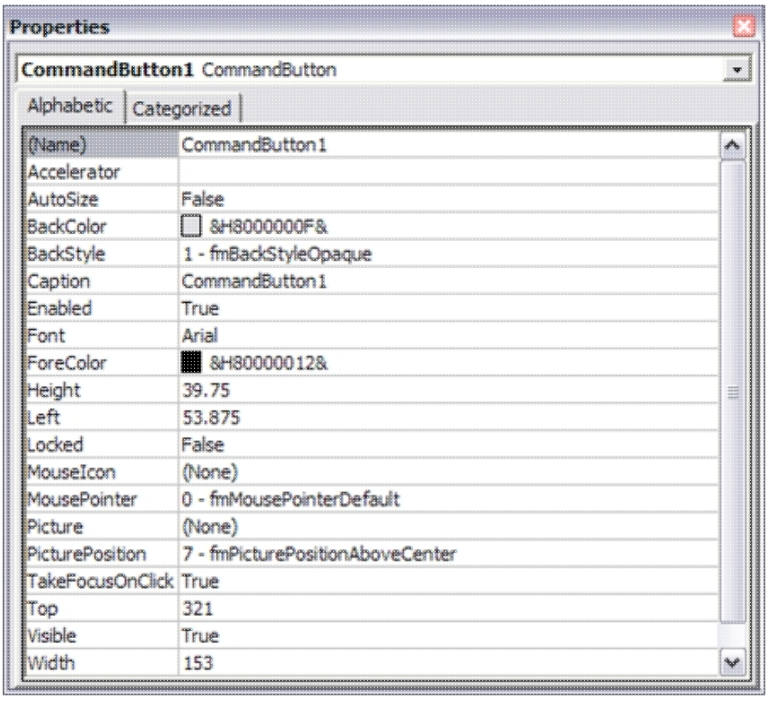
- Double-click on the new button to open the VisualBasic editor with two empty functions pre-defined. The first one pertains to the control itself and can be ignored in this context *For the second function (which is for the newly-created button), copy the following into the editor, between the two lines 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
```

6.14.1 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

6.15 Background Images

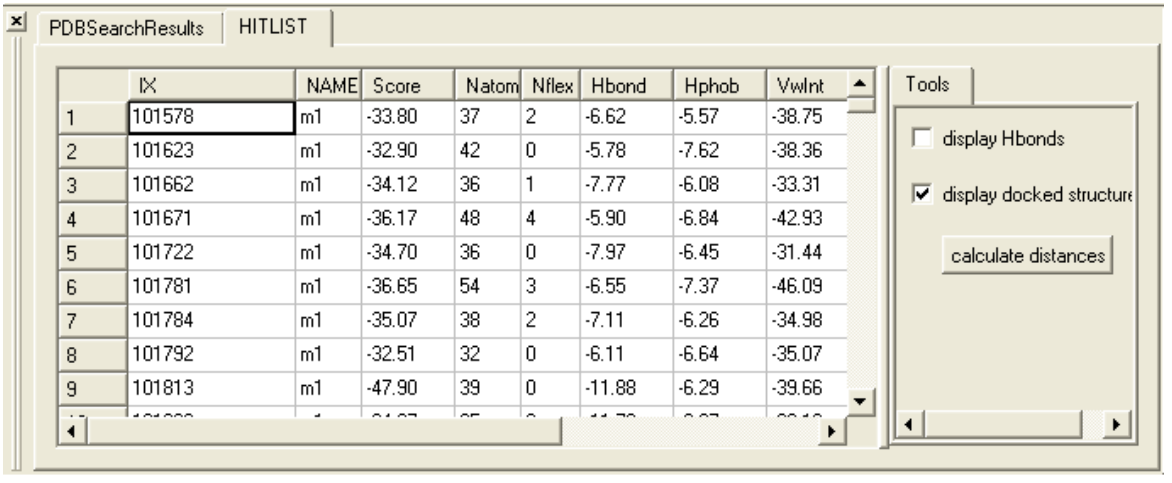
In ActiveICM version 1.1-5 and higher you can add background images to your icb file and display in PowerPoint and the web using ActiveICM. The documentation on how to insert background images can be found `here`.

7 Working with Tables

One of the easiest ways to store, sort and display data in ICM is by the use of a table. In most cases tables are automatically created, for example, if you search for a PDB file or when you load a compound database (SDF file). It is also possible for you to create your own table. Once a table is created, ICM provides easy to use tools to sort, add, edit and plot data.

Here we will concentrate on describing the actions you can perform on a table once it has been read into ICM. We will start by describing a simple table. Actions which can be performed on chemical tables are described in the section entitled Working with Chemical Spreadsheets.

A standard ICM table:



Chapter Contents:

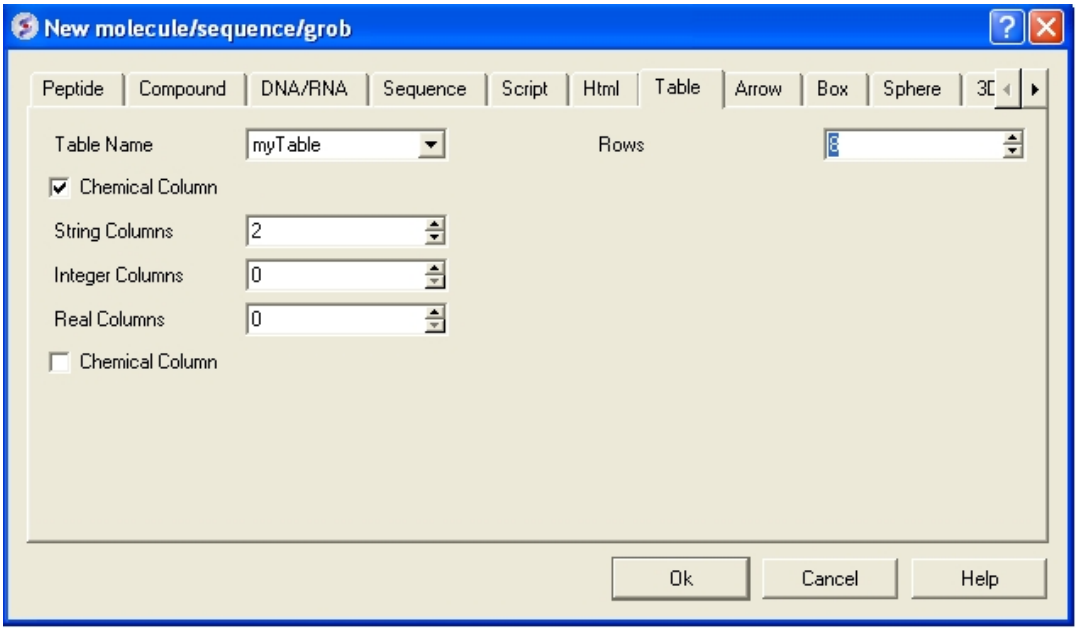
7.1 Standard ICM Tables

Available in the following product(s): ICM-Chemist | ICM-Chemist-Pro | ICM-VLS

7.1.1 Generate 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.
- If you wish to make a chemical table (chemical spreadsheet) select the **Chemical Column** box.



7.1.2 Reading a Table

A table can be read and saved as a *.csv , *.tsv or a .tab file. Saving or reading your table as a csv (comma separated value) file enables the table to be transfered or loaded from other applications such as Microsoft Excel. A compound database such as an .sdf file can also be viewed as a table in ICM, additional details on how to manipulate a `molecular table` is explained in the next section.

A table can be read into ICM by selecting:

- File/Open and then selecting the table you have saved.

OR

Sometimes data is naturally stored and displayed in a table - e.g. PDB data. A common use of tables is for compound data. An explanation of how to use compound molecular tables is in the next section entitled `ICM Molecular Tables`.

For an example of a table try the following:

- Select PDB search tab.
- Type * into data entry box.
- Click on the button next to the data entry box.

A table of all the PDB structures will be displayed at the bottom of the GUI.

NOTE: If you have loaded a table and it is not displayed it may be because the table window is hidden. To display the table, select the window menu and select table see the `Window Menu Section.`

7.1.3 Saving a table

To save the whole table:

- To save a table right click on the table header tab and select Save As..

To save a row selection:

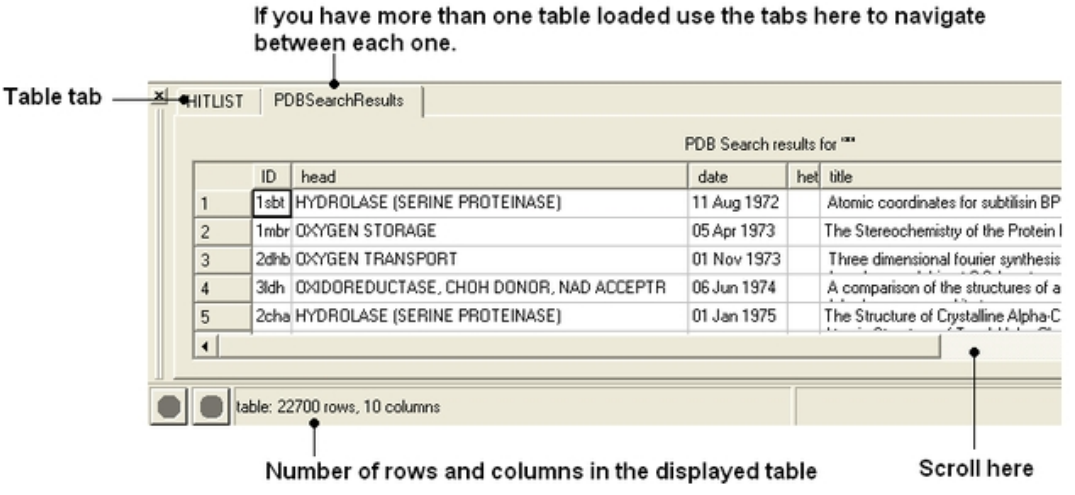
- `Select` a row(s)
- Right click and choose **Save Selection As** or **Save Selection As Csv + Headers**

7.1.4 Basic Table Navigation

To view the contents of a table you can move the table up and down using the scroll bars on the side and bottom of the display.

NOTE: If you have loaded a table and it isnt displayed it may be because the table display isnt selected. To select the table display, select the window menu and select table (See `Window Menu Section`).

If you have read more than one table in ICM you can select a table by clicking the tab on the top of the table (See Below).



NOTE: Double clicking on the tab allows two tables to be displayed at once. Double clicking again returns to the default table layout.

NOTE: Information regarding the number of rows and columns within a table is displayed at the bottom of the table.

If you would like the table to be the main window in the graphical user interface:

- Select Windows/Table->Main

7.1.5 Table View (Grid Layout)

To change the table view (layout):

- Select the columns you wish to display in grid view. No selection will place all columns in grid view
- Right click on a table row and select **Table View**
- You can view the table in **Grid View** and toggle between grid and standard view. You can define your own grid using the **Custon Grid** option or display the table in **Form View**.

NOTE: You can `save` a table view.

7.1.6 Change Row Height

To change the row height:

- Click and drag on the row separator
- Hold the Ctl key to change the height of all rows.

7.1.7 Table View Save

Once you have a `table view` that you want to keep. You can save it by:

- Right click on a table row and select **Store Views**
- Select **Save Current View**
- Enter a name for the table view and you can return to that view by repeating the first two steps above.
- You can rename, delete or restore view by right clicking on the name of the table view.

7.1.8 Table Search

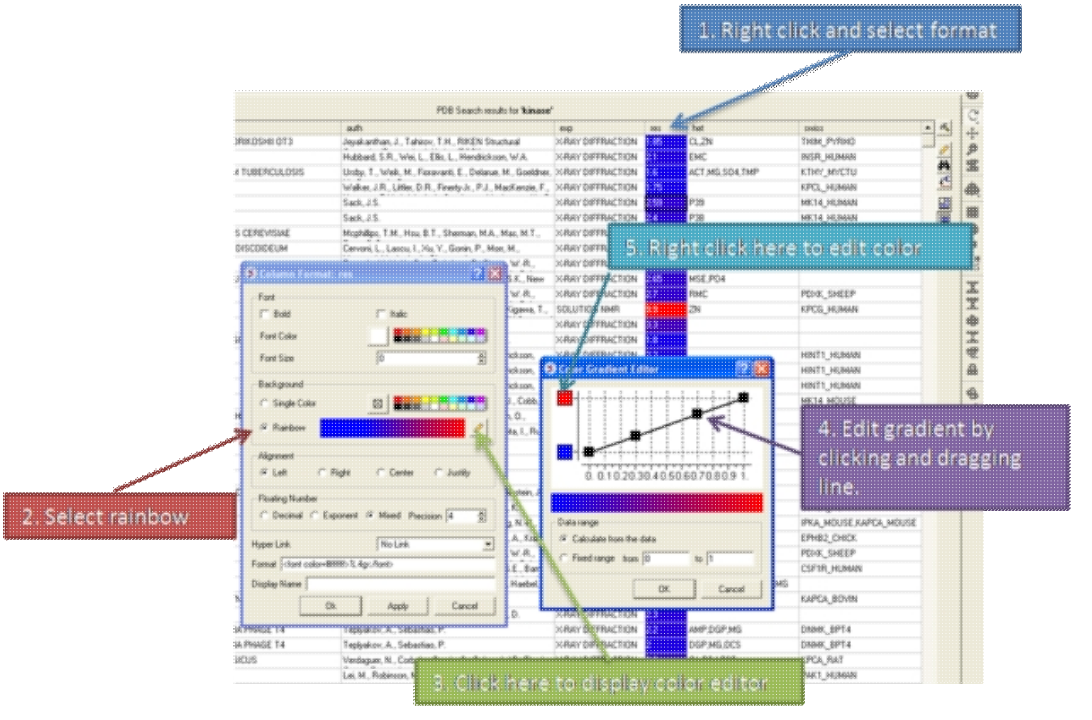
To search a table:

- Right click on a table row and select **Find and Replace**. You can also use CTRL F.
- Enter a search string.
- Press the **Find** button.

7.1.9 Table Color

You can color your table based on values within a column by:

- Right click on the column header and select **Format.**
- In the **Background** panel select the color you desire eg **Single Color** or you can by a rainbow according to the data in the column. To edit the range of values relating to each color click on the pencil (edit) button as shown below.



7.1.10 Table Font

- Right click on the column header and select **Format.**
- Change the font using the options in the **Font** panel.

7.1.11 Table Alignment

- Right click on the column header and select **Format.**
- Change the font using the options in the **Alignment** panel.

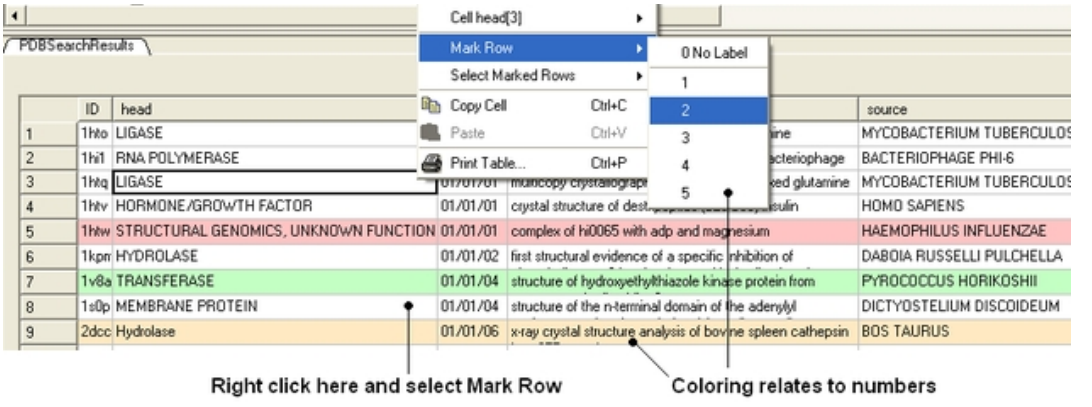
Rows can be colored by marking them as described `here`

7.1.12 Mark a Row

A row in a table can be marked and grouped by a label which enables the row(s) to be selected easily at a later time.

To mark a row

- Right click on the row in the table you wish to **mark.** Or `select` multiple rows and then right click.
- Select **Mark Row/** and then choose a number. In the GUI the number of rows that can be marked is limited to 5 but this can be increased using the command line command.
- A row that is marked will be colored - each number is assigned a color. The coloring can be changed in the `gui tab in preferences`.



To select marked rows

- Right click on the table and choose **Select Marked Rows** and choose a number which relates to the marked rows as described earlier.
- Selected rows will be highlighted blue - once rows are selected a number of right click options are activated such as copy selection to new ICM table.

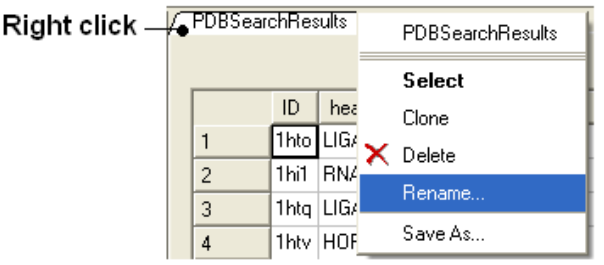
7.1.13 Table right click options

Right-click options vary according to where you click and what is selected. The options are intuitive, for example options that are performed on the whole table (eg Save and Delete) are performed by right-clicking on the Table tab. Other right-click options vary according to whether the row or column is `selected` or not.

7.1.14 Rename a Table

To rename a table:

- Right click on the table tab and select rename.
- Enter a new name and select OK.



7.1.15 Clone a Table

- Right click on the table tab and select clone.

7.1.16 Delete a Table

- Right click on the table tab and select delete.

7.1.17 Page Setup

Before `printing a table` you can change the orientation and scale.

To do this:

- Right click on the table header and select **Page Setup**.

7.1.18 Print a Table

A table can be printed by:

- Right click on the table tab and a menu will be displayed.
- Select the "Print" option. You may want to change the setup of the table (eg orientation and scale. You can do this using `Page Setup` option.

7.1.19 Export to Excel

To export a table to excel.

- Right click on the table header.
- Select the option to **Export to Excel**.

7.1.20 Save a Table

- Right click on the table tab and select Save As..

NOTE: You can save your table in comma separated format if you want to read it into another program such as Microsoft Excel.

7.1.21 Change Column and Row Width

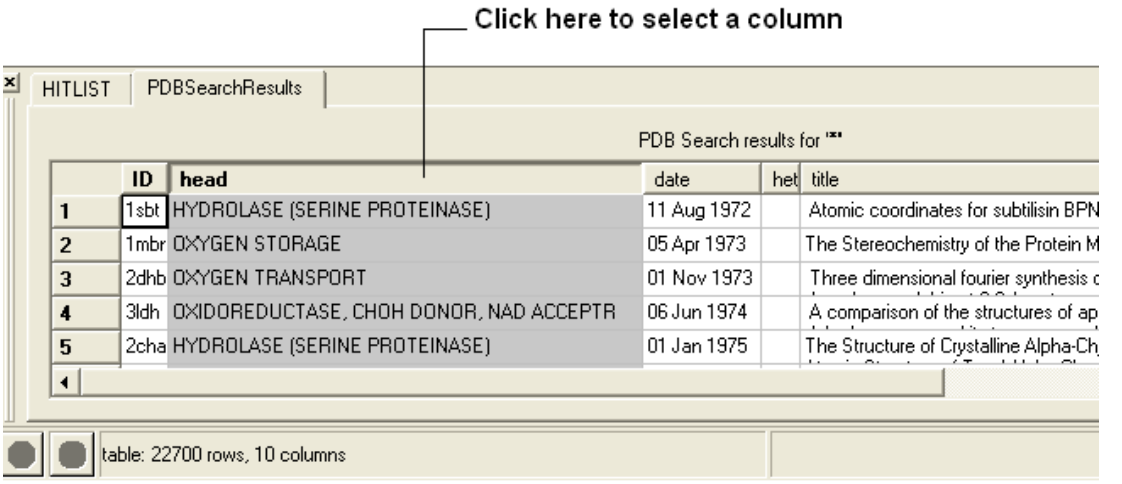
To change the width of column and rows:

You can change the width of a row or column by clicking on the separating line and dragging. You can make each row the same width by holding down the **Shift** key and dragging one of the row edges.

7.1.22 Making Table Selections

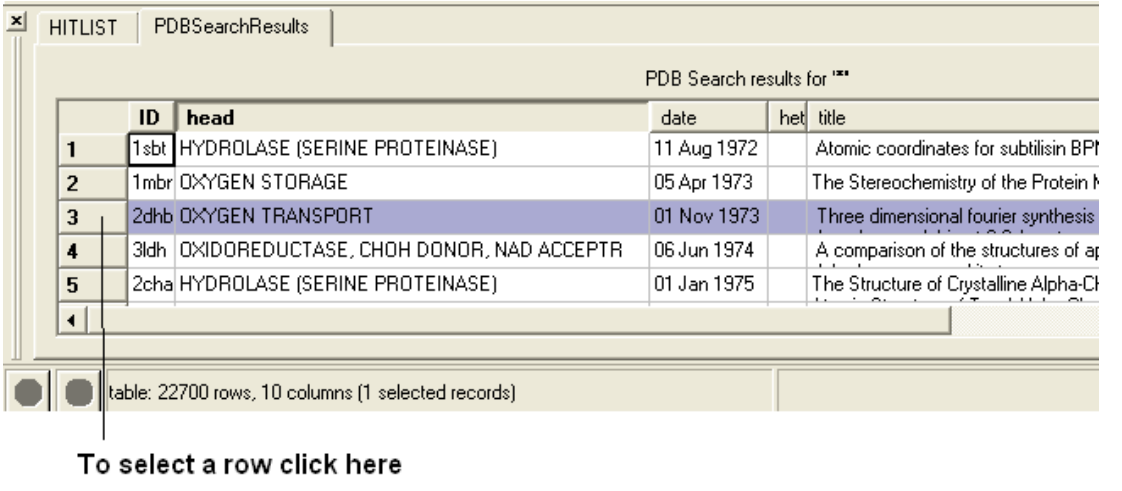
To select one column of a table:

- Click on the column header



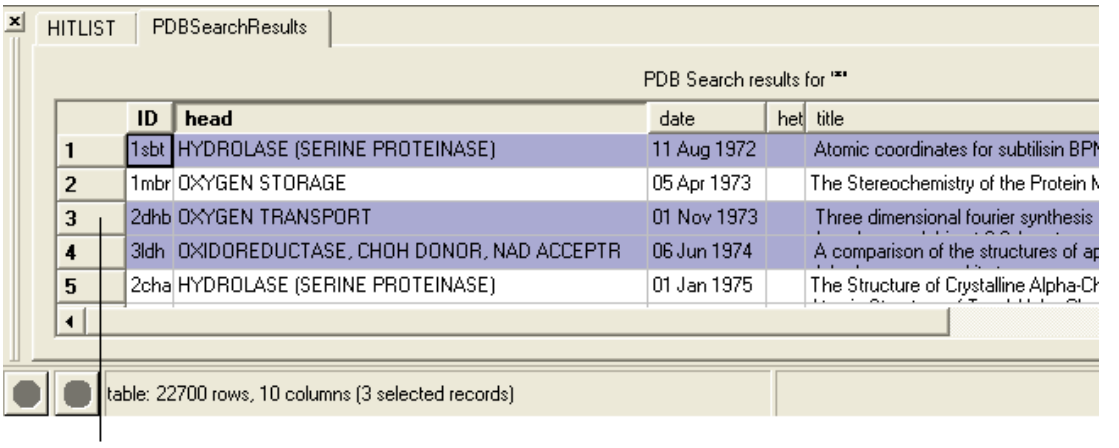
To select one row of a table:

- Click on the row header



To select more than one row or column:

- Click on one row or column whilst pressing the Ctrl key
- Select multiple number of rows or columns whilst still pressing the Ctrl key



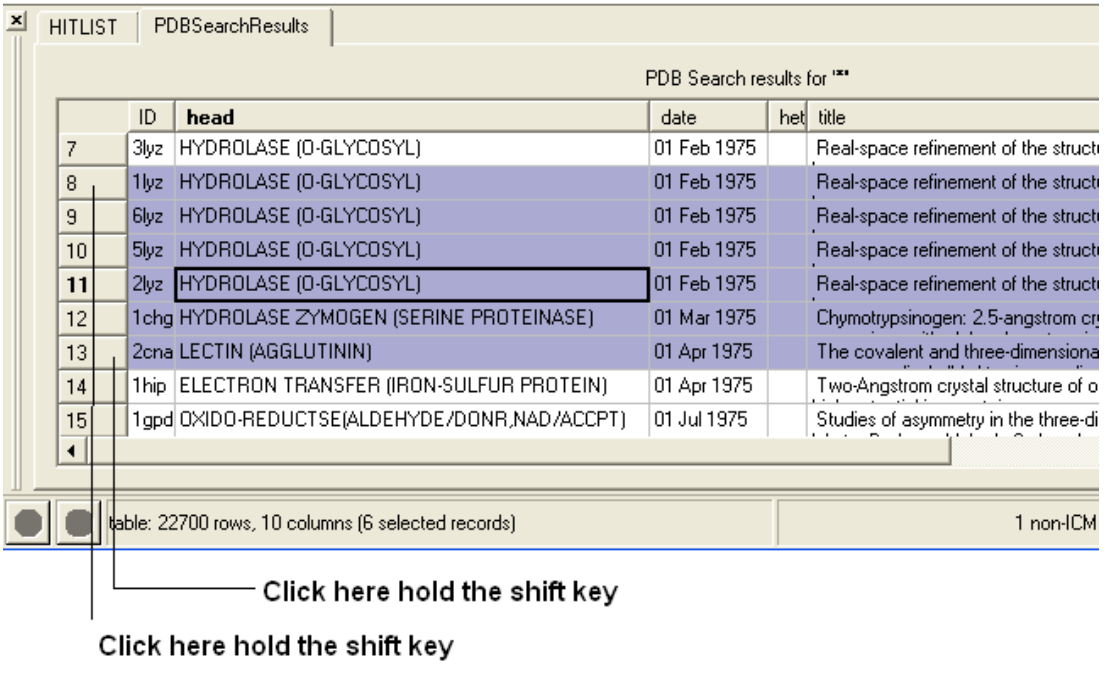
Select multiple rows and columns by clicking and selecting whilst pressing the Ctrl key.

NOTE: The Ctrl key acts as a toggle enabling select and unselect.

To select a range of columns or rows:

- Click on the first row or column in the range whilst pressing the Shift key.
- Click on the last row or column in the range whilst pressing the Shift key.

To select a range of columns or rows - click on the first member of the range and the last whilst pressing the shift key.



To invert a selection:

- Right click on the original selection and a menu will be displayed.
- Select the Row Selection/Invert selection option.

NOTE: Invert selection can only be used on rows.

To select the whole table:

- Right click in the table and a menu will be displayed.

- Select the Row Selection/Select All option.

To remove a selection:

- Click anywhere within the table.

A selection can also be made from a plot select(`table-plot{See Select plot section}).

7.1.23 Editing a Table

To edit the contents of a table column:

- `Select` the column and then right-click on a column header and a menu will be displayed.
- Select the "Edit Mode" option. A tick will be displayed if it is selected.

OR

To edit the text or values within a cell:

- Right click on the table and select **Edit Cells by Double-click** .

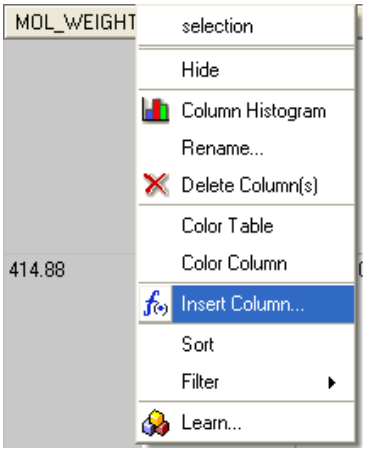
To edit the name of a column:

- Right click on the column header and a menu will be displayed.
- Select the option "Rename Column..." and enter the appropriate new text.

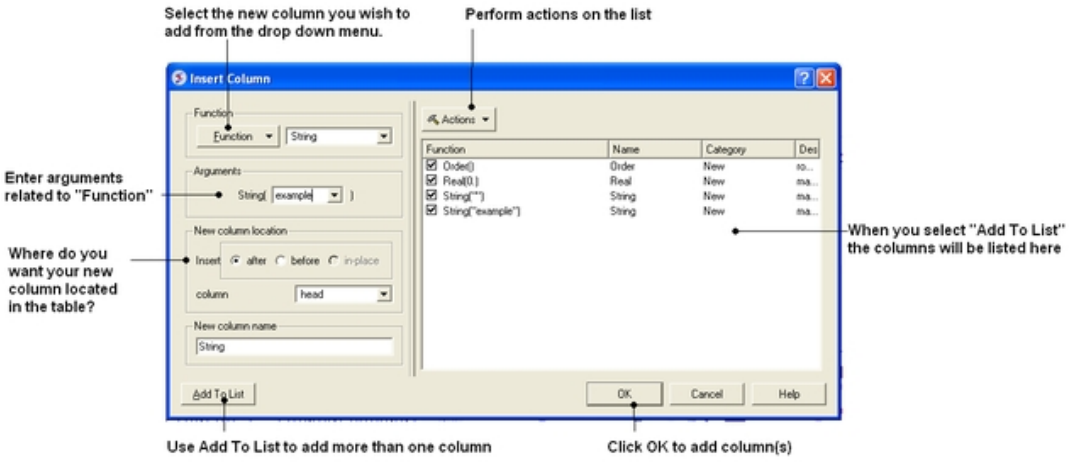
7.1.24 Inserting Columns

To insert a column:

- Identify the position within the table where you wish the column to be inserted.
- Right click on the column header and a menu will be displayed.
- Select "Insert Column"



A dialog box will then be displayed as shown below.



- Select the function you wish to add to the new column. Functions can be applied to many columns e.g. add etc..
- A set of arguments related to the function selected will then be displayed.
- Enter the appropriate arguments related to the function selected.
- Select where you want the new column to be located in the table.
- Enter the new column name
- If you wish to add multiple columns then use the **Add to List** option.

Many different functions are available:

- **New** Add a new column containing a real number, integer, string,or random number.
- **Transformations** A number of transformations can be selected and applied to a table column as shown below.
- **Mathematical** A number of mathematical functions
- **Text** Apply a number of different functions to the text in a column.
- **Chemical** Calculate a number of different chemical properties.
- **Convert Units** Radian to Degrees and Degree to Radian

Once the function and the correct arguments have been entered:

- Select whether you wish the new column to be added before,after or in place of this column.
- Enter the name of the new column.

NOTE: If you want to add more than one column choose **Add to List** and the action will be added to a list on the right hand side of the dialog box.

7.1.25 Column Statistics

To calculate various statistics describing columns and inter-column relationship:

- Right click on the column header and a menu will be displayed.
- Select "Column Statistics"

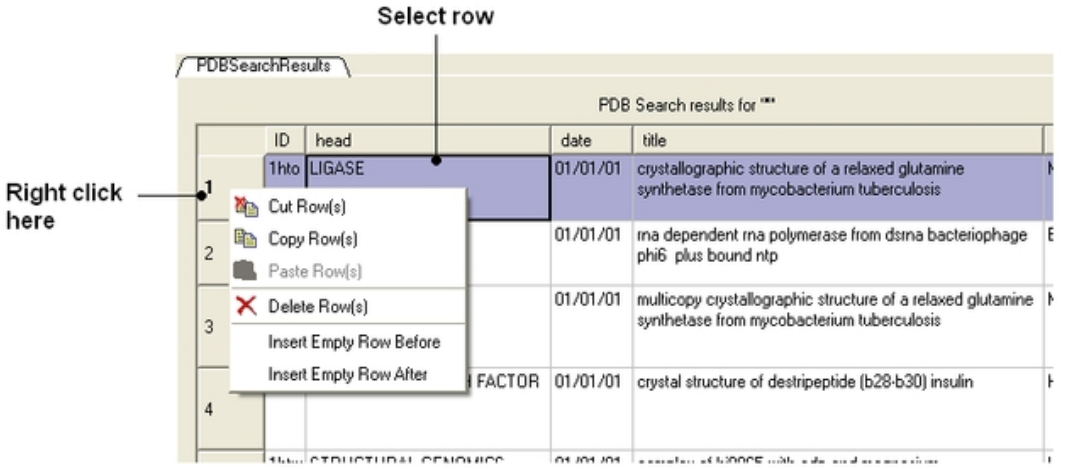
The output is printed into the ICM Terminal window and the Column Statistics Window.

7.1.26 Inserting Rows

To insert a row:

- Identify the position within the table where you wish the row to be inserted and `select` the row.
- Right click on the row name (eg the number of the row) and a menu will be displayed.
- Select **Insert Row Before or Insert Row After**.

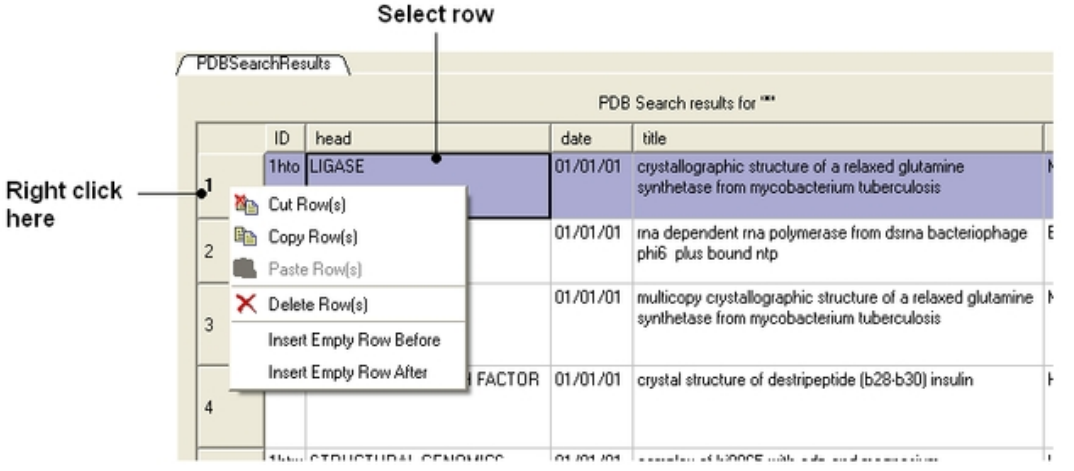
A blank row will be inserted. You can add data to this row by following the instructions in the `edit table section`.



7.1.27 Copy Cut and Paste Row

Copy, Cut and Paste Row:

- Select the row(s) `See table selection section`.
- Right click on the row header
- Select **Copy Row(s)**.
- To paste a row select the row header under which you wish to paste the row. Right click and select **Paste Row(s)**



7.1.28 Copy Cell

To copy a table cell:

- Right click on cell.
- Select Copy Cell - you can then paste it into a new table.

7.1.29 Copy Selection to an ICM Table

To copy a selection to a new table:

- Select the row(s) `See table selection section`.
- Right click on the row header
- Select **Copy Selection to ICM Table** and then choose Auto (ICM will name the table or New and you can enter a new table name.

7.1.30 Deleting Columns and Rows

To delete a column or row:

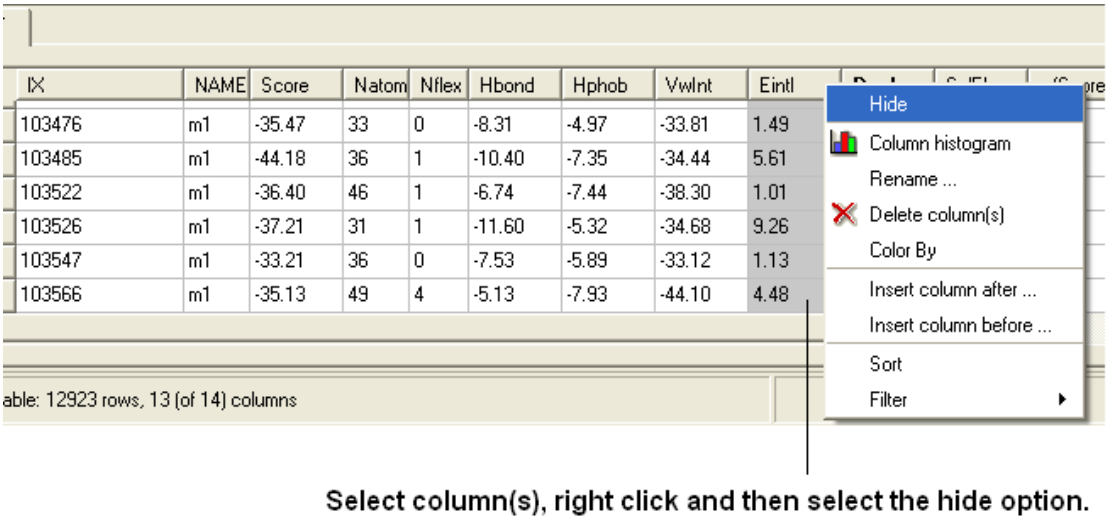
- Select the column(s) or row(s) you wish to delete. See the `select table` section for information on how to make table selections.
- Right click on the row to delete a row or right click on the column header to delete a column and select the delete option from the menu.

7.1.31 Hide and Show Columns

If you have a large table you may wish to only show and display certain columns and hide others. By default any loaded table will have all the columns displayed.

To select which columns you wish to hide:

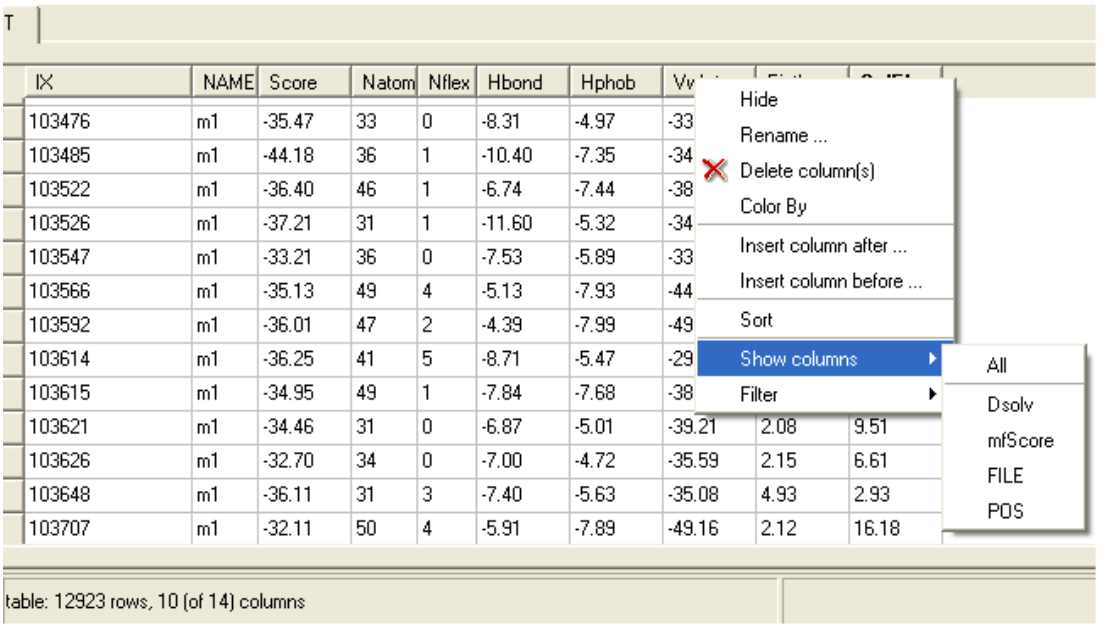
- Select the column(s) you wish to hide. See the `select table` section for information on how to make table selections.
- Right click and select the hide option from the menu.



Select column(s), right click and then select the hide option.

To show hidden columns:

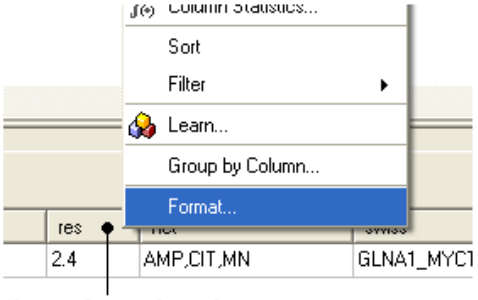
- Right click on the column header and a menu will be displayed.
- Select the **Show Columns** options.
- Select which column you wish to show from the drop down list.



7.1.32 Column Format and Custom Actions

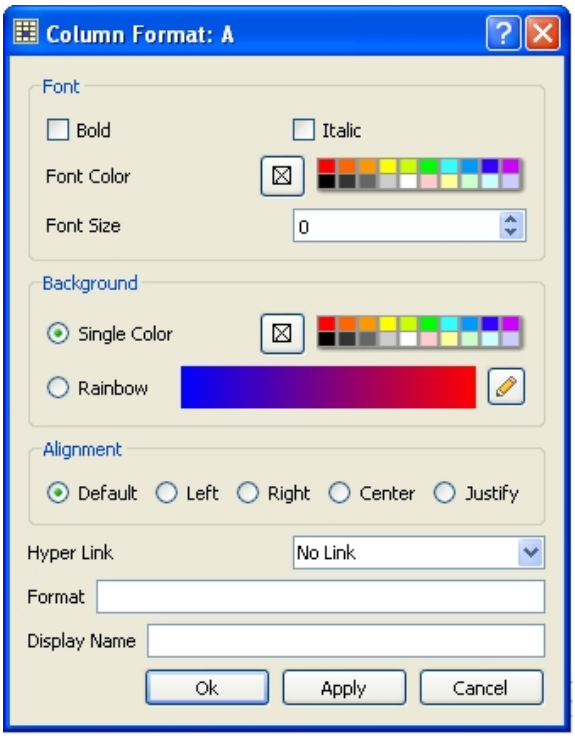
To change the **font** color or size, the **alignment** of the column data, the background color, add hyperlink, or script:

- Right click on the column header and select **Format**



Right click on the column header

- A window as shown below will be displayed.
- Make the desired changes and click **Apply**



To add a hyperlink to PubMed, PDB or Uniprot:

- Click on the drop down hyper link button.
- If the data in the column is a **PDB**, **Uniprot/SwissProt** or **PubMed** code then choose the built in format from the menu.
- Click Apply and the data in the column will become blue hyperlinks.

To add a user-defined hyperlink:

- Click on the drop down hyperlink button.
- Choose "Simple link" See below for details on how to access cell data.
- Click Apply and the data in the column will become blue hyperlinks.

To add an internal ICM link:

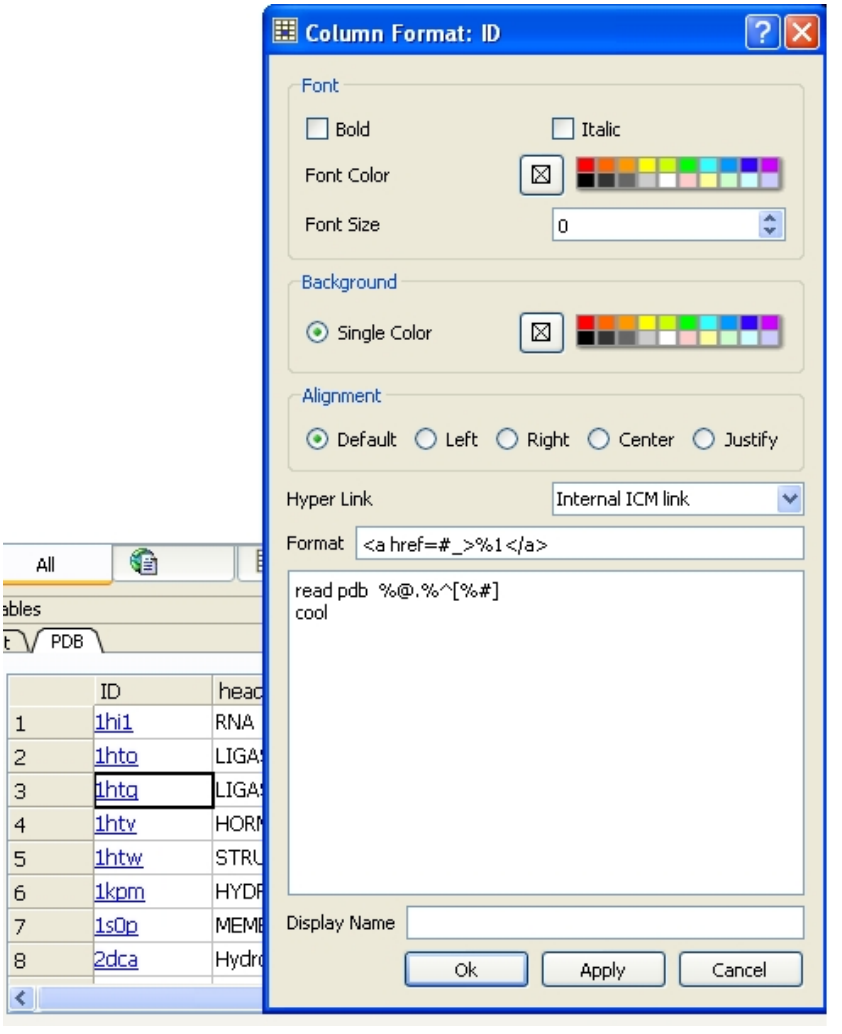
- Click on the drop down hyperlink button.
- Choose "Internal ICM link" See below for details on how to access cell data.
- Enter ICM scripting language in the panel that opens (see image below).
- Click Apply and the data in the column will become blue hyperlinks.

The value of the clicked cell is accessed as %1. To refer to the other cells and/or table itself the following shortcuts can be used:

- %@ # table name
- %# # clicked row number
- %^ # clicked column number

Example:

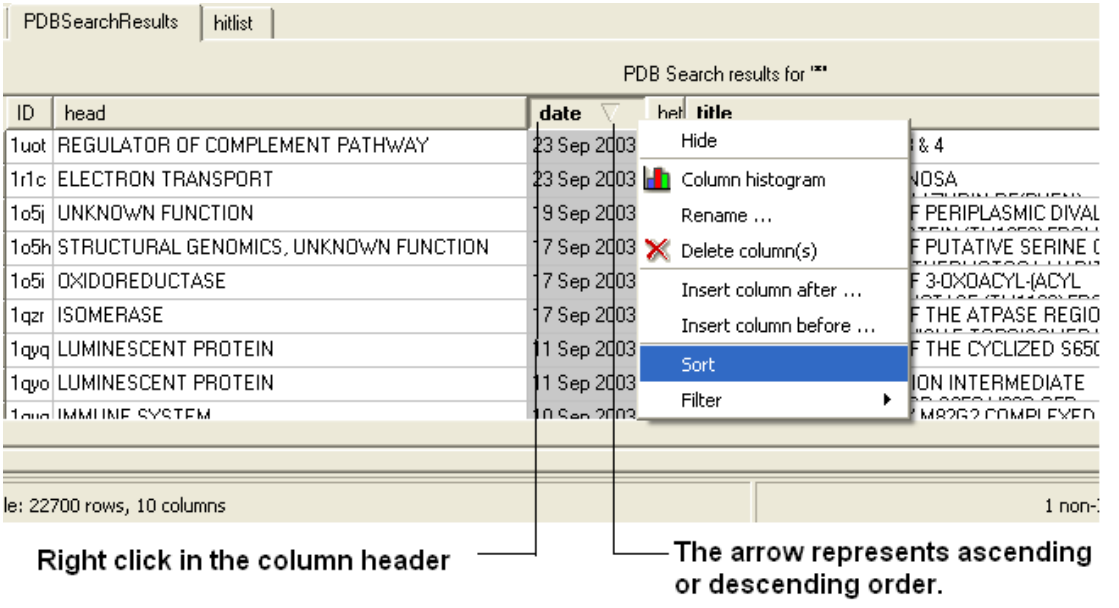
To add a an internal ICM link that reads a pdb dile and then displays it you could use the following ICM commands in the link:



7.1.33 Table Sorting

To sort a table by a column value:

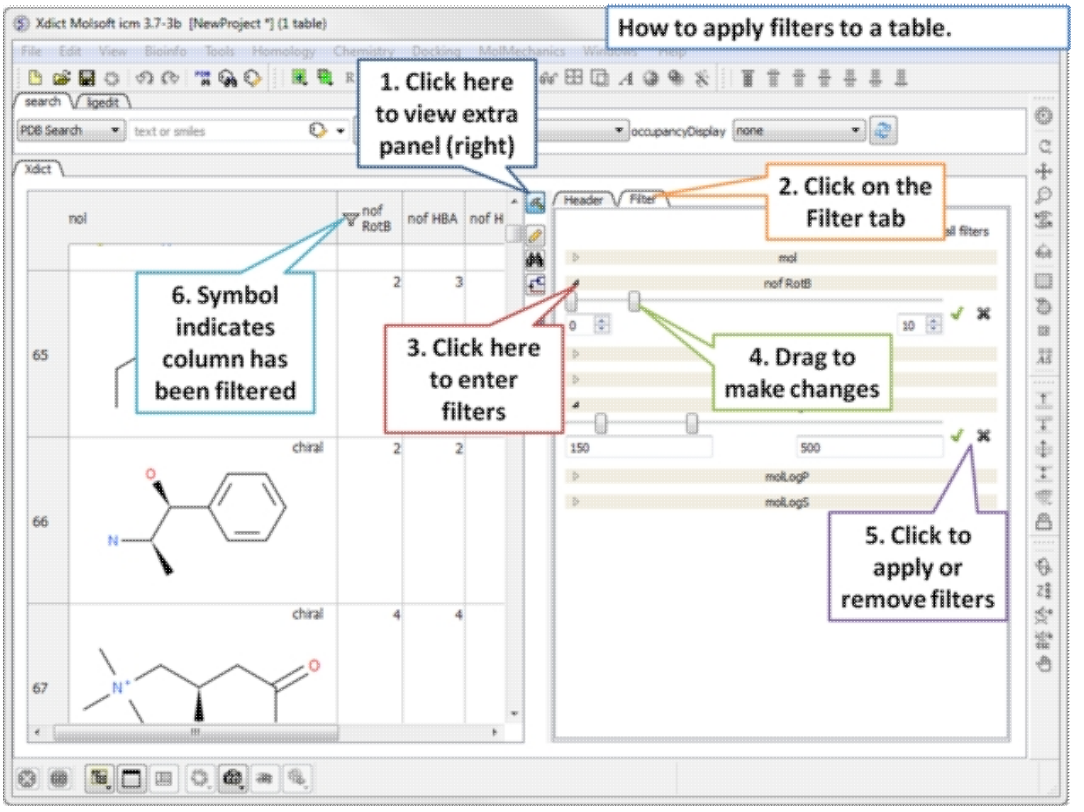
- Right click on the column header.
- Select the **Sort** option.



7.1.34 Table Filtering and Appending

There are two ways to filter table content one is via the table panel or by using the right click column header options.

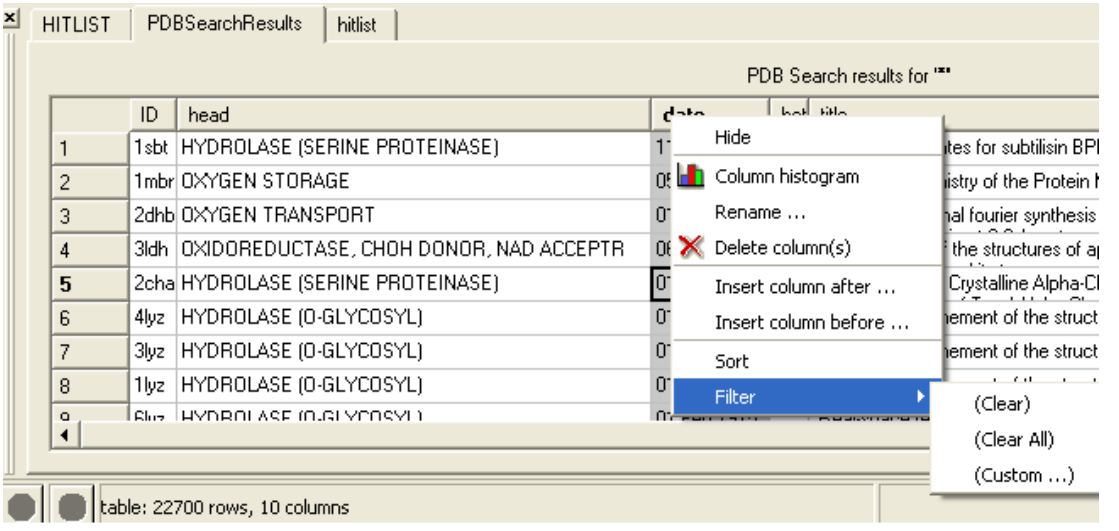
To filter a table using the extra panel sliders:



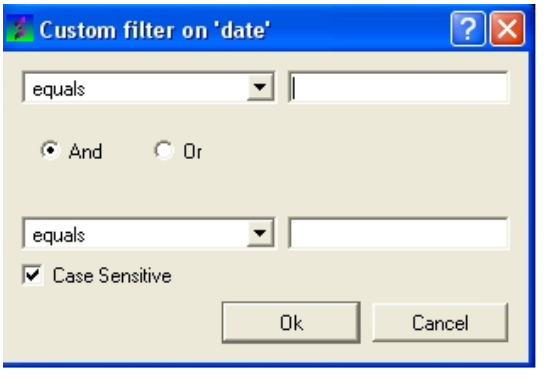
Open the extra panel and choose the filter tab. Click and drag on the sliders to conveniently choose the filtering values or enter the values directly. Click on the green 'tick' to apply filters.

To filter a table using the column header:

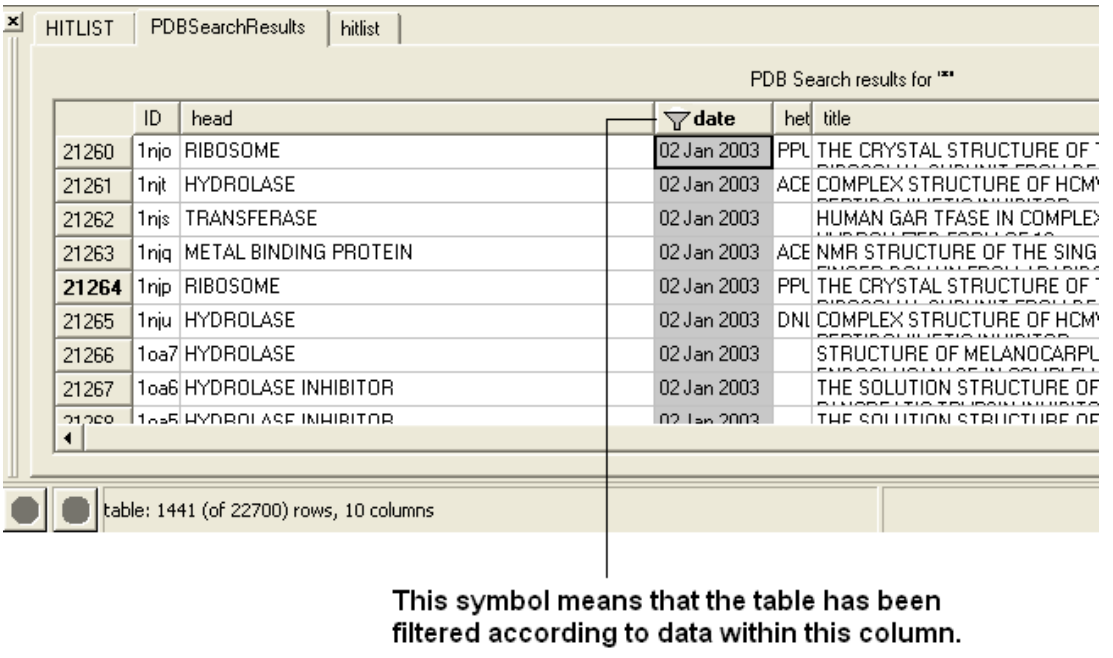
- Select the column you wish to filter. See the `select table` section for information on how to make table selections.
- Right click on the column header.
- Select the **Filter** option.



- Select the "Custom" option and a data entry box as shown below will be displayed.
- Enter the appropriate operations and filter values for your search.
- Click OK.



NOTE: When a column has been filtered a symbol as shown below will appear in the header of the column.



To append the filtered information into a new table:

- Select the whole table either by right clicking or pressing Ctrl A.
- Right click on the table and select "Append to other table".
- Enter a new name for the table you are appending with your filter results.

OR

Selected rows can be appended to a new table by:

- Right clicking on the selected rows and a menu will be displayed.
- Selecting the "copy selection to ICM table" option.

A table can be filtered by a cell value:

- By clicking once in a cell.
- Right click and a menu will be displayed.
- Select the option "Filter by cell value".

A filter can be cleared by:

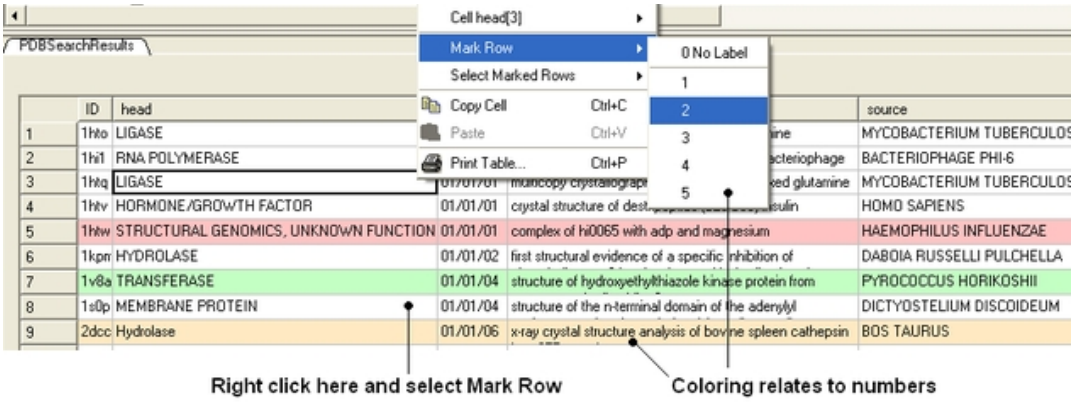
- Right clicking on the column selection and selecting Filter/Clear or Filter/Clear All

7.1.35 Mark and Select Rows

A row in a table can be marked and grouped by a label which enables the row(s) to be selected easily at a later time.

To mark a row

- Right click on the row in the table you wish to **mark.**
- Select **Mark Row/** and then choose a number. In the GUI the number of rows that can be marked is limited to 5 but this can be increased using the command line command.
- A row that is marked will be colored - each number is assigned a color. The coloring can be changed in the `gui tab in preferences`.



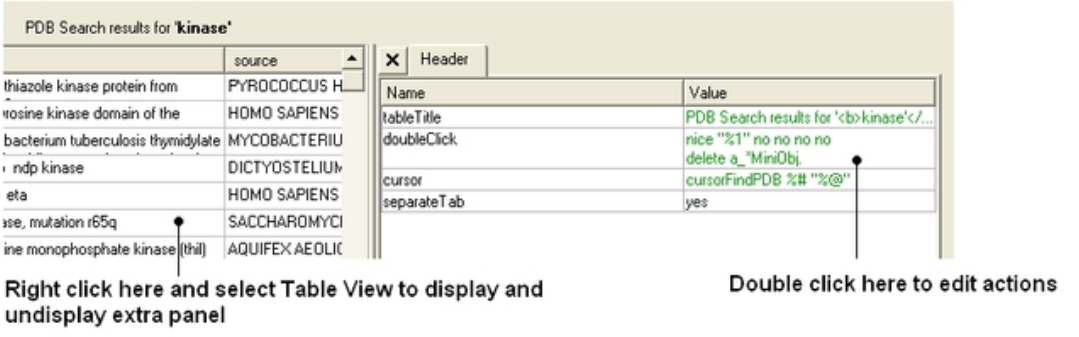
To select marked rows

- Right click on the table and choose **Select Marked Rows** and choose a number which relates to the marked rows as described earlier.
- Selected rows will be highlighted blue - once rows are selected a number of right click options are activated such as copy selection to new ICM table.

7.1.36 Mouse and Cursor Actions on a Table

The actions resulting from a mouse click or cursor on a table can be changed by:

- Right click on a table and select Table View/Show Extra Panel
- A panel as shown below will be displayed.



- Double click in the **Value** column and the column can be edited. Add ICM commands for the action you want. A value in a column can be referred to using "%" e.g. column two would be referred to as "%2". In the example shown above the function nice is acting on the contents of column one for the double click action.

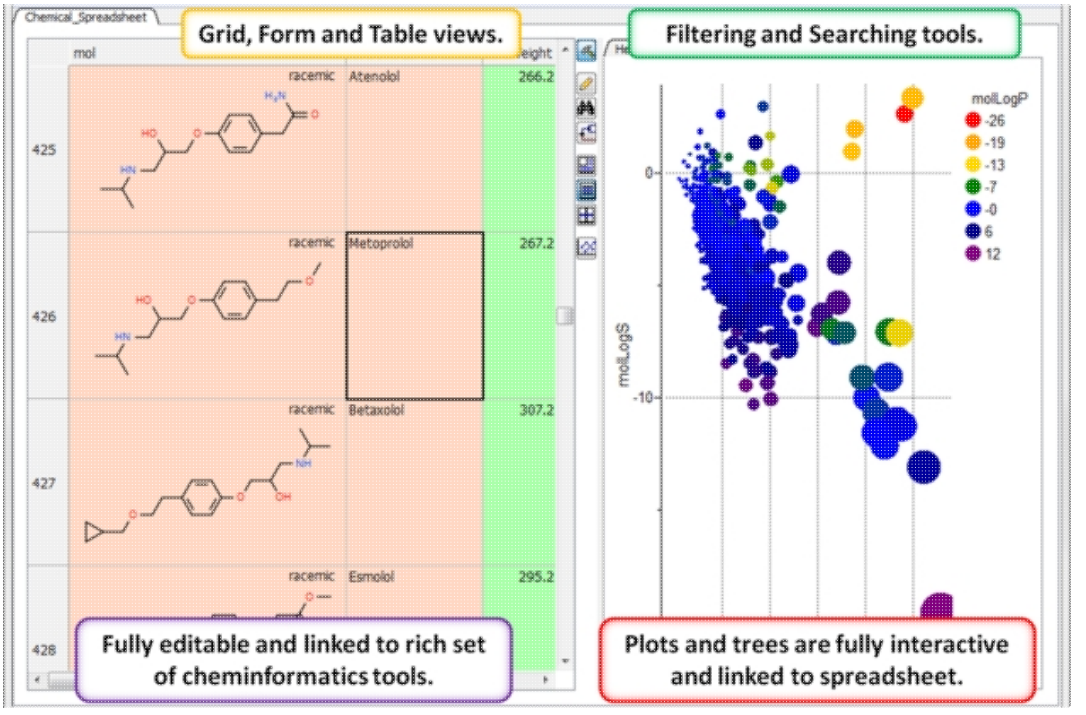
NOTE: The action associated with cursor and double click is placed in a variable name TableName.cursor and TableName.doubleClick

7.2 Molecular Tables

Available in the following product(s): `ICM-Chemist` | `ICM-Chemist-Pro` | `ICM-VLS`

An ICM molecular table is created when an SDF or Mol file is read into ICM. To read and open a mol or sdf file go to File/Open `(See Open an ICM file section)` All of the table functions described in the previous section `Standard ICM Table` can be applied to molecular tables. Molecular tables are described in more detail in the Cheminformatics chapter.

An example of an ICM molecular table:



7.3 Insert Interactive Objects into Table Cell

Available in the following product(s): `ICM-Chemist` | `ICM-Chemist-Pro` | `ICM-VLS`

NOTE: This option is available in Version 3.7-2b and above.

To store objects in a table please use the following:

Example:

```
read pdb "1crn"
display a_
add column t Parray( object a_ preview )
```

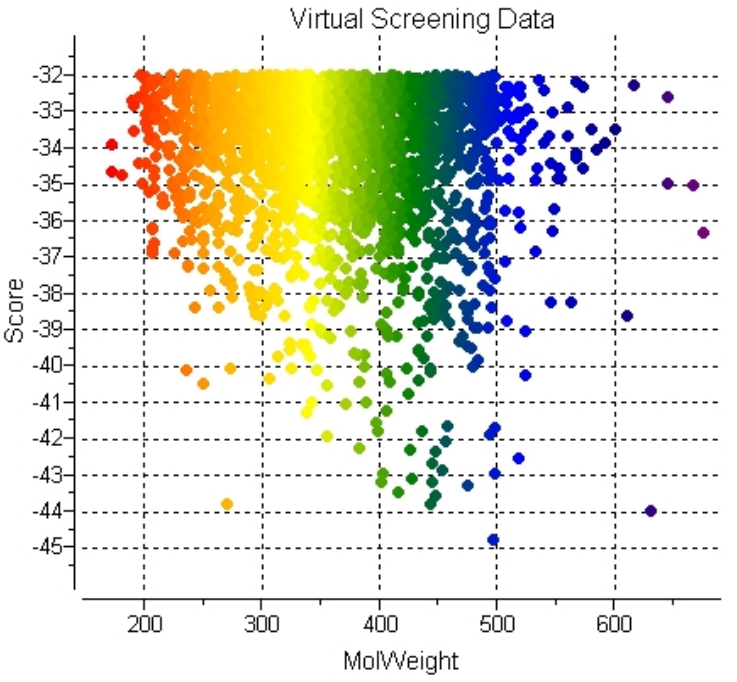
Viewing Objects from the table can be dragged and dropped into the ICM Workspace to display them again.
How to make the objects in the table fully interactive

- Right click on the column header and select "Live Rotatable View"

7.4 Plotting Table Data

Available in the following product(s): `ICM-Chemist` | `ICM-Chemist-Pro` | `ICM-VLS`

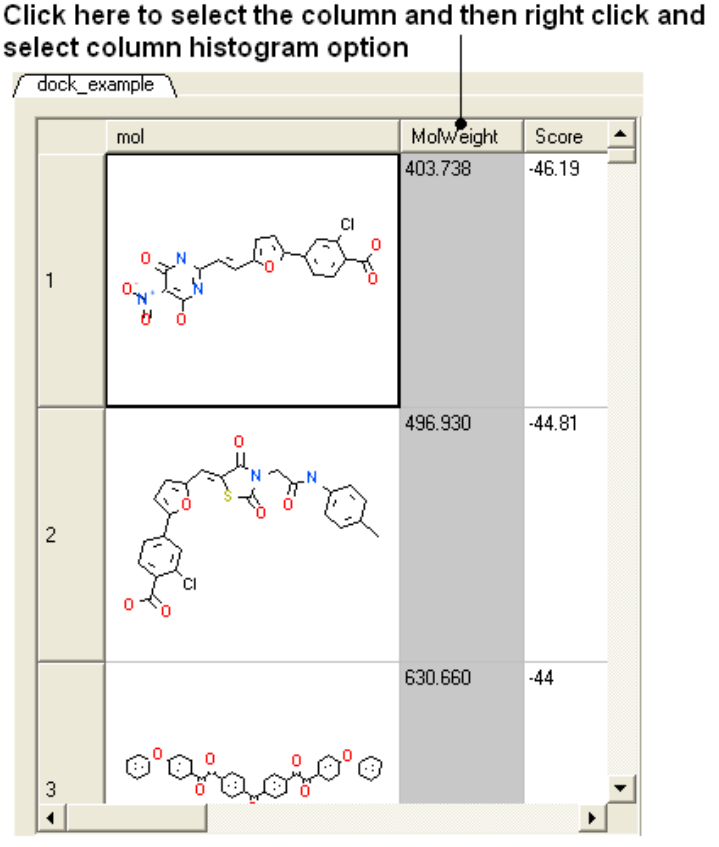
The data within a table can be plotted graphically. A histogram can be made for the data within one column or a plot can be constructed for the data within two columns.



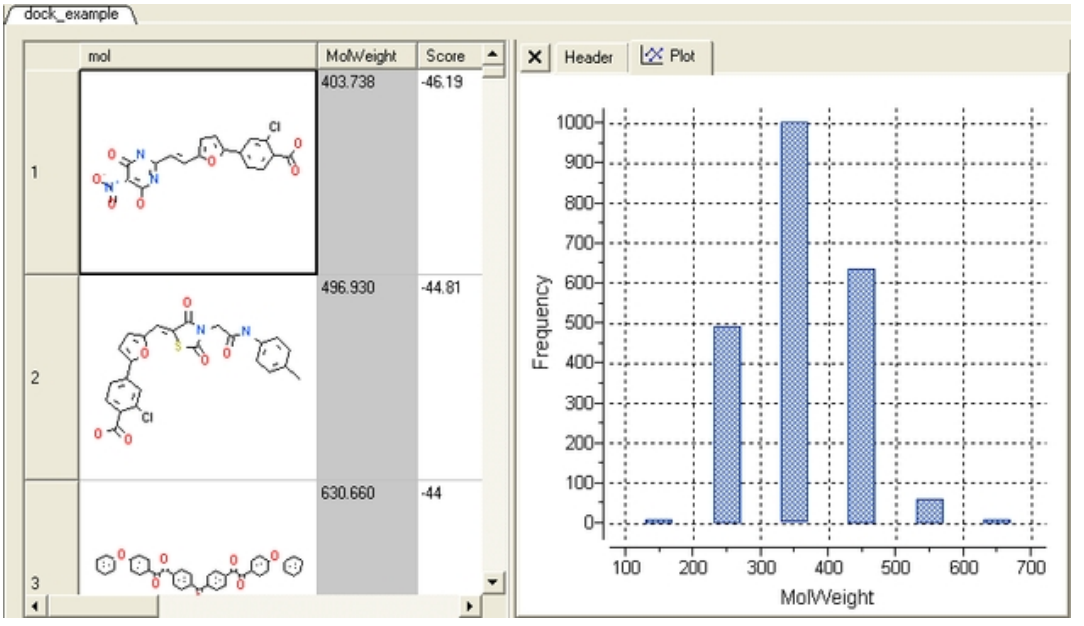
7.4.1 Column Histogram

To plot a histogram of the data within one column:

- Select the column by clicking on the column header.
- Right click on the column header.
- Select the **Column histogram** option.



A plot will then be displayed next to the table.

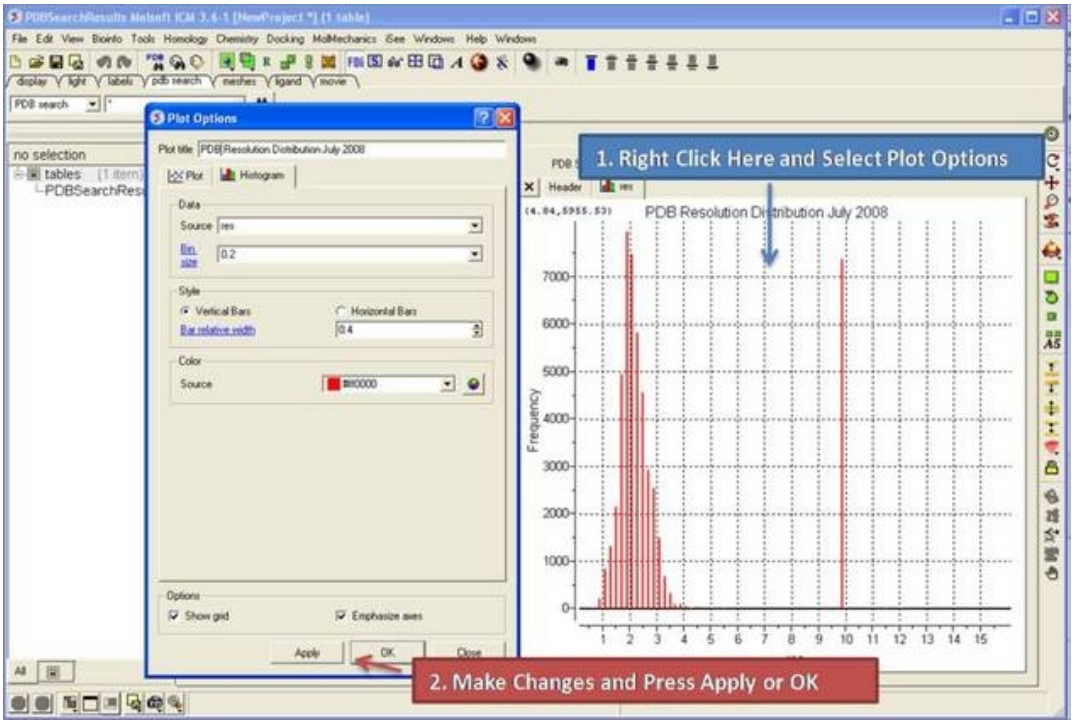


7.4.2 Histogram Options

Once you have created a histogram you can change the following parameters by right clicking on the plot and selecting options

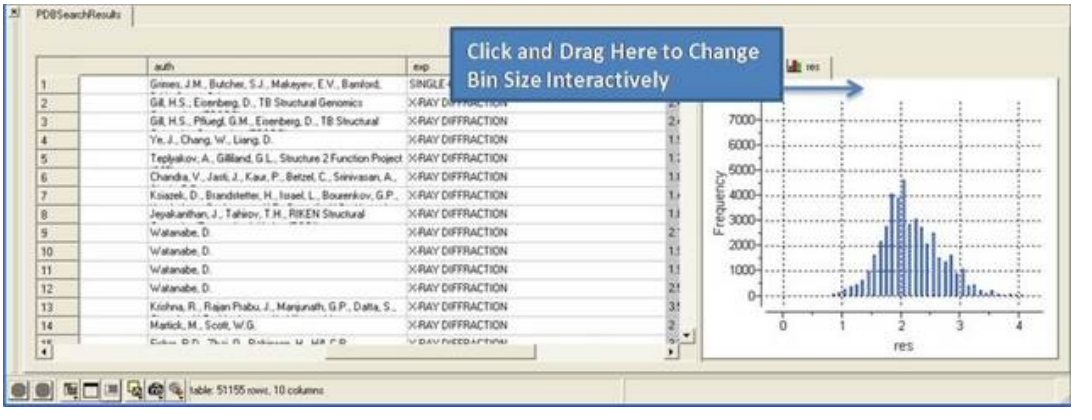
Options:

- Change plot title.
- Change the data source using the drop down button and select another column in the table.
- Change the histogram bin size.
- Change the bars positioning from vertical to horizontal.
- Change the bar relative width compared to bin size. Bigger values give thicker bars.
- Color the bars



7.4.3 Histogram Bins

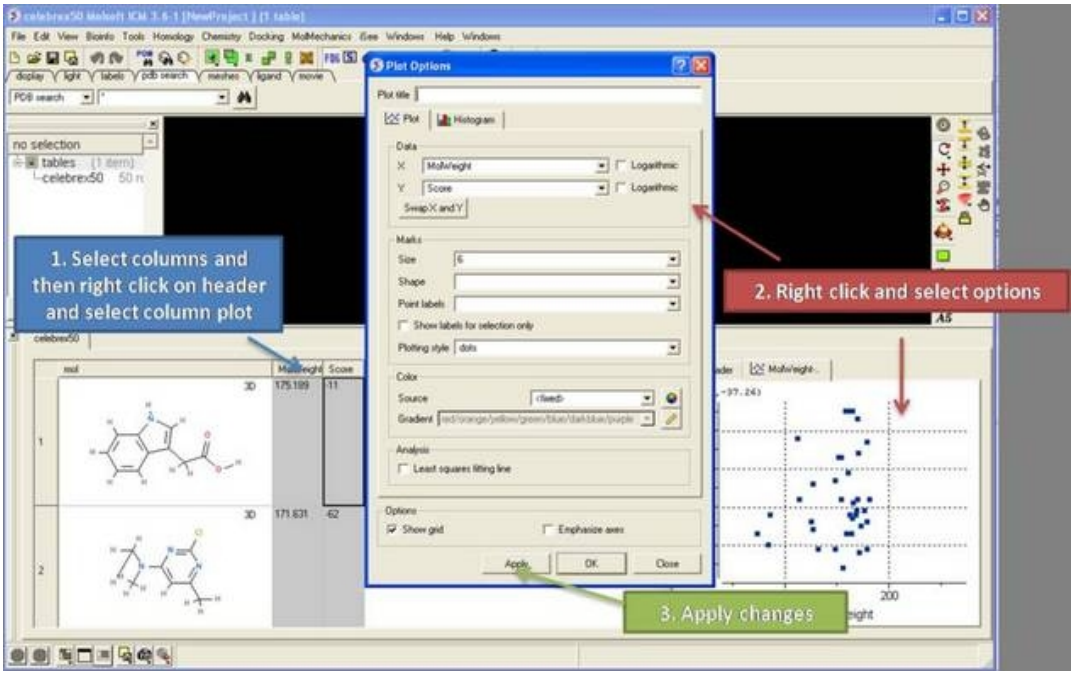
There are two ways to change the bin size. 1. Using the **options** dialog box or 2. interactively by left clicking and dragging at the top of the plot as shown below - this will allow you to find the best density estimation picture.



7.4.4 Plotting two columns

To construct a plot from data within two columns:

- Select the two columns.
- Right click on the column header.
- Select the **Columns plot** option.



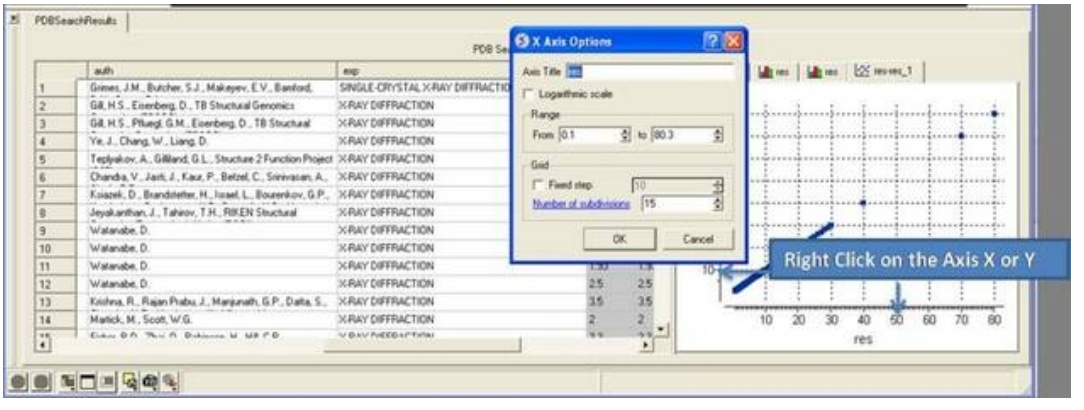
7.4.5 Add a title to a plot

To add a title to a plot:

- Right click on the plot and select **Edit Title** or choose **Options**

7.4.6 Axis Options

Each axis has a set of options which can be accessed by right clicking on the axis and selecting **Options.**



To change the title of the X or Y Axis:

- Right click on the axis and select **options**

To change the data range:

- Right click on the axis and select **options**
- Change the **From** and **to** values in the **Range** box

To change the Grid steps (ticks) on the X or Y axis:

- Select either a fixed step e.g. 10 and you can define the number of subdivisions (ticks) in each step. Choosing 1 will display zero ticks between divisions.

To change the axis to logarithmic

- Right click on the axis and select **options**
- Select the Logarithmic scale check box

7.4.7 Change Axis Data

To swap the X and Y axis:

- Right click on the plot and select **Options**.
- Select the **Swap X and Y** button.
- Click OK.

To change the data source for either the X or Y axis:

- Right click on the plot and select **Options**.
- Select the drop down arrow as shown below and select a different column from the table.
- Click OK.

7.4.8 Logarithmic Plots

To change the scale of the axis to logaritmic:

- Right click on the plot and select **Options**.
- Select the **Logarithmic** check box.

7.4.9 Change Mark Shape or Size

To change the plot mark, shape, style or label:

- Right click on the plot and select **Options**.
- Select the desired size and shape using the drop-down buttons in the **Marks** section of the window.

To add point labels:

- Right click on the plot and select **Options**.
- Select the drop down arrow in the **Point labels** dialog box
- If you only want to label selected points check the **Show labels for selection only** option. Making plot selections is described `here`.

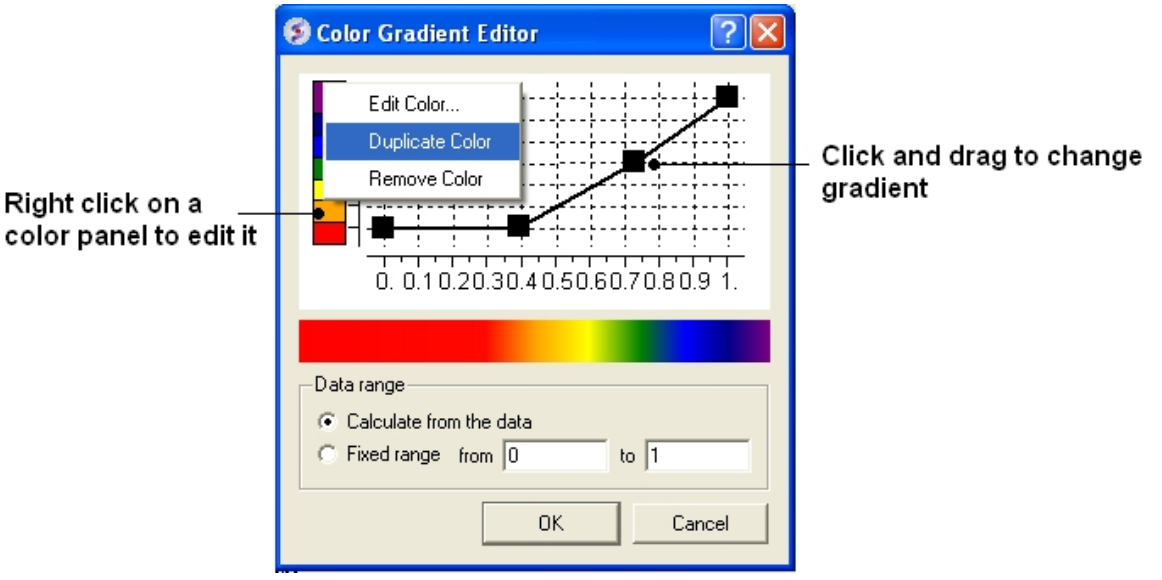
7.4.10 Change Mark Color

To change the color of the plot marks:

- Right click on the plot and select **Options**.
- In the **Color** section of the window select the **Source** (column name plotted as X or Y) you wish to color.
- Select the color palette and choose the desired color or you can choose a Gradient of colors.

To edit the color gradient

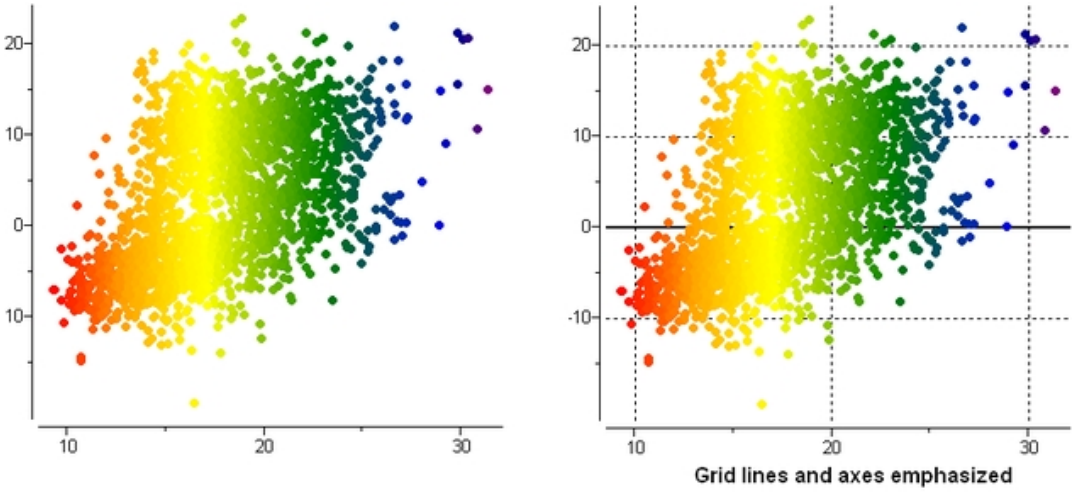
- Click on the **Color gradient editor** button and a window as shown below will be displayed.
- Click and drag on a mark in the gradient plot to change the color gradient.
- Right click on a color in the Y-axis to - **Edit, Duplicate or Remove Color**.
- The color gradient can be applied to all points in the data or for a fixed range.



7.4.11 Grid and Axis Display

To remove the grid display and/or highlight the axes:

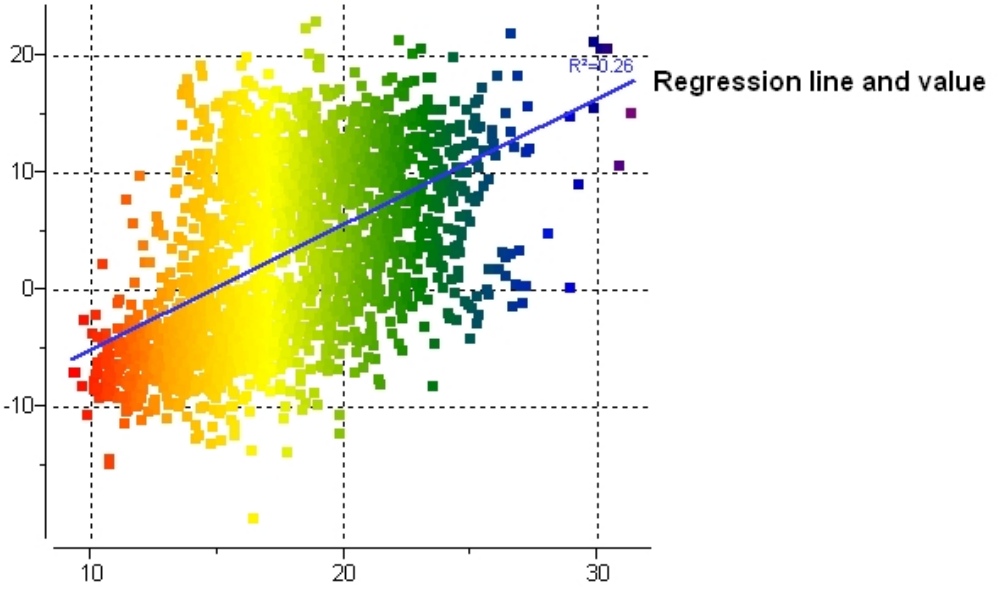
- Right click on the plot and select **Options**.
- Check the **Show grid** or **Emphasize axes** options.



7.4.12 Least Squares Fitting

To fit the data to a straight line using least square fitting

- Right click on the plot and select **Options**.
- Select the check box for **Least squares fitting line**.



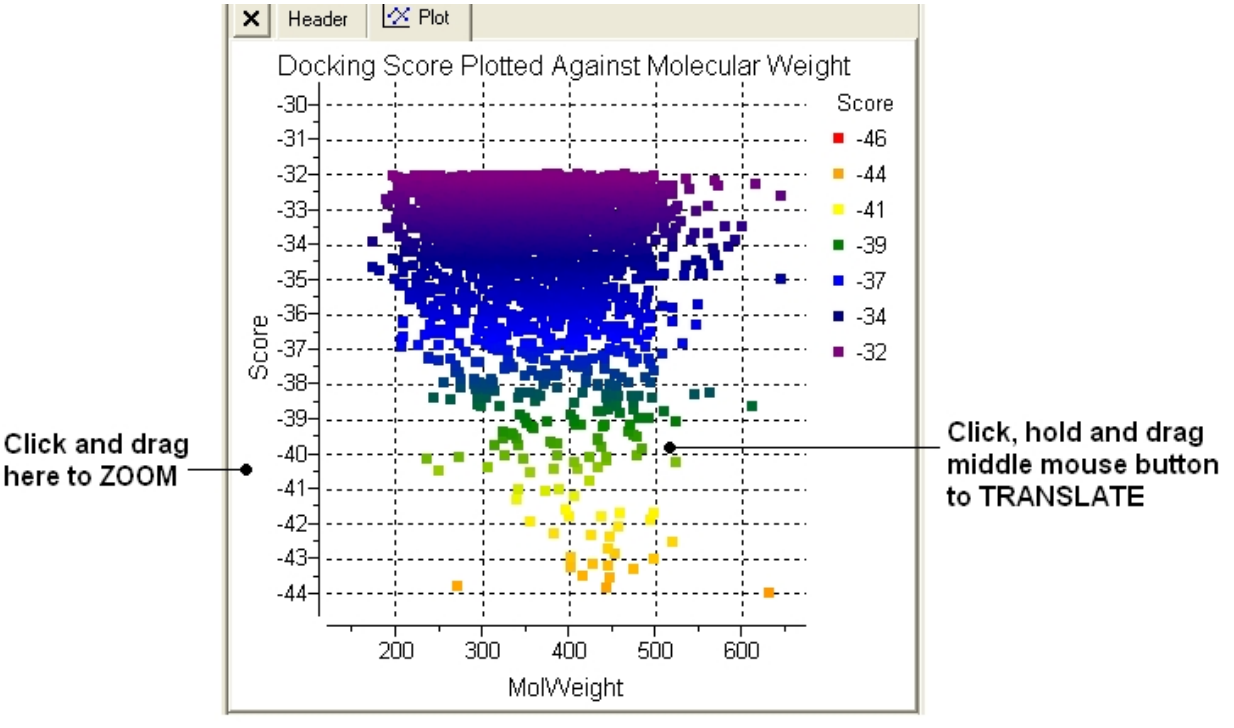
7.4.13 Zoom, Translate and Center

To zoom into a plot:

- Click outside the plot on the left-hand-side and drag the mouse or use the middle mouse wheel to zoom in and out.

To translate a plot

- Click, hold and drag using the middle mouse button on the plot.



To center onto a plot

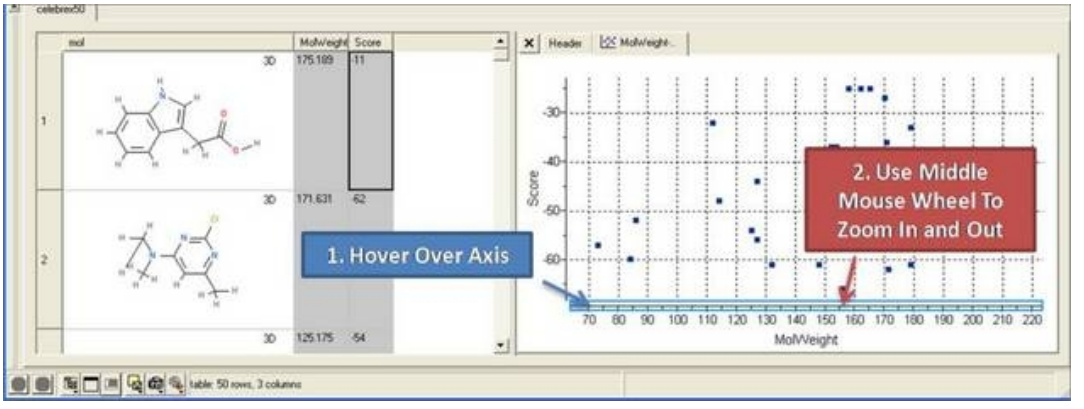
- Right click on the plot and select **Center all** or **Center Selection**. Making selections in a plot is described in the next section.

To center into an axis

- Right click on the axis and select **center.**

To zoom into an axis

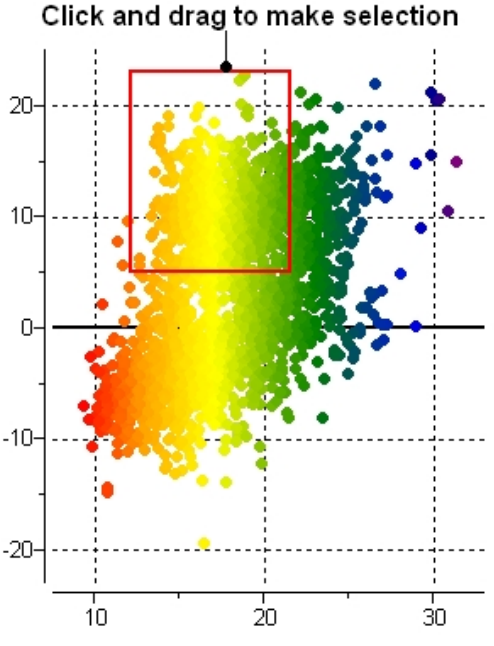
- Hover the mouse over the axis until you see a blue rectangle surrounding the axis.
- User the middle mouse wheel to zoom in and out as shown below.

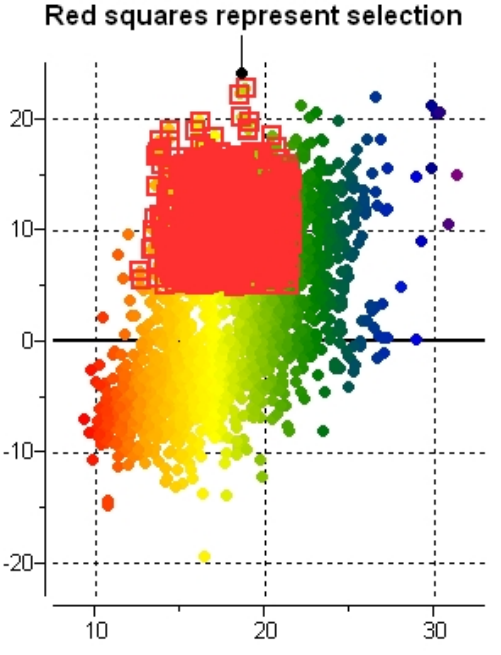


7.4.14 Plot Selection

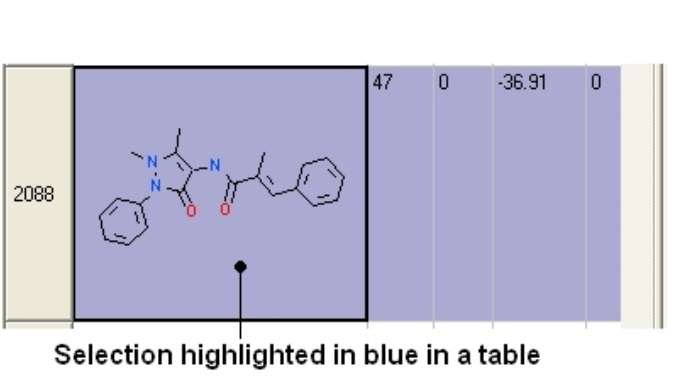
To make a selection in a plot:

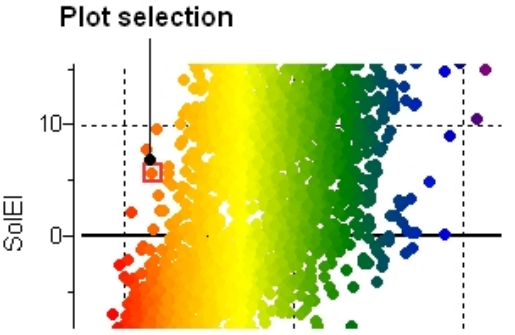
- Click and drag in the plot to make a selection. Individual points can be selected with a single click.



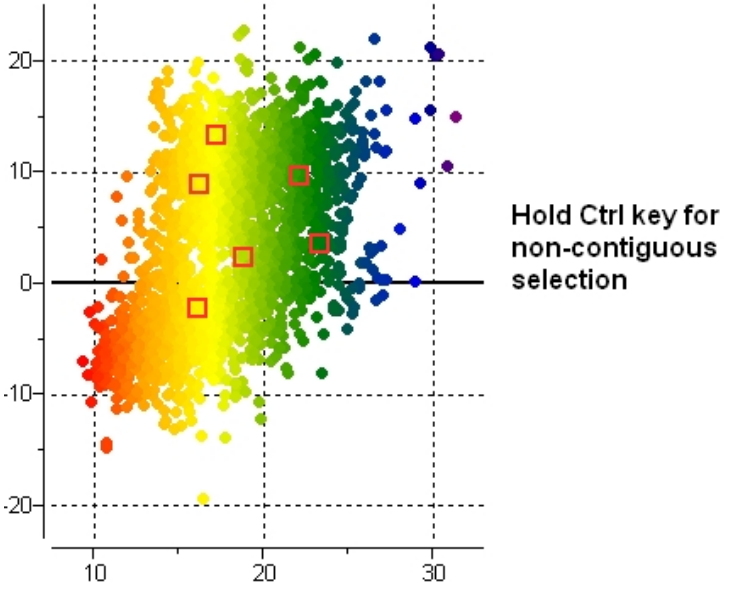


All selections are directly linked to the table from which the plot was made. Selections in the table are highlighted in blue.





Non-contiguous selections in the plot can be made by holding the CTRL key.



7.4.15 Print Plot

To print a plot:

- Right click on the plot and a menu will be displayed.
- Select the print option.

7.4.16 Saving a Plot Image

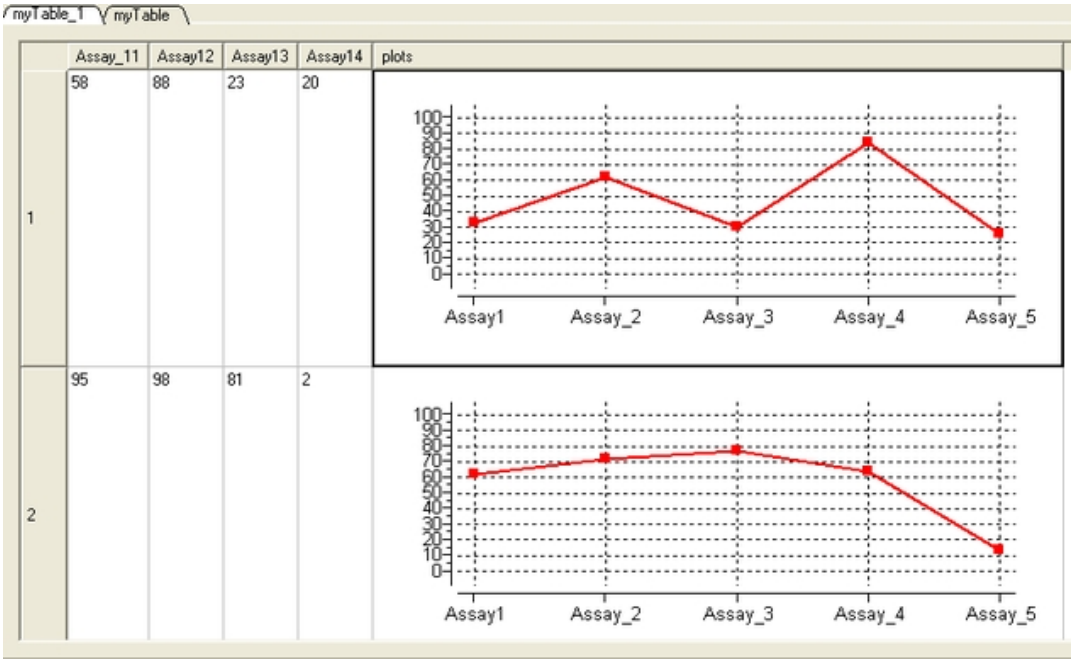
To save a plot image or copy to clipboard:

- Right click on the plot and a menu will be displayed.
- Select the **Save/Export Image** option.

7.4.17 Table Inline Plots

Plots can be inserted into a table row by:

- Select the columns you wish to plot.
- Right click on the column header and select **Inline Plots**
- The plot will then be displayed in each row of the table.


myTable_1
myTable
Assay_11
Assay12
Assay13
Assay14
plots
1
58
88
23
20
2
95
98
81
2
100
90
80
70
60
50
40
30
20
10
0
Assay1
Assay_2
Assay_3
Assay_4
Assay_5

8 Tutorials

'; winRef.document.write(str); }

Graphics Tutorials		
Molecule Representation, Coloring, Labeling and Annotation	HTML	
Creating Fully Interactive Slides for PowerPoint and the Web	HTML	Also see ActiveICM Reference Guide
Sequence and Alignment Tutorials		
Read Sequences and Align	HTML	
Link Sequence to Structure	HTML	
Protein Structure Tutorials		
PDB Search	HTML	
Convert PDB to ICM Object	HTML	
How to display hydrogen bonds between a ligand and receptor.	HTML	
PDB Preparation: Symmetry	HTML	
PDB Preparation: Occupancy & B-Factors	HTML	
PDB Preparation: Alternative Orientation	HTML	
PDB Preparation: Biomolecule	HTML	
Protein Modeling Tutorials		
Building an Homology Model	HTML	
Kinase Homology Modeling Example	HTML	
Loop Modeling	HTML	
Predicting the Effect of a Mutation on Binding	HTML	
Cheminformatics Tutorials		
Chemical Sketching using the Molecular Editor	HTML	also see Reference Guide
Chemical Substructure and Fingerprint Searching	HTML,	Also see Refrence Guide
Chemical Clustering	HTML,	
3D Pharmacophore Search	HTML	Also see video
2D Pharmacophore Search	HTML	Also see video
How to convert 2D chemicals to 3D	HTML	Also see video
Chemical Superposition	HTML	Also see Reference Guide
How to Build and Apply QSAR Prediction Models	HTML	Also see video Pt.1 video Pt.2
How to Create a Markush Structure	HTML	Also see video
How to Enumerate a Markush Library	HTML	Also see video
How to Decompose a library based on a Markush Library	HTML	Also see video
How to Enumerate a library by reaction	HTML	Also see video
ICM Interactive 3D Ligand Editor Tutorials		
Working with the ICM Interactive 3D Ligand Editor	HTML	Also see Reference Guide.
Ligand Docking Tutorials		
Dock Biotin to the Streptavidin Receptor	HTML	Also see video
Re-Dock an Inhibitor to Ricin Crystal Structure	HTML	

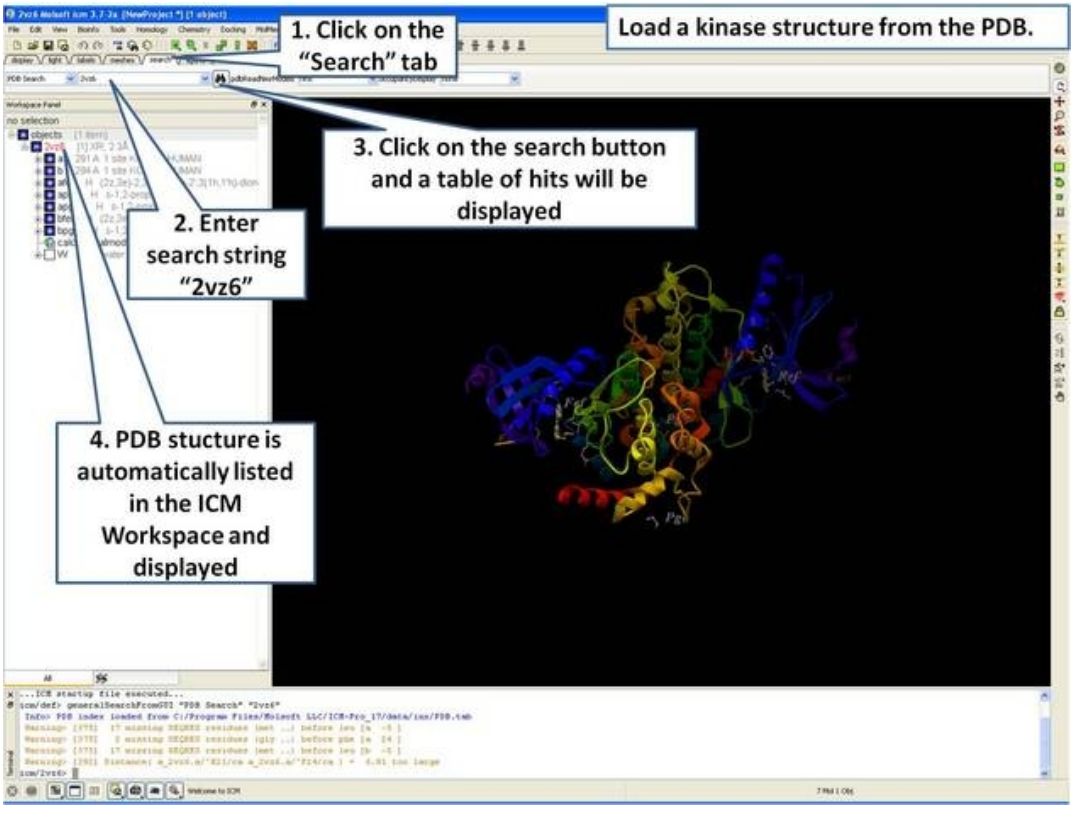
Covalent Docking	HTML	
Virtual Screening Tutorials		
Virtual Ligand Screening to Ricin Receptor	HTML	
Virtual Ligand Screening to Cyclooxygenase	HTML	Also see `video Pt.1.` video Pt.2
Docking a Markush Library	HTML	
Methods for Incorporating Receptor Induced Fit (Flexibility) Tutorials		
Multiple Receptor Conformation Ensemble Docking Example	HTML	
Explicit Group Docking	HTML	

8.1 Graphics Tutorials

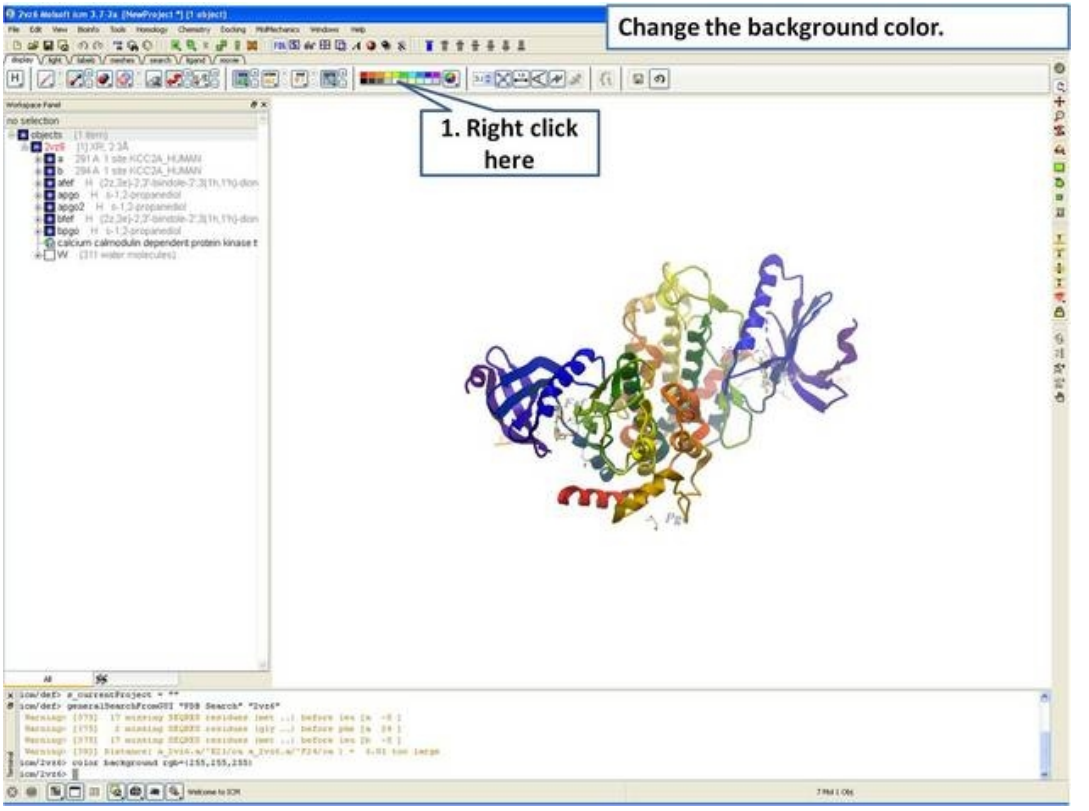
8.1.1 Change Molecule Representation and Color

This tutorial shows you how to:

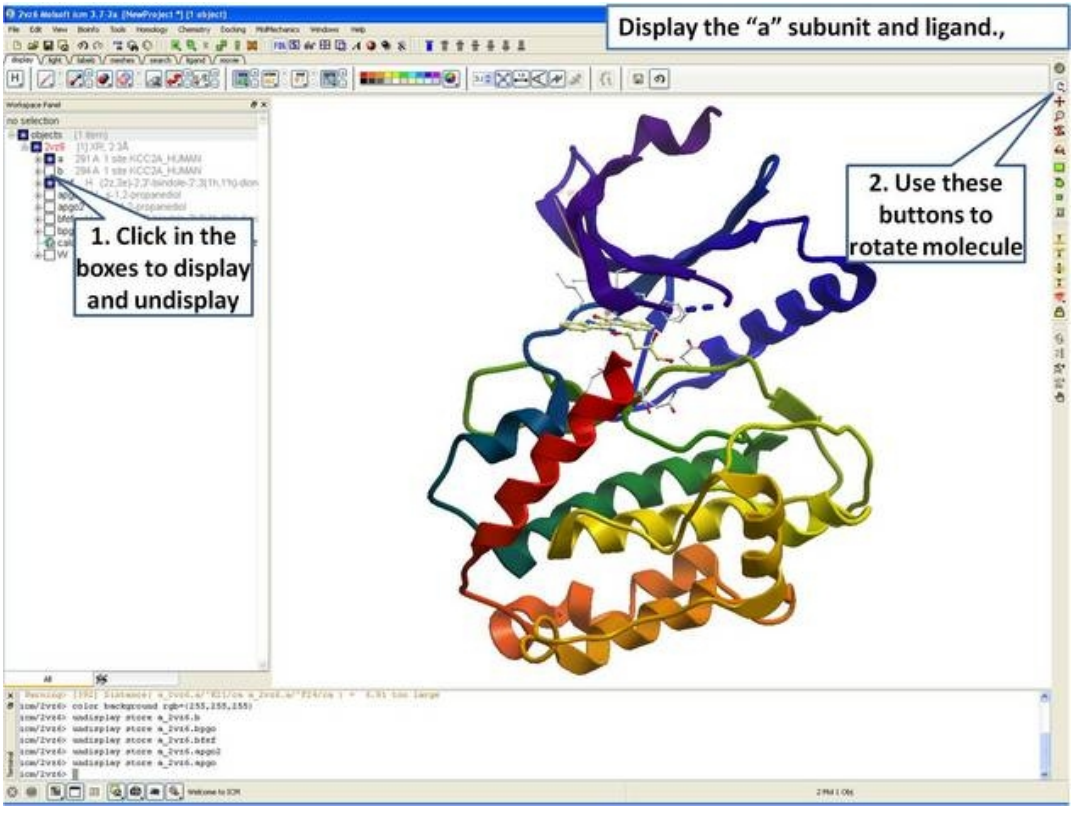
- How to load a PDB structure into ICM.
- How to change the background color.
- How to display and undisplay a molecule.
- How to color ribbon representation.



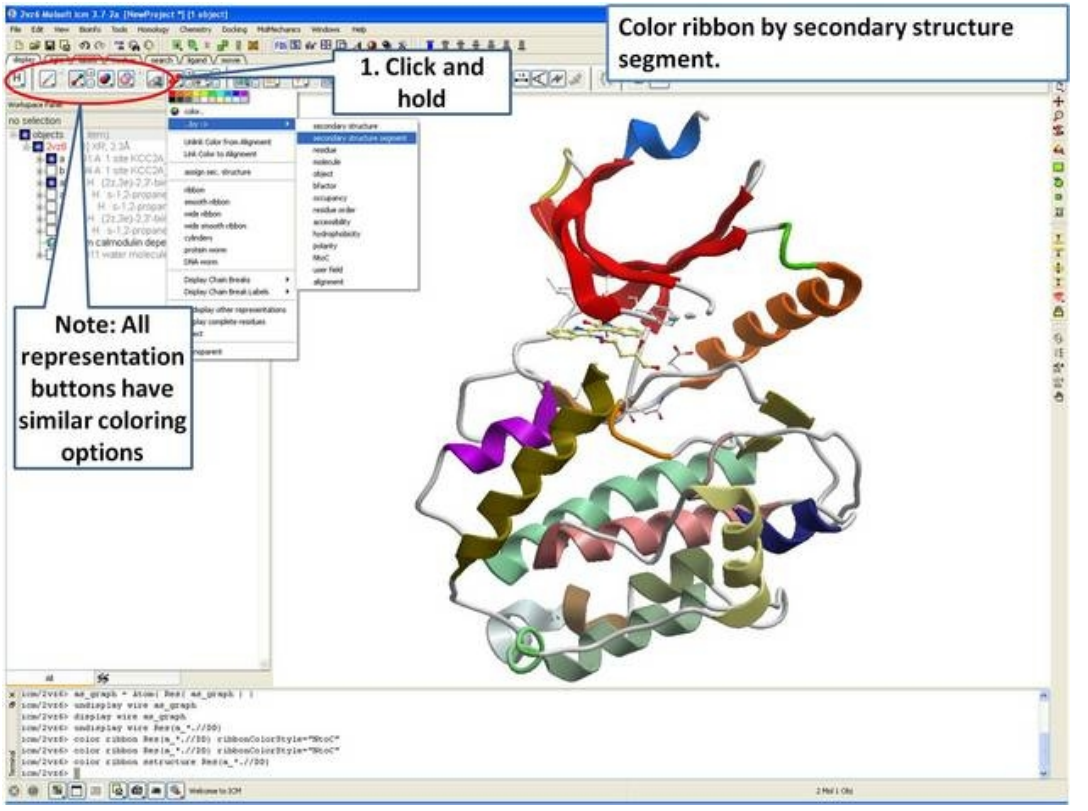
Step 1: Click on the search tab to load and display the PDB structure 2vz6



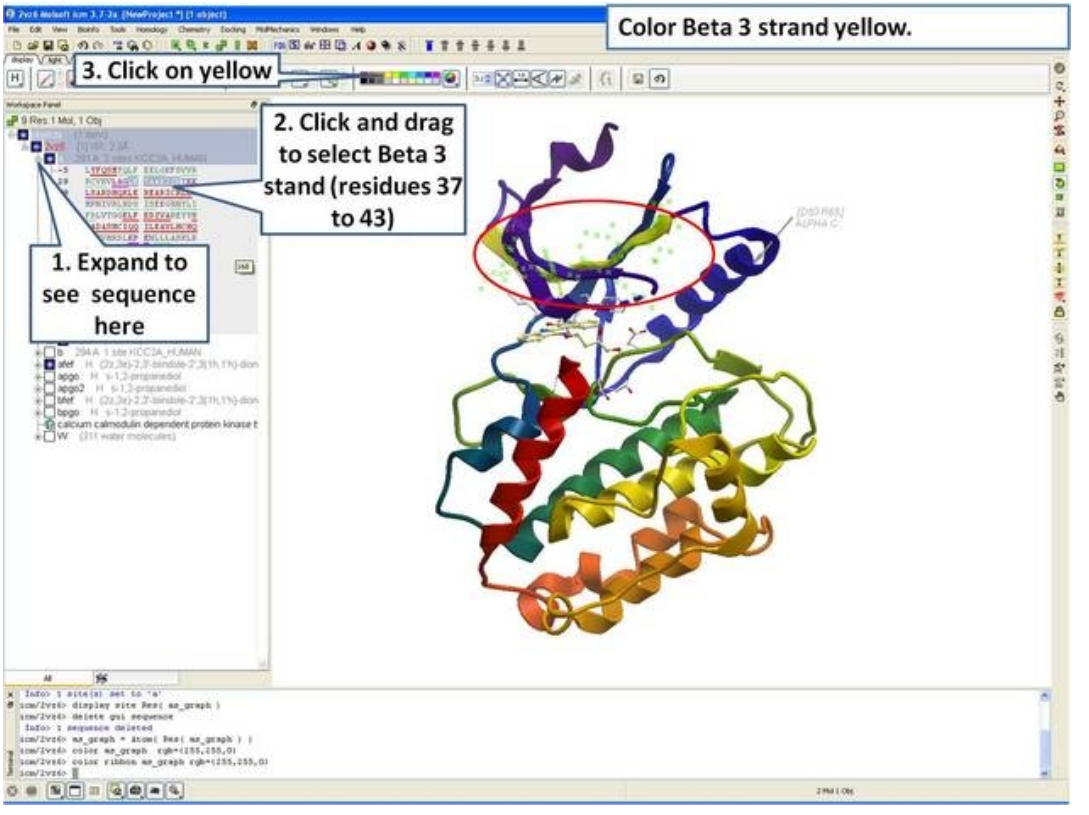
Step 2: Change the background color by right clicking on the color palette.



Step 3: Display the "a" subunit of the kinase.



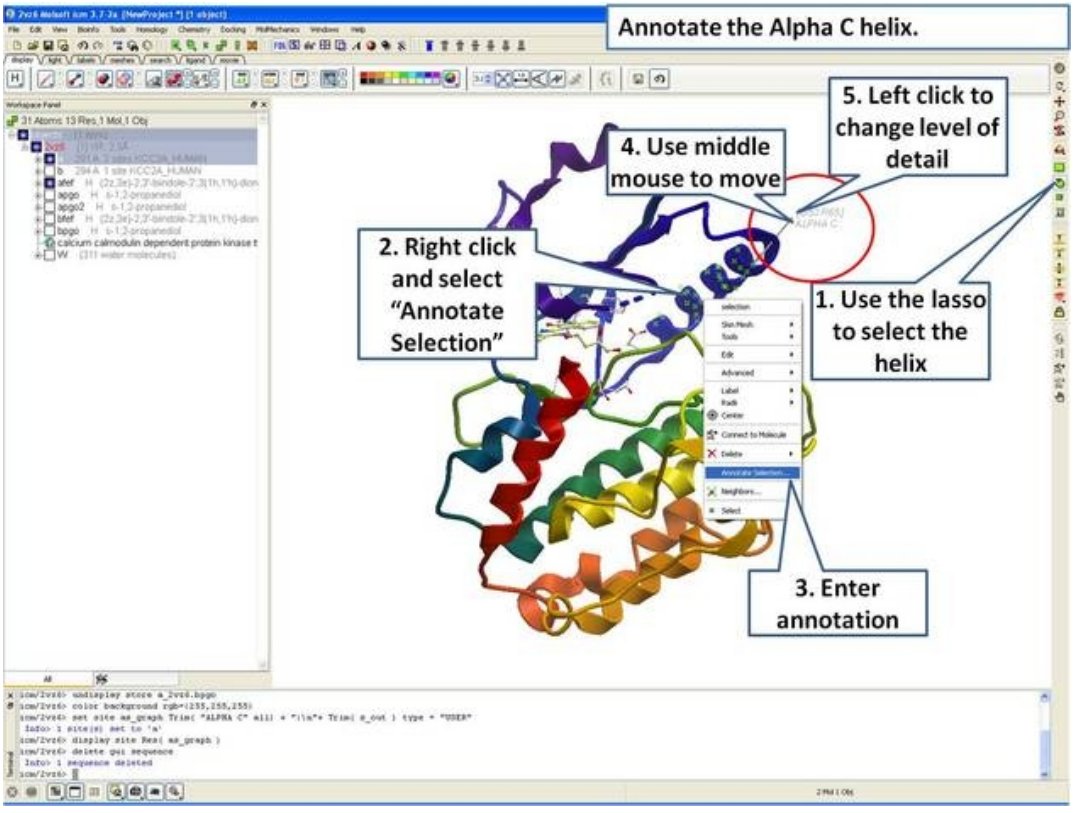
Step 4: Use the options in the "Display Tab" to color the ribbon.



Step 5: Select the beta 3 strand (residues 37:43) and color yellow.

8.1.2 Annotation

This tutorial shows you how to add user defined annotation to a particular region of a protein structure.

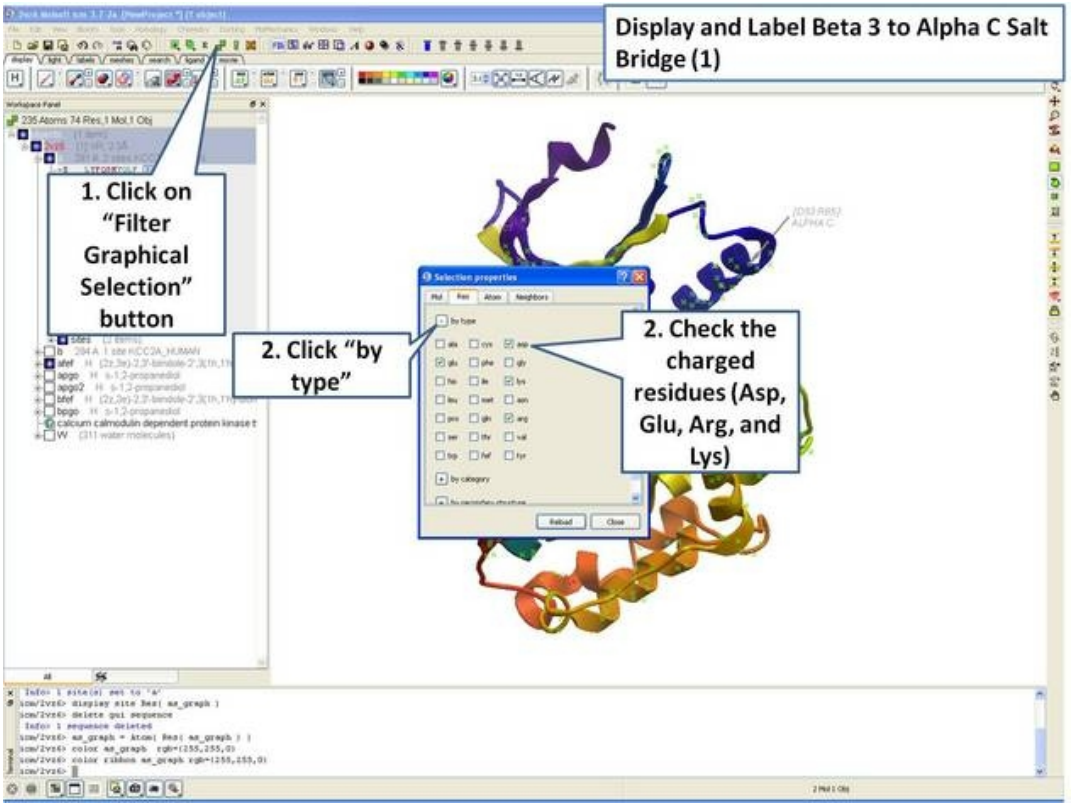


Step 6: Select the region you wish to annotate and right click on the selection for options.

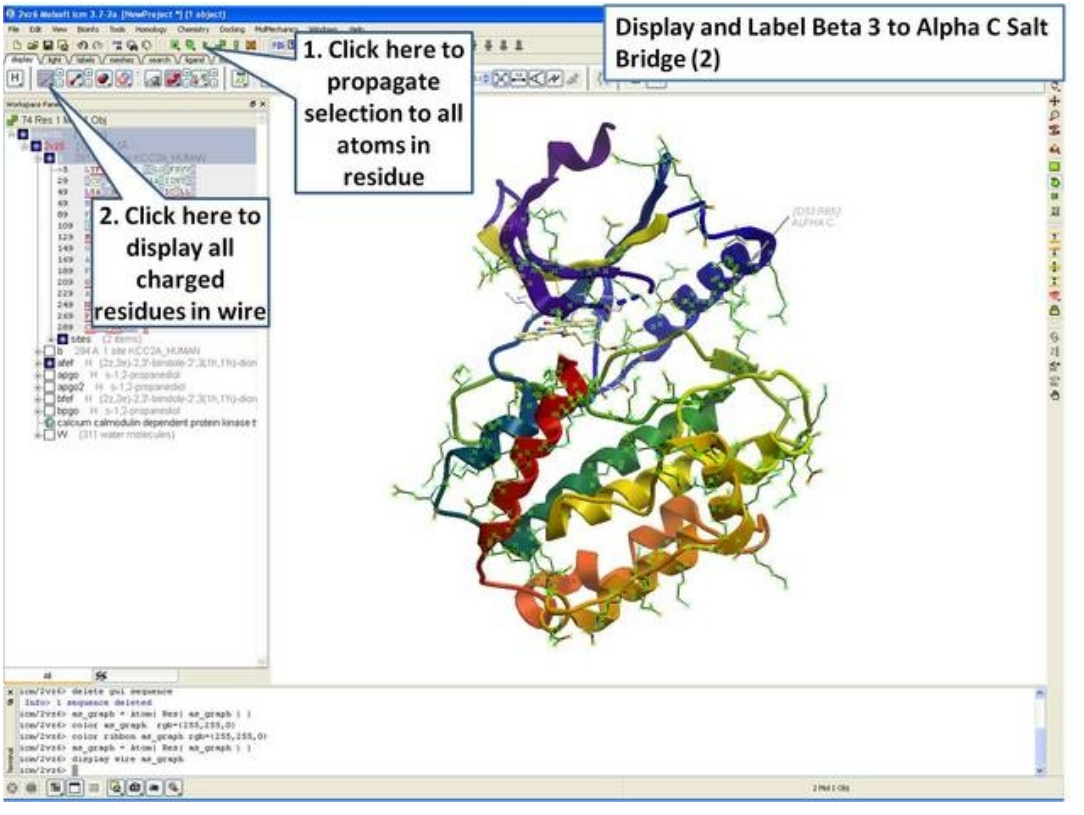
8.1.3 Labels

This tutorial is a continuation from the previous tutorials in this section and shows you how to:

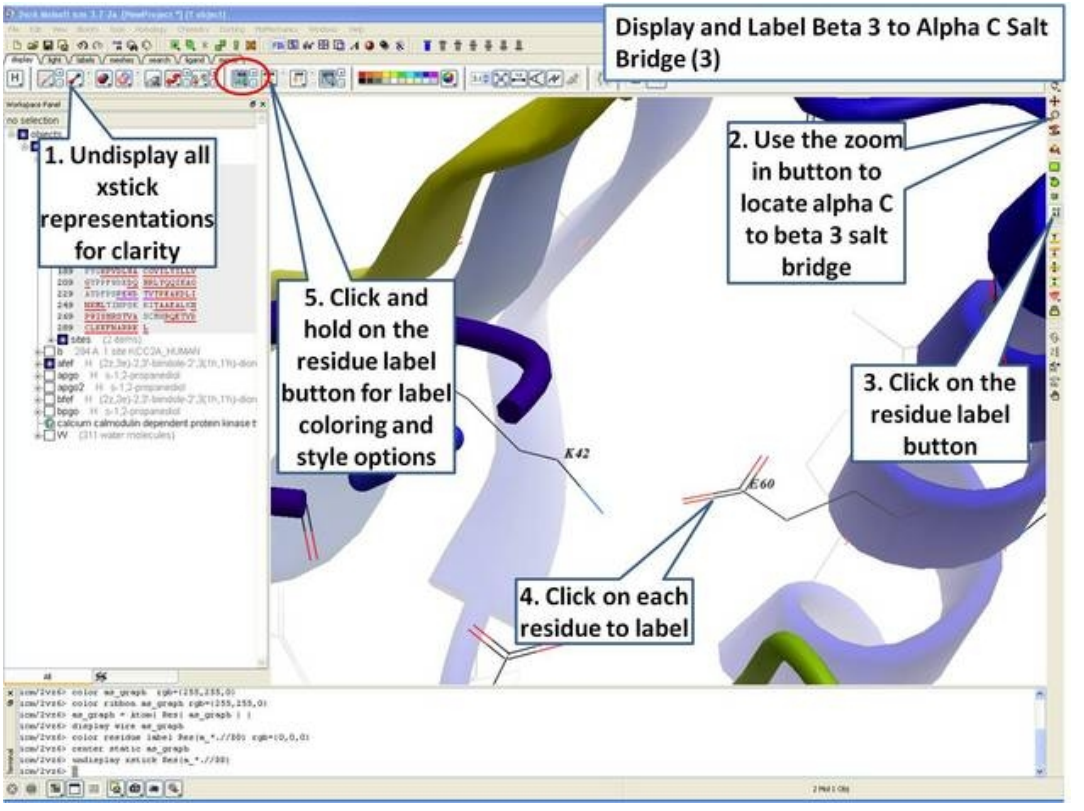
- How to select individual residue types.
- How to propagate a selection from one atom to all.
- How to use the residue label button.
- How to make a spherical selection.
- How to label a residue selection.



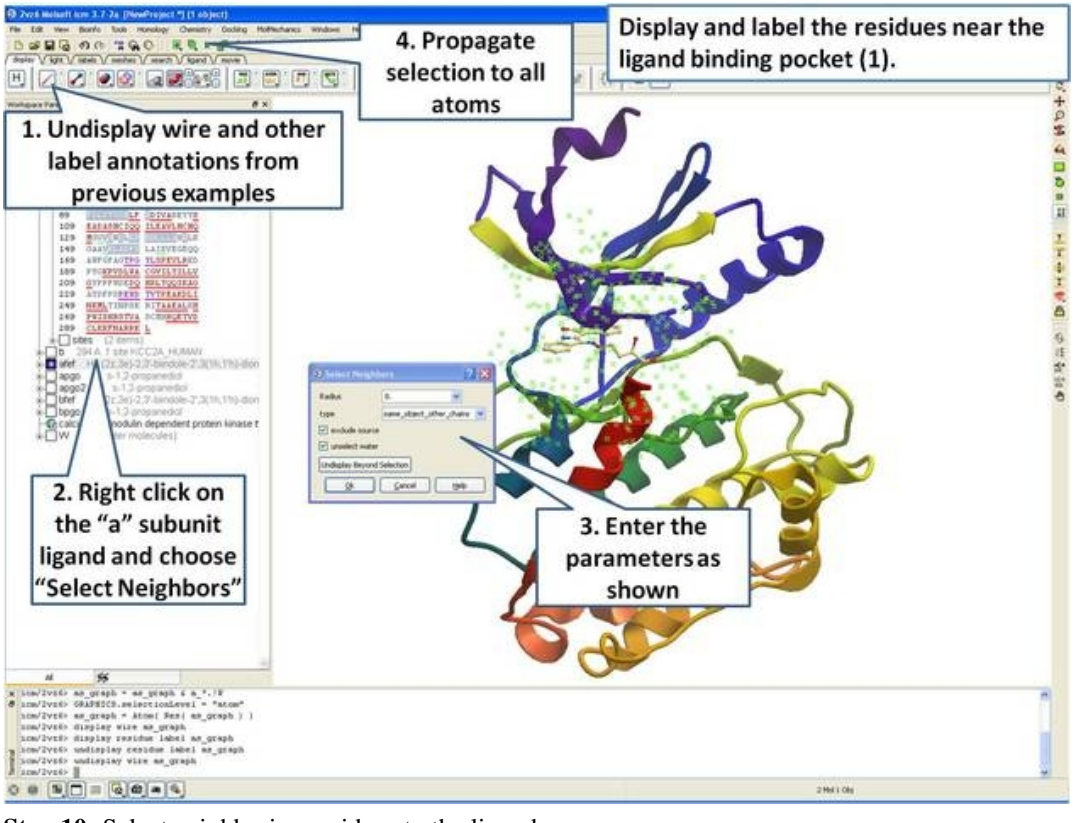
Step 7: Use the "Filter Graphical Selection" button to select charged residues.



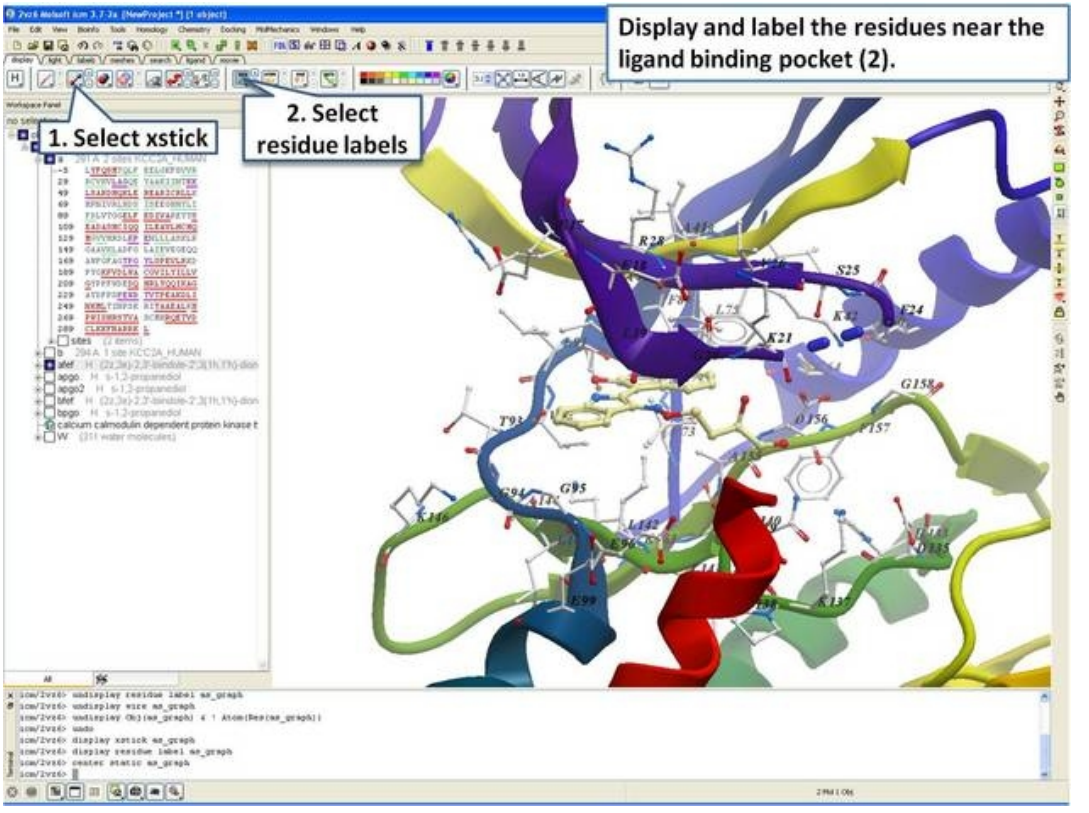
Step 8: Propagate selection to all taoms to display all atoms of the side chain.



Step 9: Locate the B3 to AlphaC salt bridge (K42- E60) and label using residue label button. **Note:** Once you have selected the two residues you can invert selection (click on invert selection button) and then undisplay all the other charged residues.



Step 10: Select neighboring residues to the ligand.

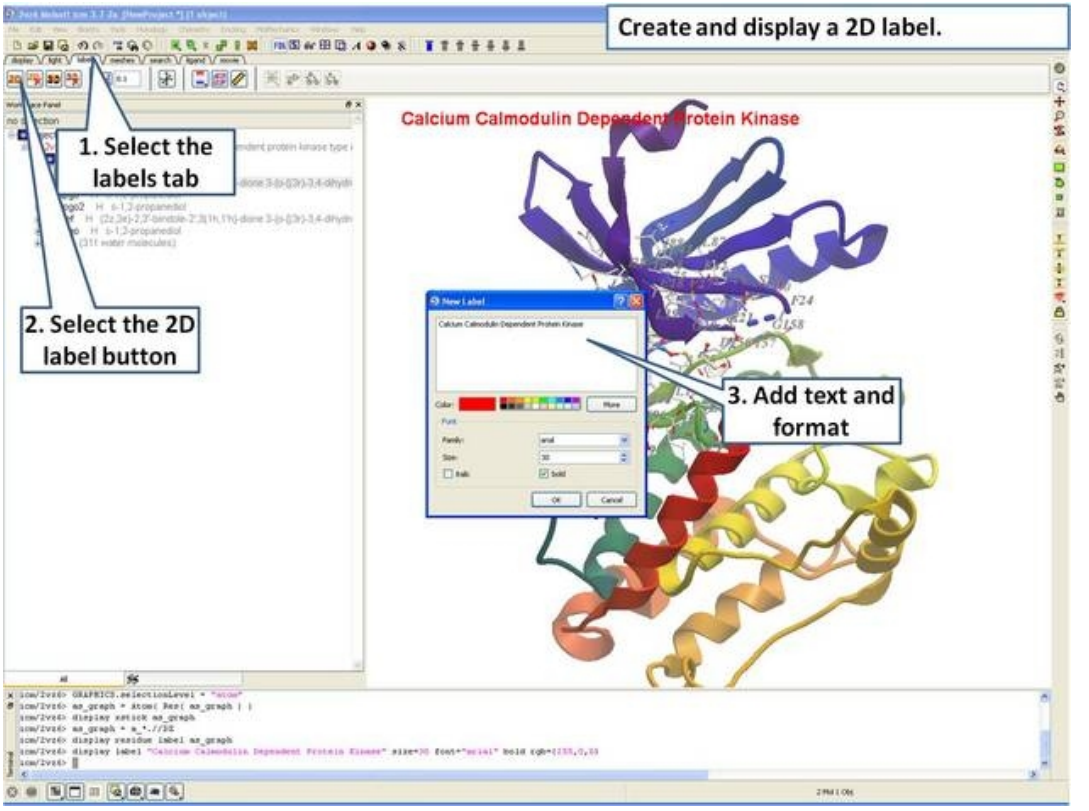


Step 11: Display the residues and label them.

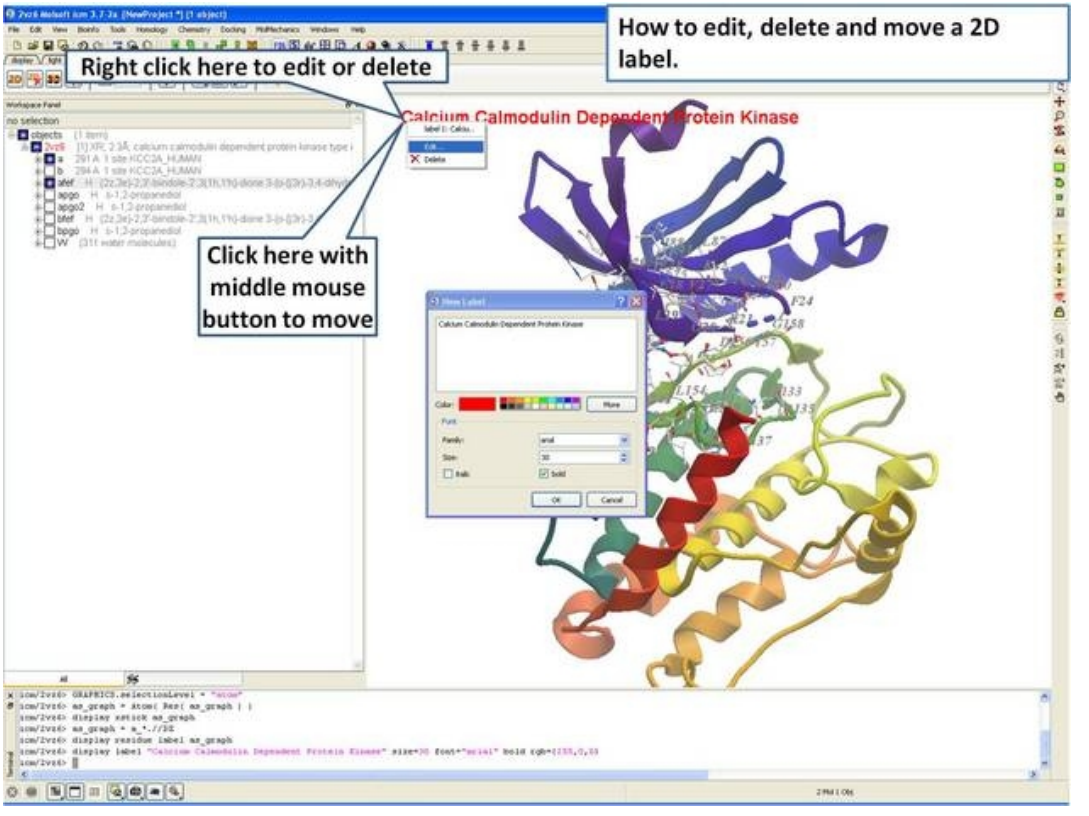
8.1.4 2D and 3D Labels

This tutorial is a continuation from the previous tutorials in this section and shows you how to:

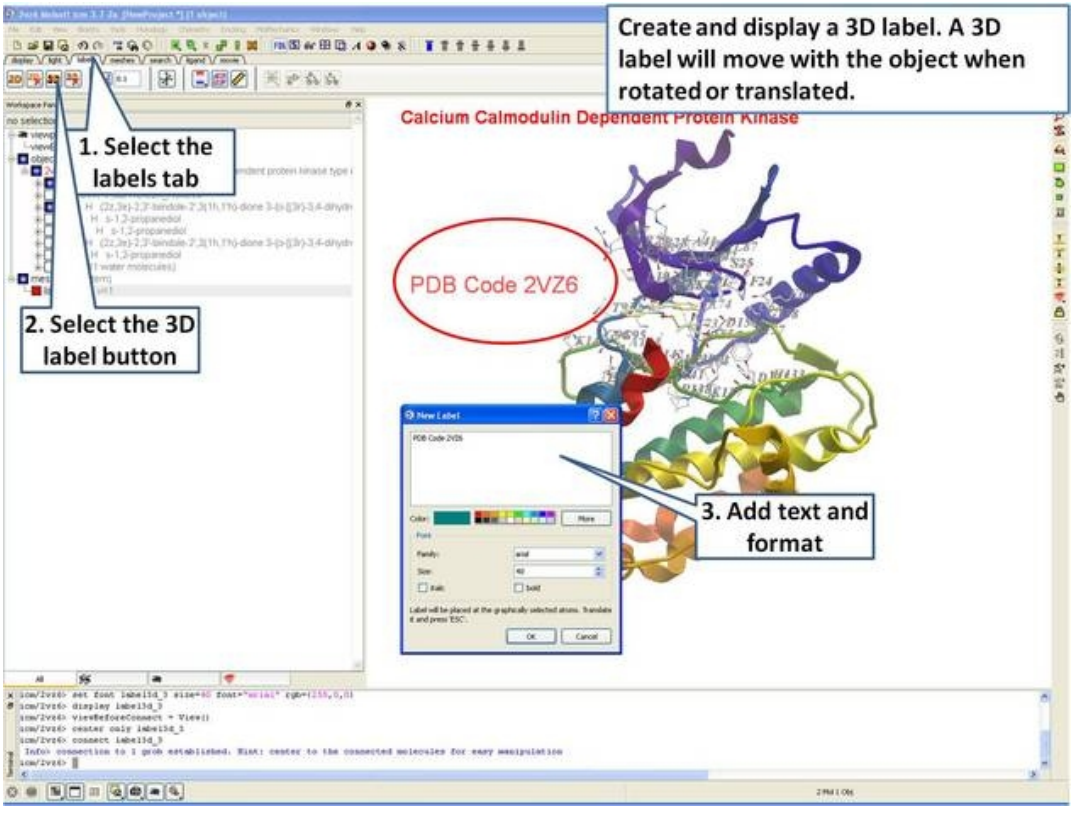
- Create and display a 2D label.
- Delete and move a 2D label.
- Create and display a 3D label.
- Delete and move a 3D label.



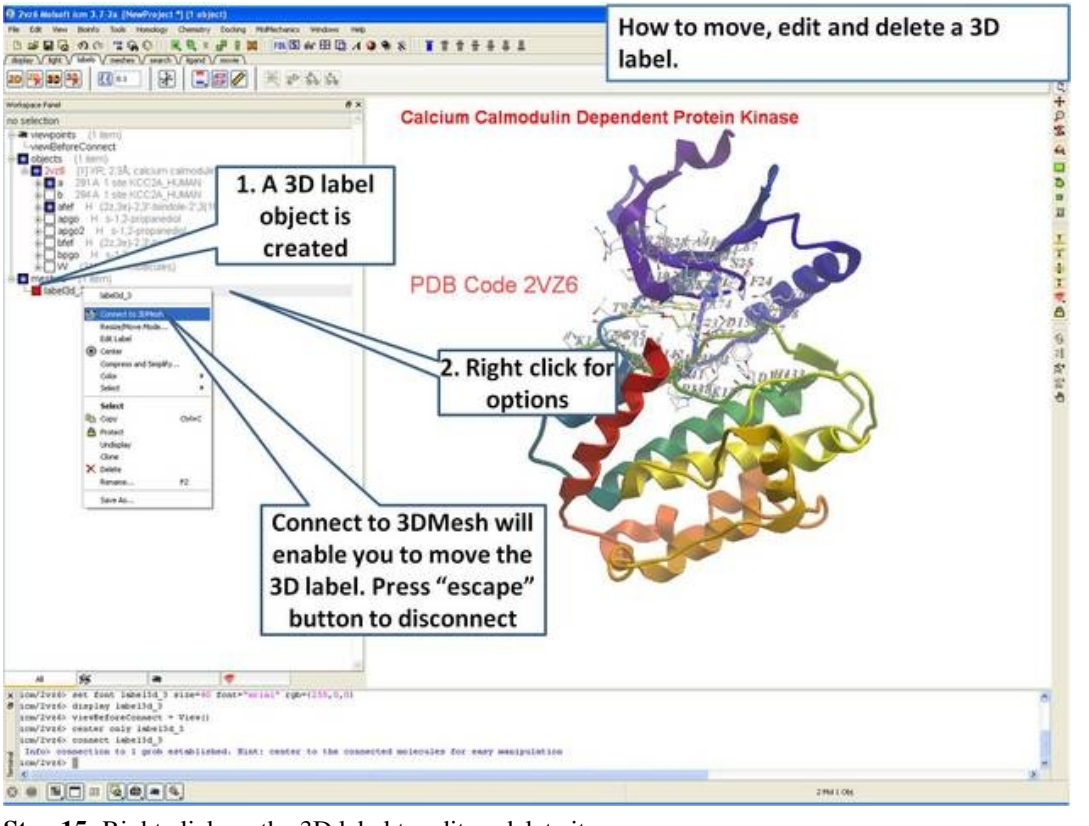
Step 12: Create a 2D label using the options in the "labels" tab.



Step 13: Right click on the 2D label to edit or delete it.



Step 14: Create a 3D label using the options in the "labels" tab.



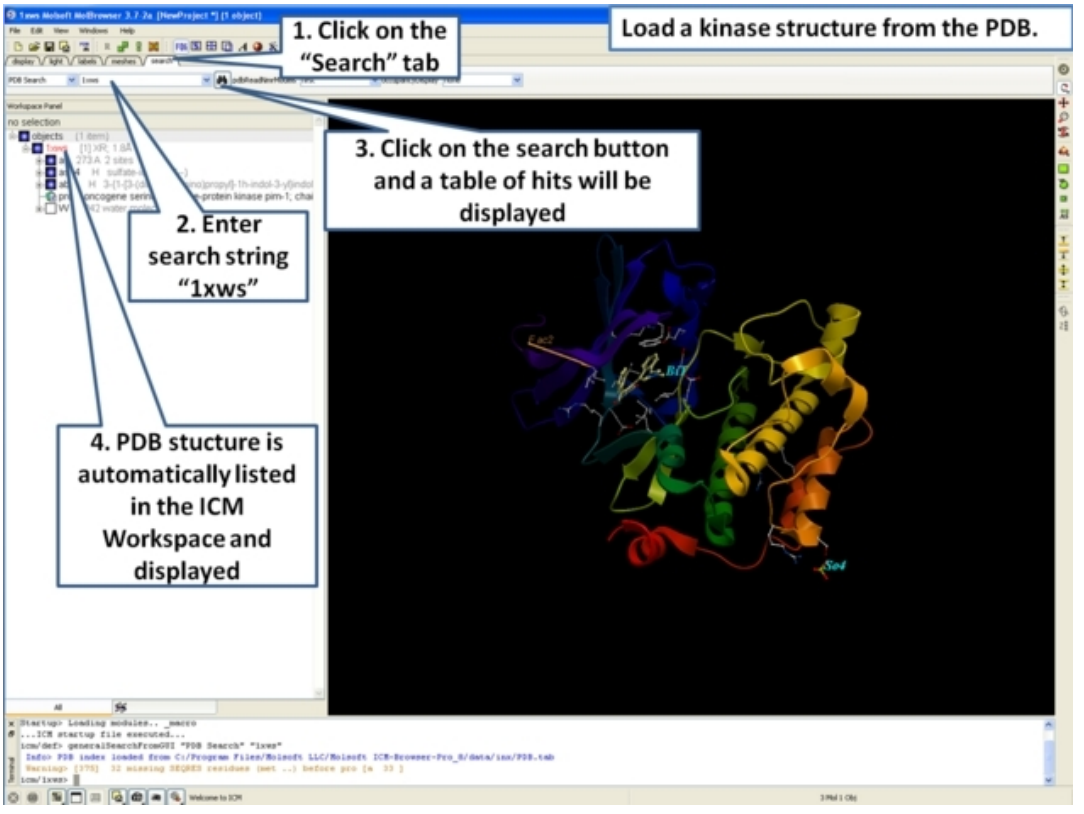
Step 15: Right click on the 3D label to edit or delete it.

8.2 Creating Fully Interactive Slides for PowerPoint and the Web Tutorial

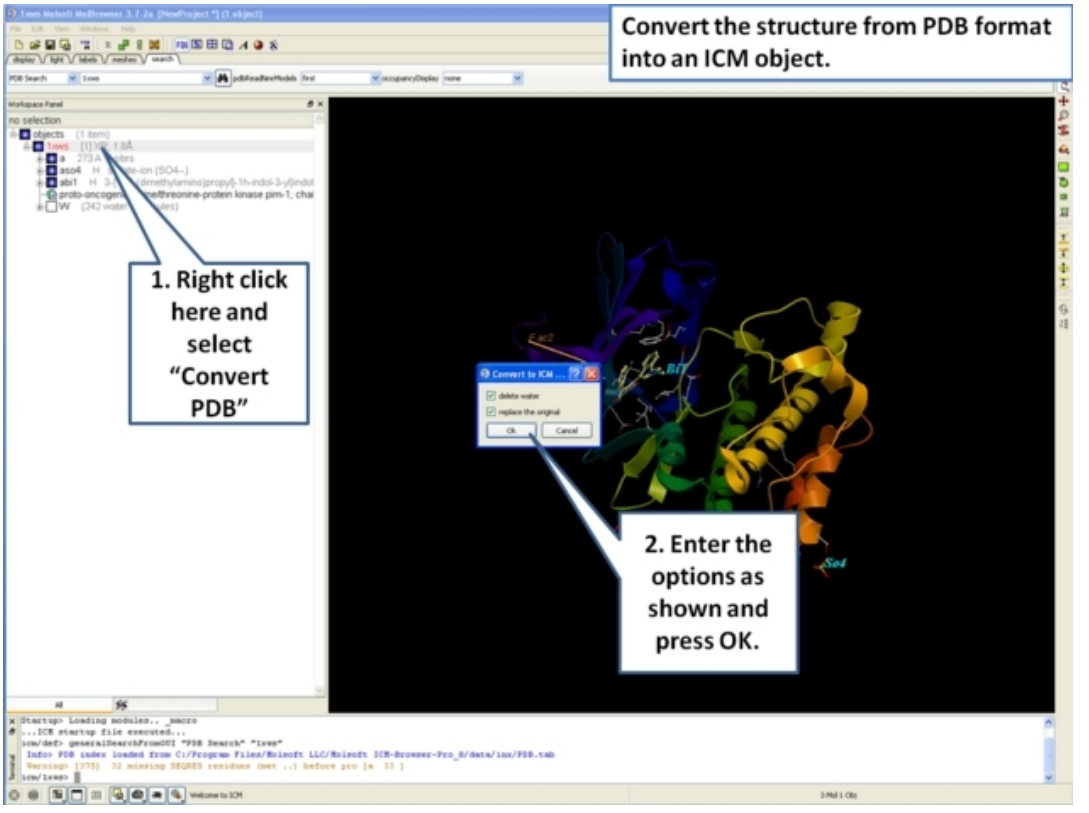
In this tutorial you will learn how to:

- How to make a fully interactive 3D slide.
- How to include HTML text
- How to link HTML text to 3D slides.

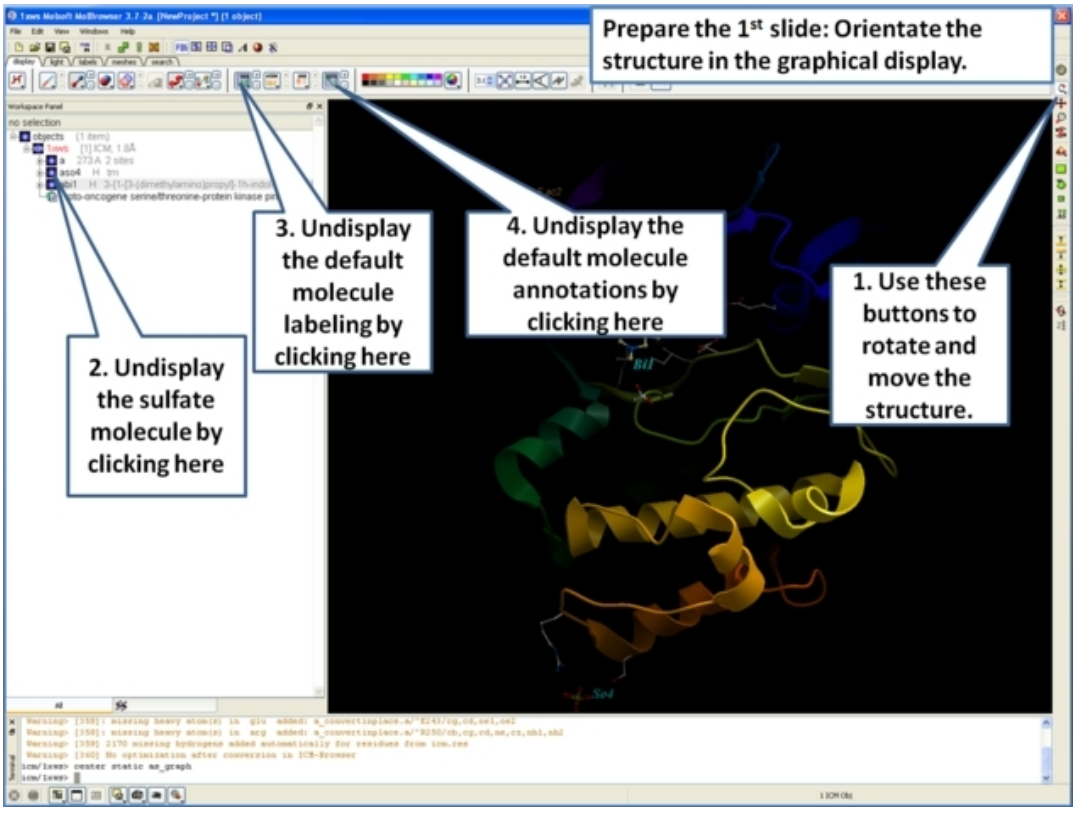
See the `ActiveICM Reference Guide` for instructions on how to view the fully interactive slides on the web and PowerPoint.



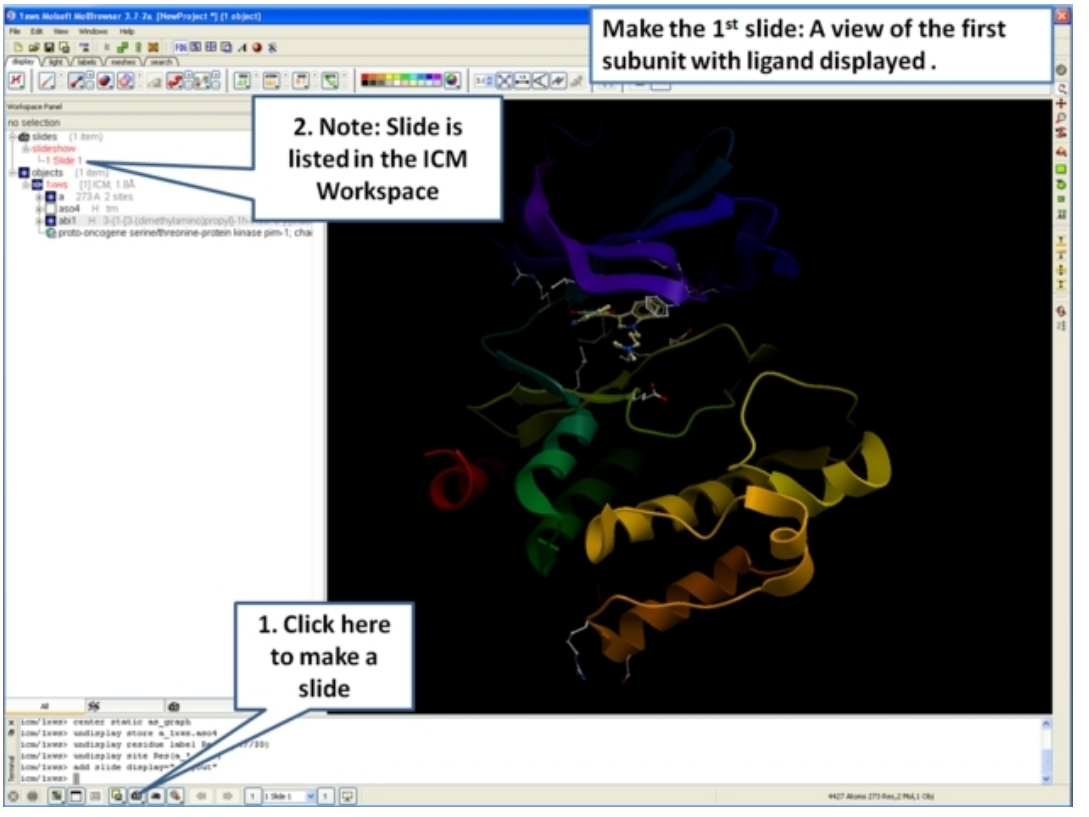
Step 1: Load the structure(s) you wish to include in a slide(s).



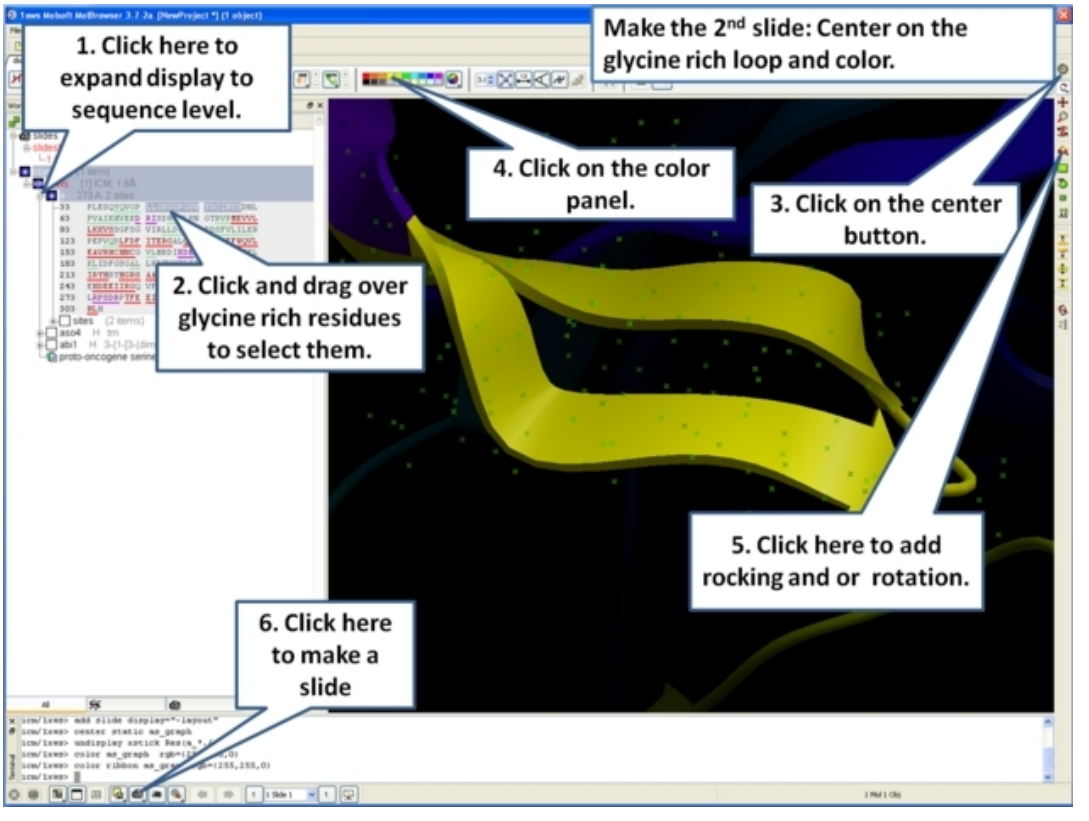
Step 2: You need to convert a PDB file to an ICM object if you wish to display surfaces colored by binding properties.



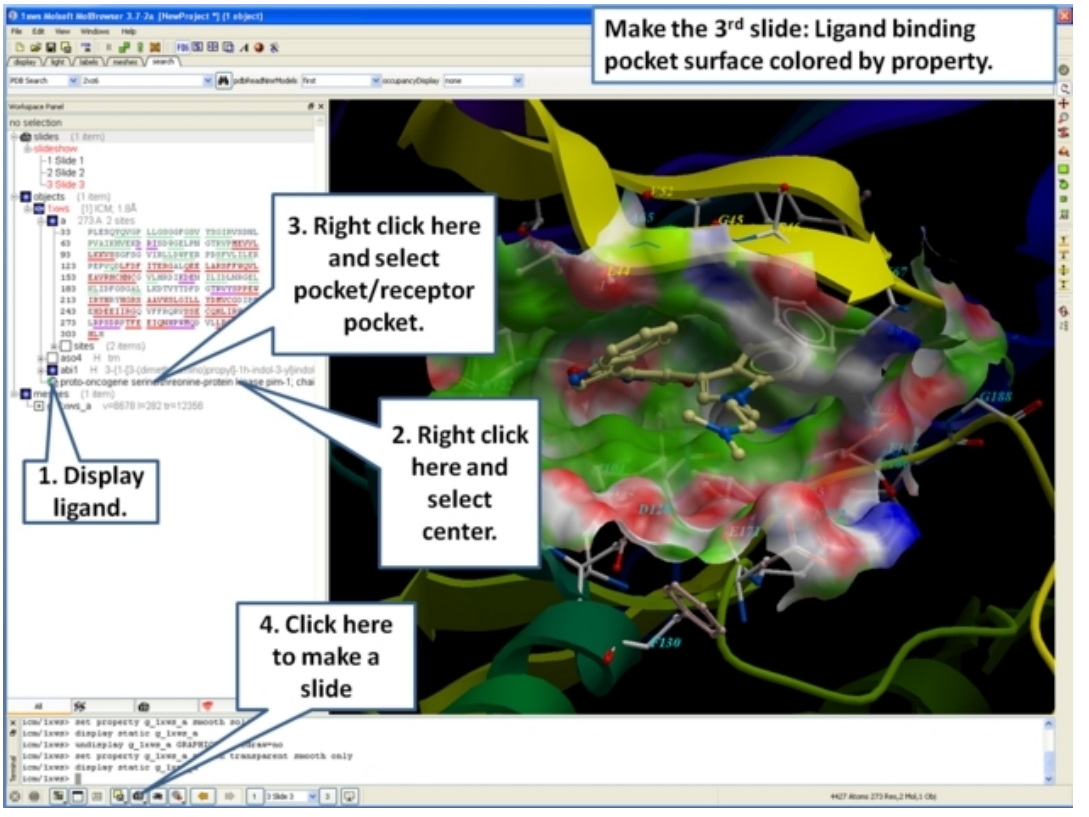
Step 3: Prepare the display for the slide.



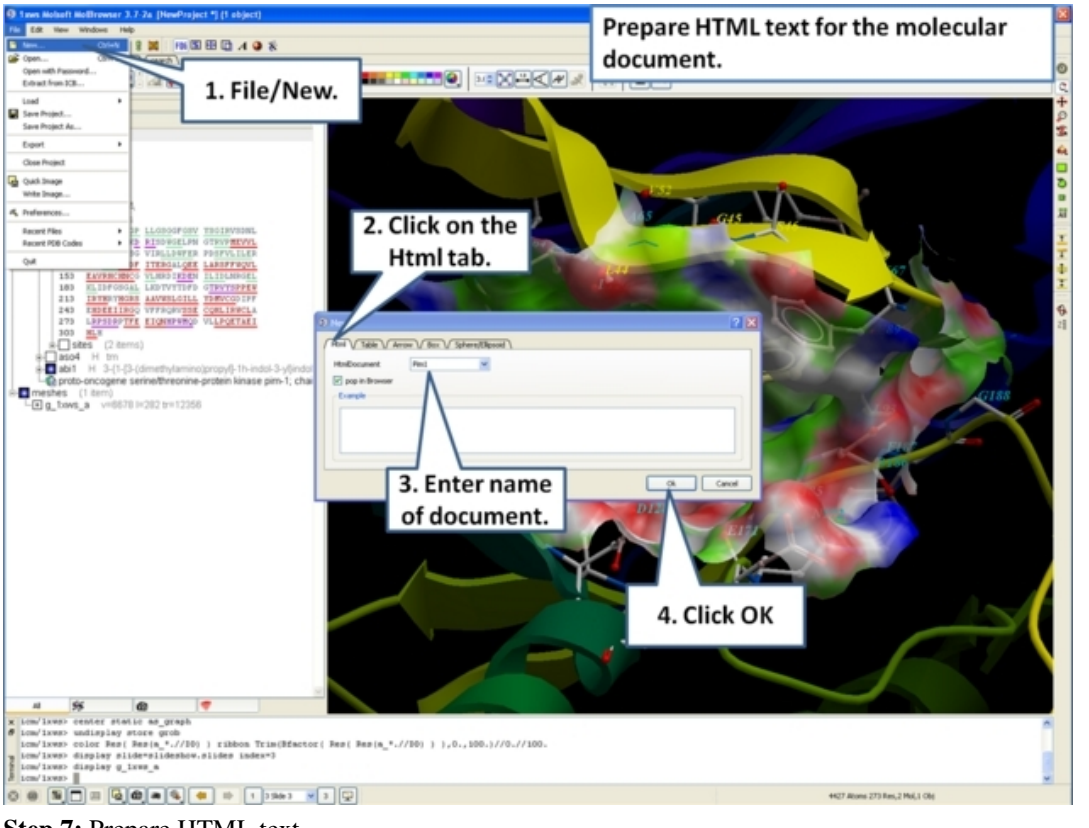
Step 4: Make a slide by clicking on the camera button.



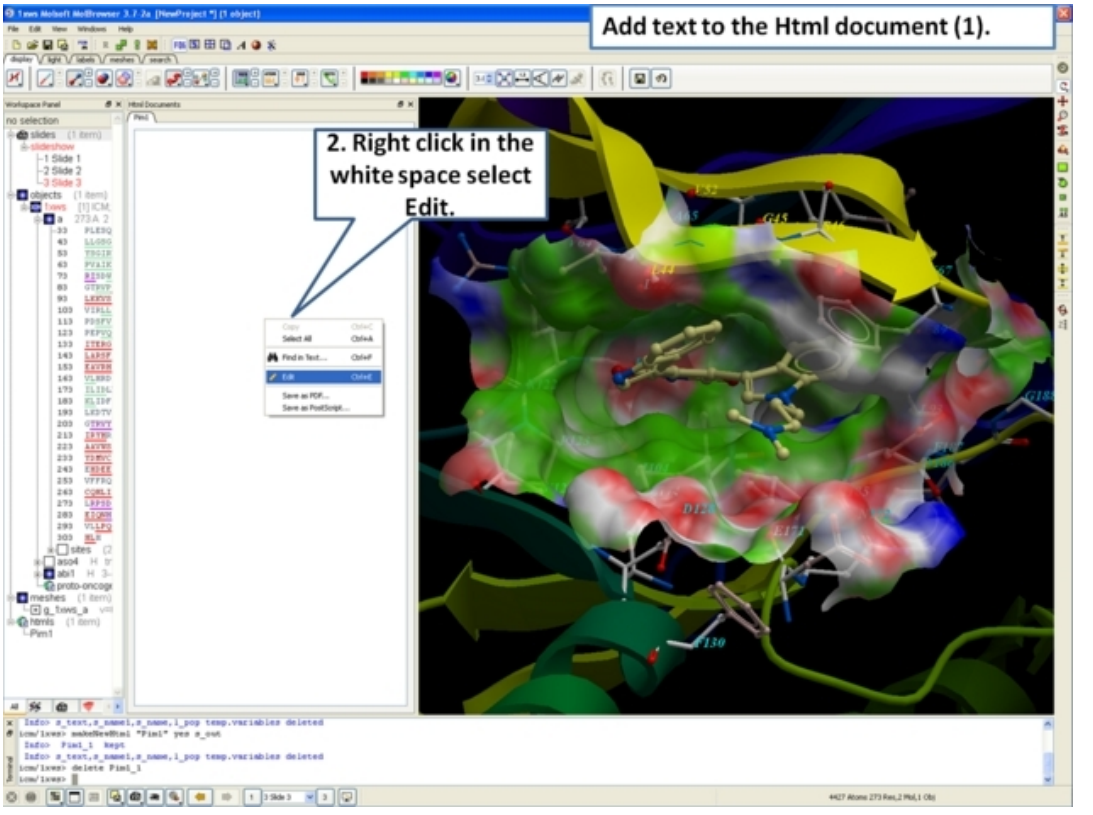
Step 5: Make another slide, in this example we color the glycine rich loop.



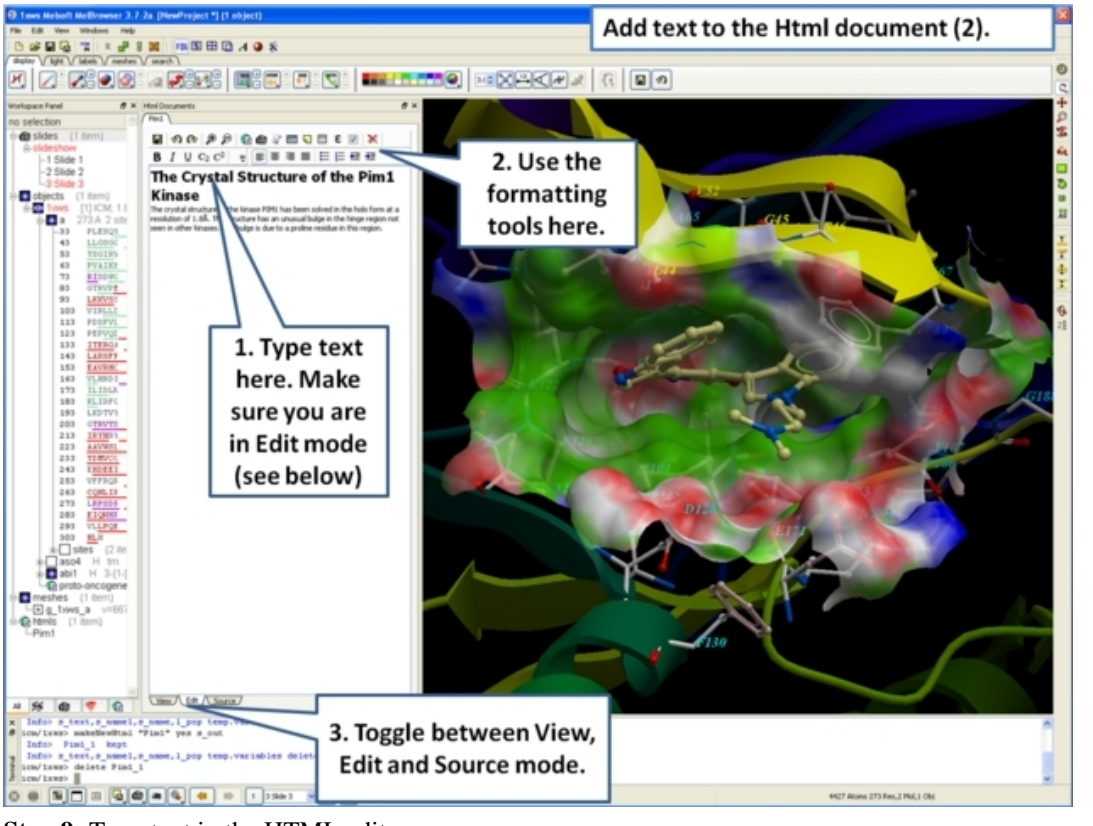
Step 6: Display the pocket surface.



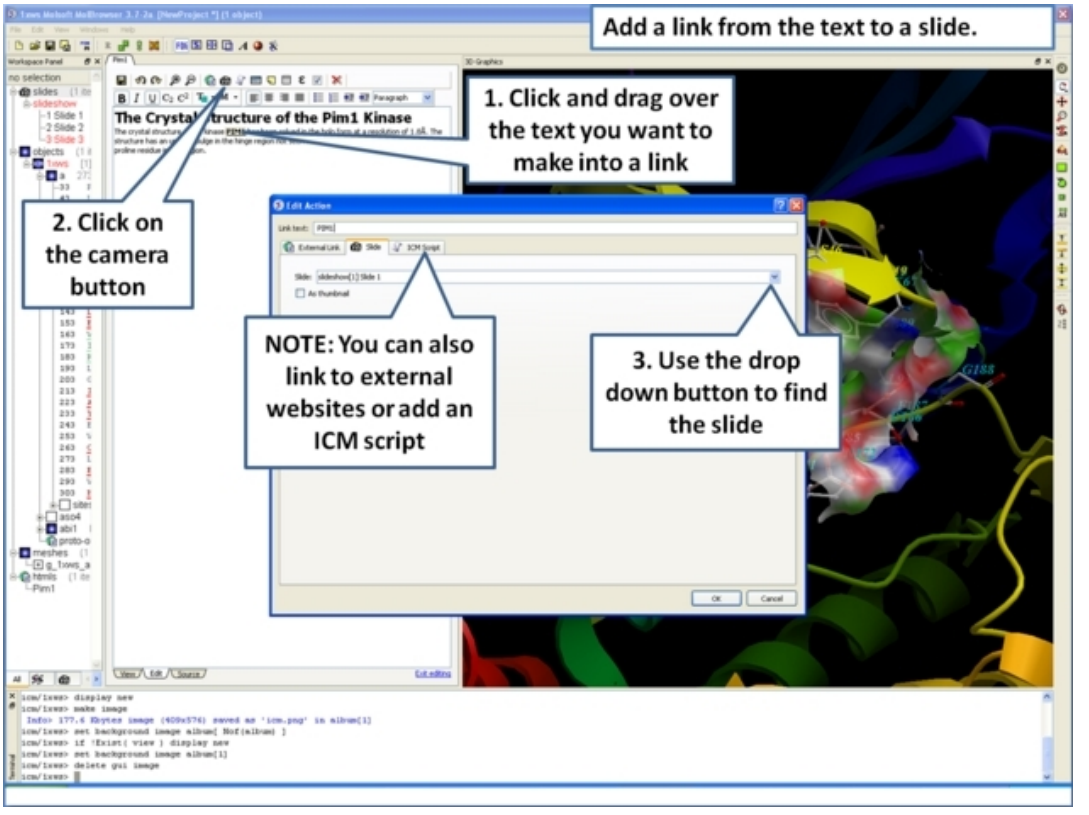
Step 7: Prepare HTML text.



Step 8: Right click in the HTML panel for editing options.



Step 9: Type text in the HTML editor.

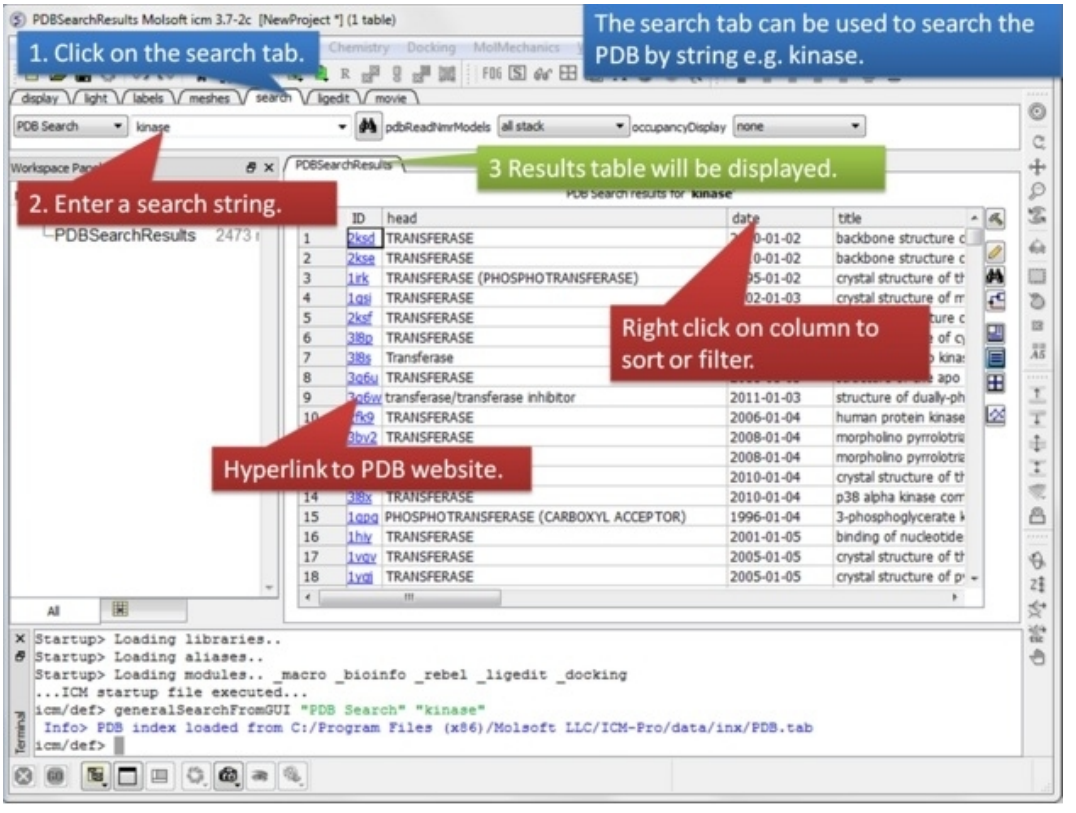


Step 10: Add a link from the text to a slide.

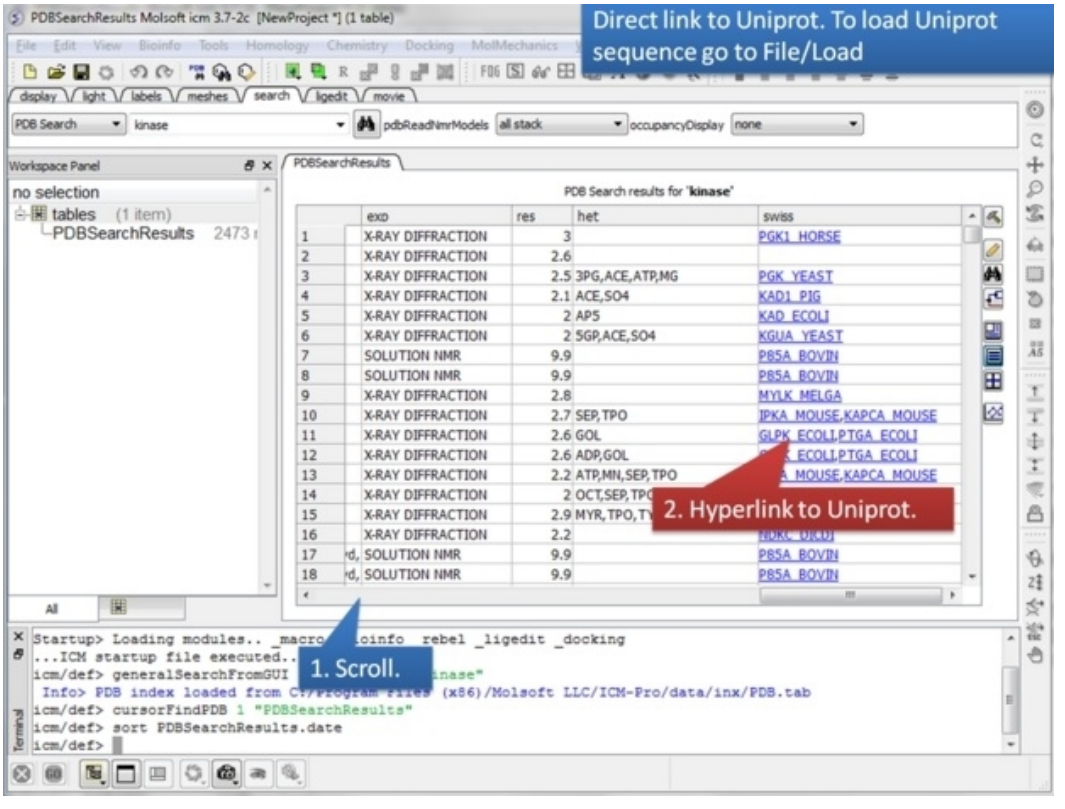
See the `ActiveICM Reference Guide` for instructions on how to view in the web and PowerPoint.

8.3 Protein Structure Tutorials

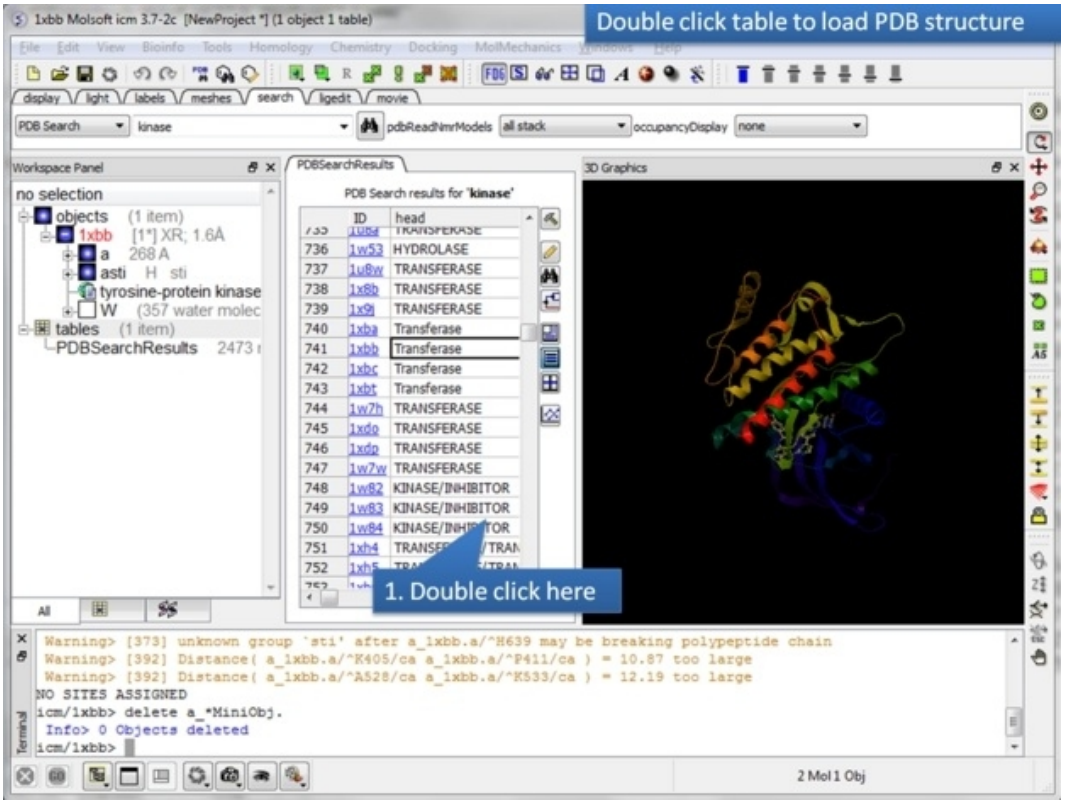
8.3.1 PDB Searching



Step 1: Use the search tab to search for a PDB by a string e.g. kinase or the pdb code: 1xbb. The table can be sorted and filtered by right clicking on the column header. A hyperlink to the PDB website is provided for each entry.



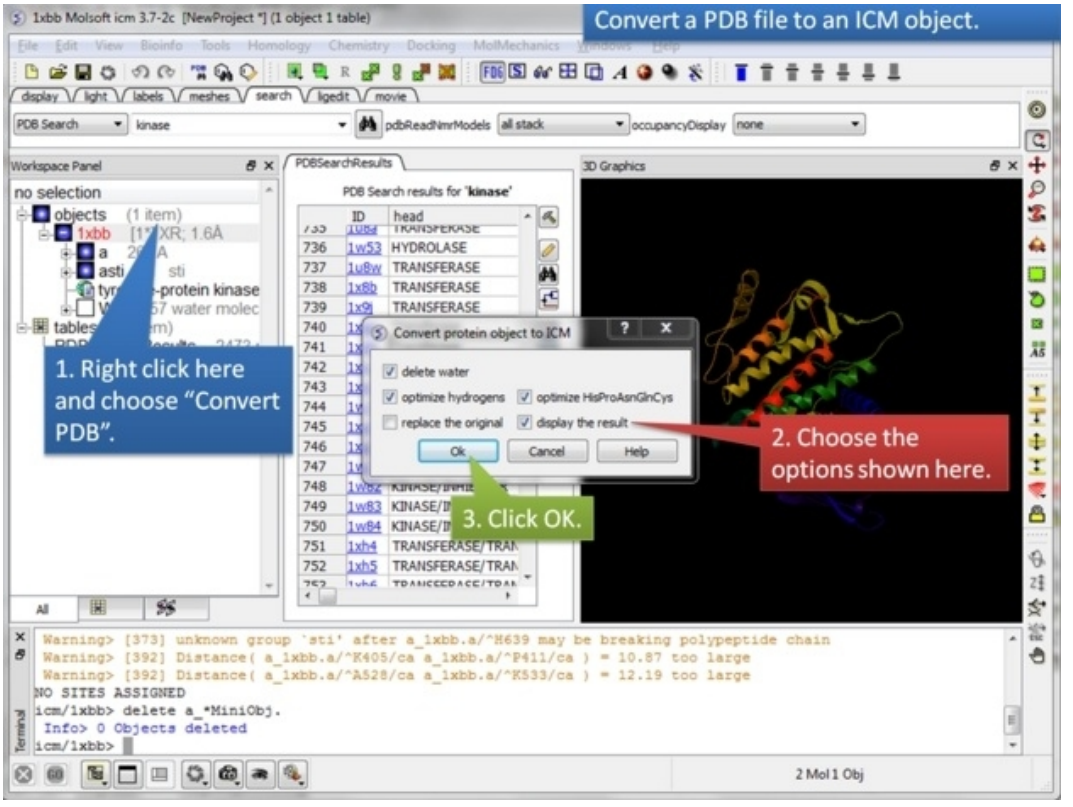
Step 2: Scroll along the table to find out more information such as resoultion (res), hetero atoms (het) and a direct link to the Uniprot website.



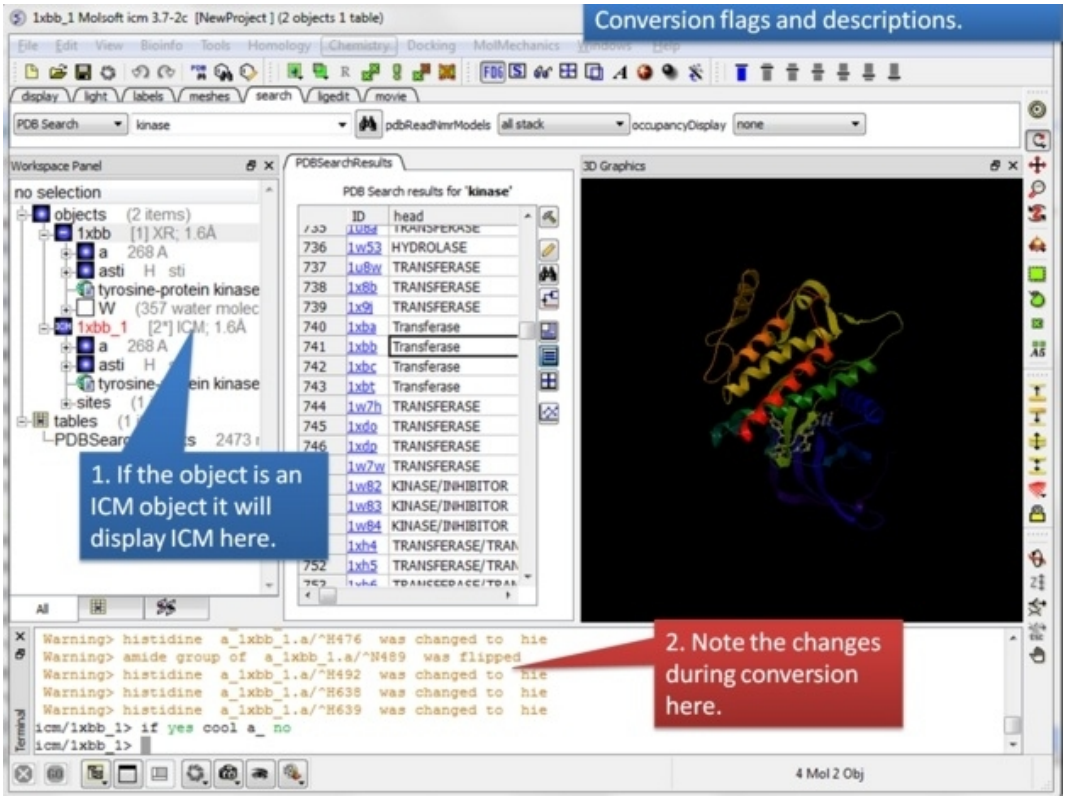
Step 3: Double click on the table to load and display the pdb structure.

8.3.2 Converting a PDB File into an ICM Object

Sometimes it is necessary to have a PDB file in the form of an ICM molecular object. For example, it's a convenient way to list and/or to change a torsion angle (or a series of them). It is also necessary to convert PDB files into ICM objects for ICM functions such as docking. There are two principally different modes of conversion. In the default mode the program looks at the residue name and tries to find a full-atom description of this residue in the icm.res file. This search is suppressed with the exact option. Hydrogen atoms will be added if the converted residues are known to the program and described in the icm.res library.



Step 1: Read in a PDB file and then right click on the pdb name in the ICM Workspace and choose the option "Convert PDB".

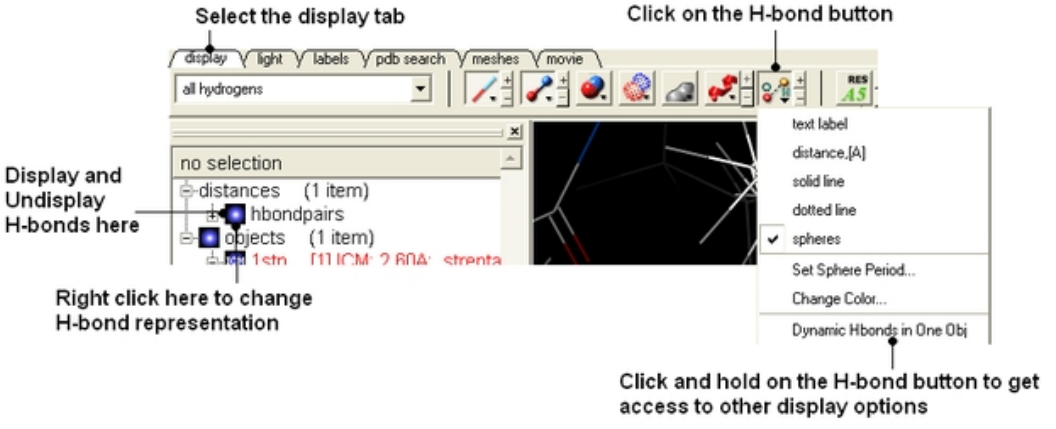


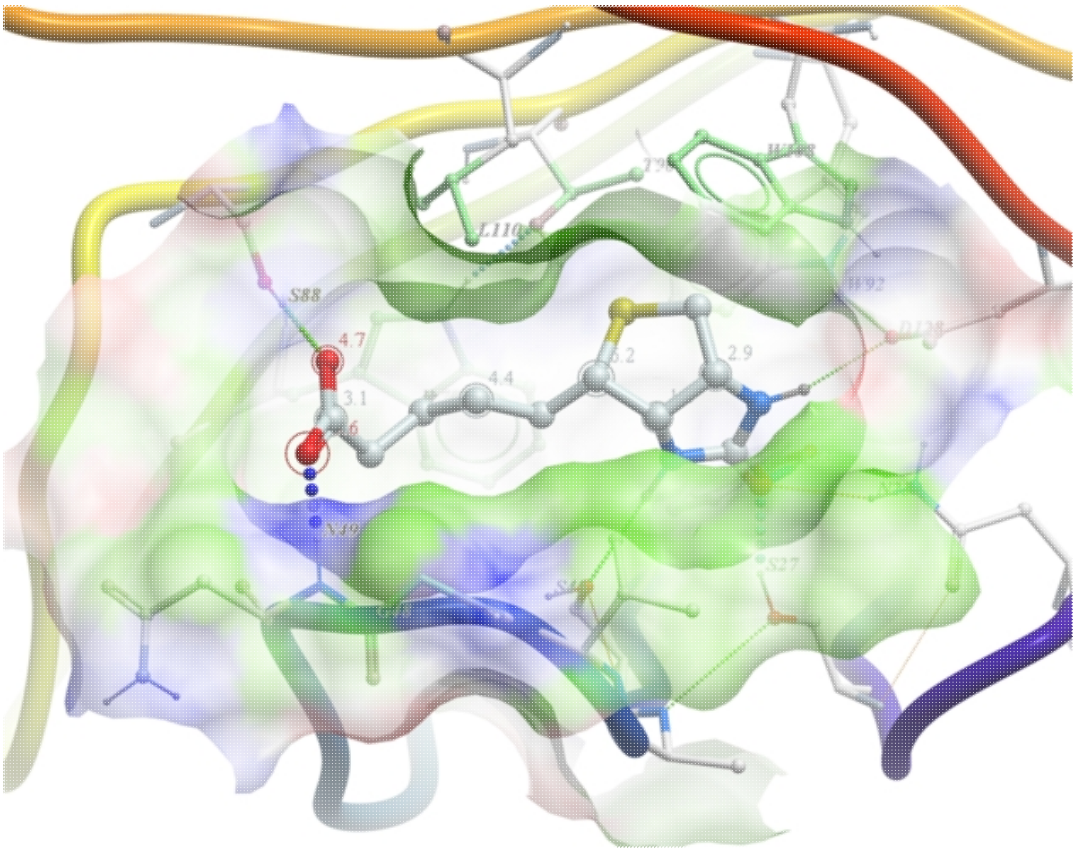
Step 2: Note the new object will have "ICM" next to its name in the ICM Workspace. Also a log of the changes made are listed in the terminal window.

8.3.3 How to display hydrogen bonds between a ligand and receptor.

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. To convert 1STP into an ICM object follow the instructions `Converting a Protein 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.





NOTE: Different options for displaying the H-bond can be accessed by clicking and holding on the H-bond button in the "Display" tab.

8.3.4 Protein Preparation and Crystallographic Analysis Tutorial

8.3.5 PDB Preparation - Symmetry

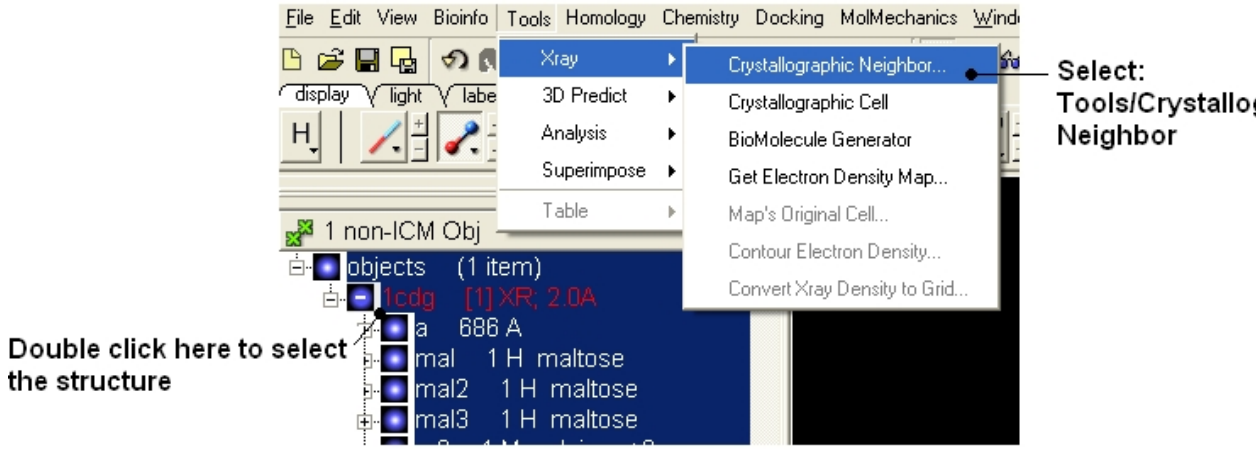
Background When inspecting a ligand binding pocket it is important to check that the true pocket is formed by chains which are not explicitely present in a PDB entry. Therefore it is necesary to use **Tools/X Ray/Crystallographic Neighbor** to find all molecules/subunits or chains involved in the interaction with the ligand. Molecular objects and 3D density maps may contain information about crystallographic symmetry. It consists of the following parameters:

1. Crystallographic group eg. P2121 that determine N (depends on a group) transformations for the atoms in the asymetric unit.
2. Crystallographic cell parameters A, B, C, Alpha, Beta and Gamma

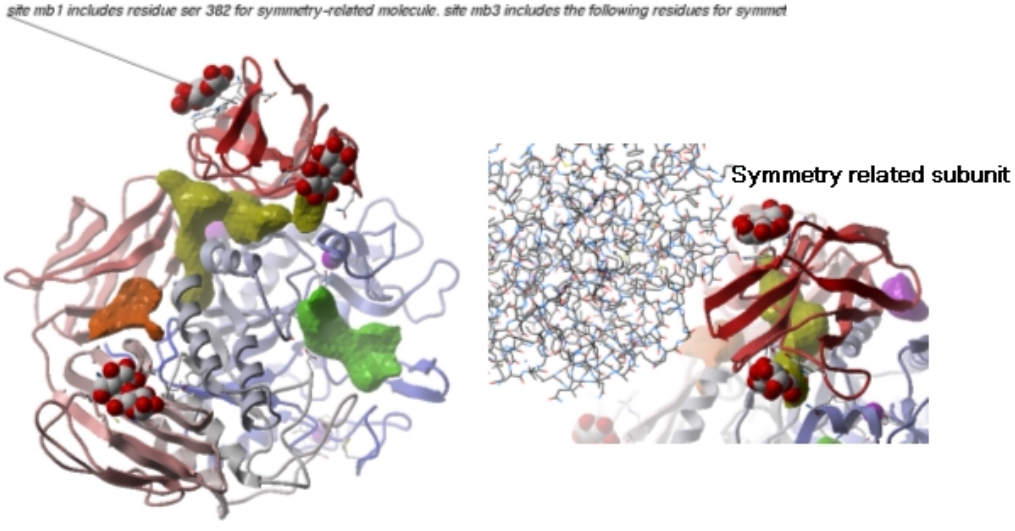
To generate the coordinates within one cell one needs to apply N transformations and then to generate neigboring cells the content of one cell needs to be translated in space according to the cell position.

Example As an example let us look at Cycloldextrin glycosyltransferase (PDB Code: 1CDG). The problem with docking to this receptor is that the true pocket is formed by chains which are not explicitly present in the PDB entry. Site mb1 includes serine 382. This cannot be predicted just by looking at the structure. Therefore we need to identify symmetry related molecules to this protein.

- Use the PDB search tab to load the crystal structure 1cdg.
- Inspect the ligand binding pocket of **maltose** (mal)
- To identify if there are any other chains involved in the interaction with the ligand select the whole structure in the ICM Workspace.



- Tools/Crystallographic Neighbor
- Select a 7A radius
- Check "create symmetry related molecules" and "display symmetry neighbors".
- Inspect the neighbors surrounding **maltose(mal).** Each symmetry related subunit can be colored by object by clicking and holding the representation button in the display tab and selecting color-by.



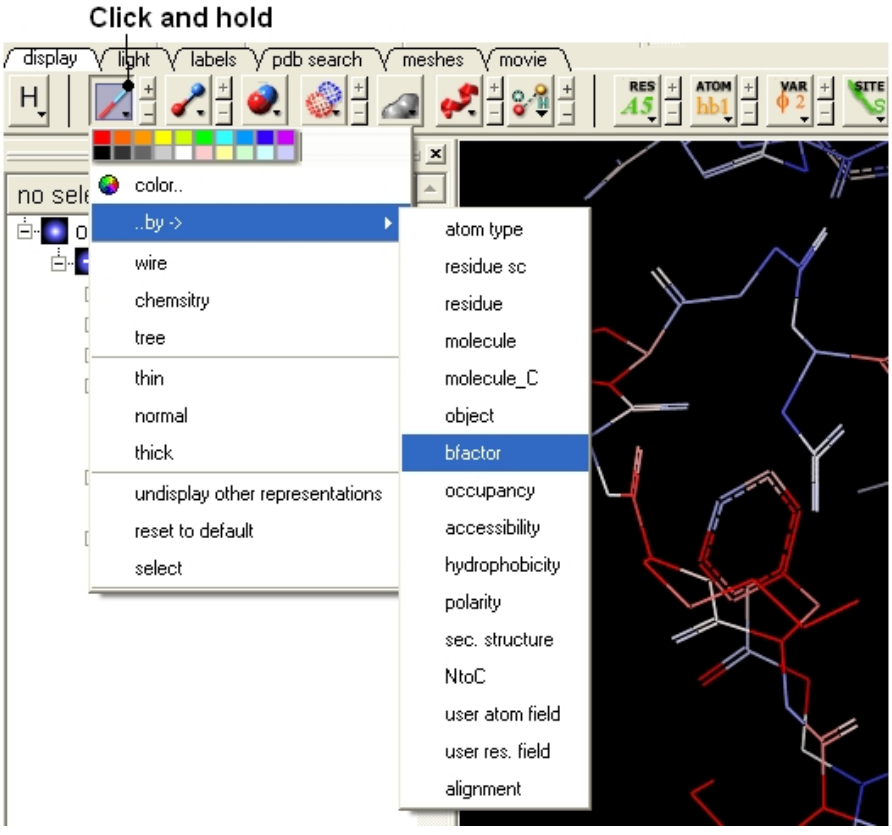
8.3.6 PDB Preparation - Occupancy and B-Factors

Background When preparing a PDB for analysis (eg docking or modeling) it is important to check the reported occupancies and b-factors. The occupancy is a fraction of atimic density at a given center. If there are two eqally occupied conformers both will have an occupancy of 0.5 - the normal value is 1 range 0-1. The *{B-Factor} is the mean-square displacement of atom from its position in the model - the normal range is 5-50.

One way of visualizing the occupancy and b-factor is by coloring the structure by these values. You can do this by clicking and holding on a representation button in the **display** panel and selecting Color-by.

As an example let us look at the crystal structure 1ATP

- Type in the PDB search tab 1atp and the structure will be displayed in the graphical display.
- Use the ICM workspace to undisplay everything except for the "e" subunit. You can do this by clicking in the blue boxes in the ICM Workspace.
- Display the "e" subunit in wire representation using the wire button in the **display** tab.
- Click and hold on the wire button and select Color-by B-Factor. Regions of high B-factor are colored red.

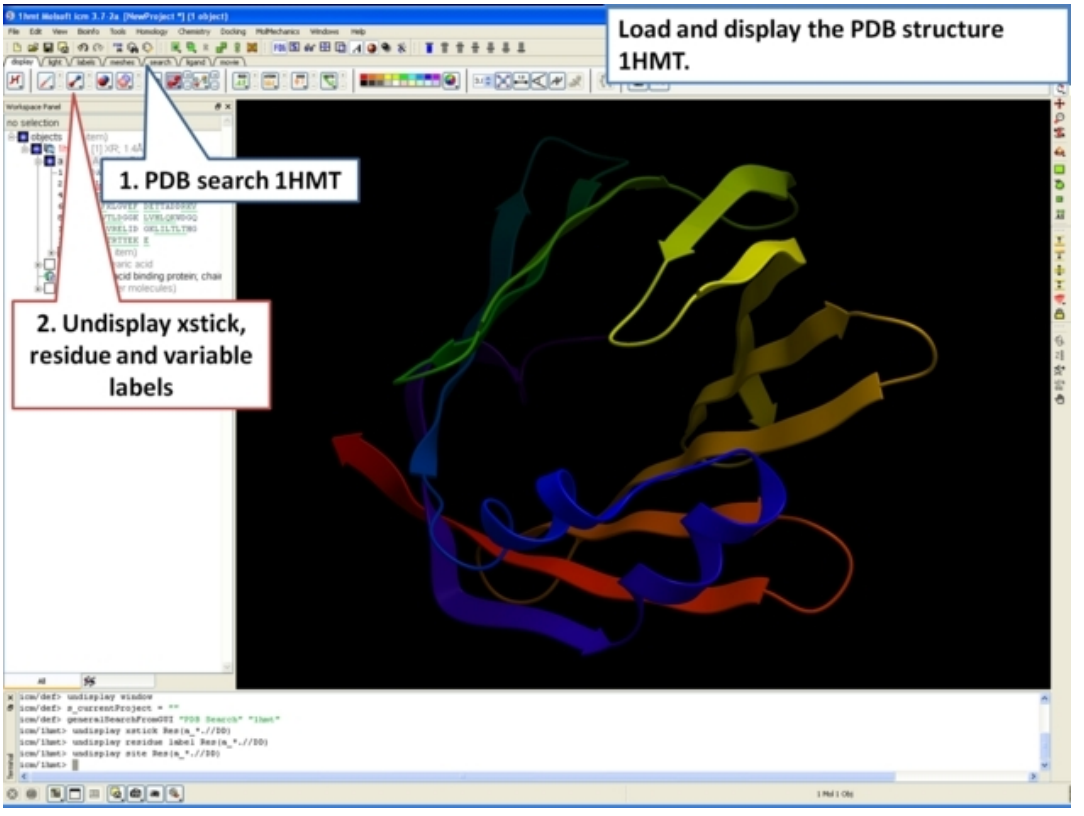


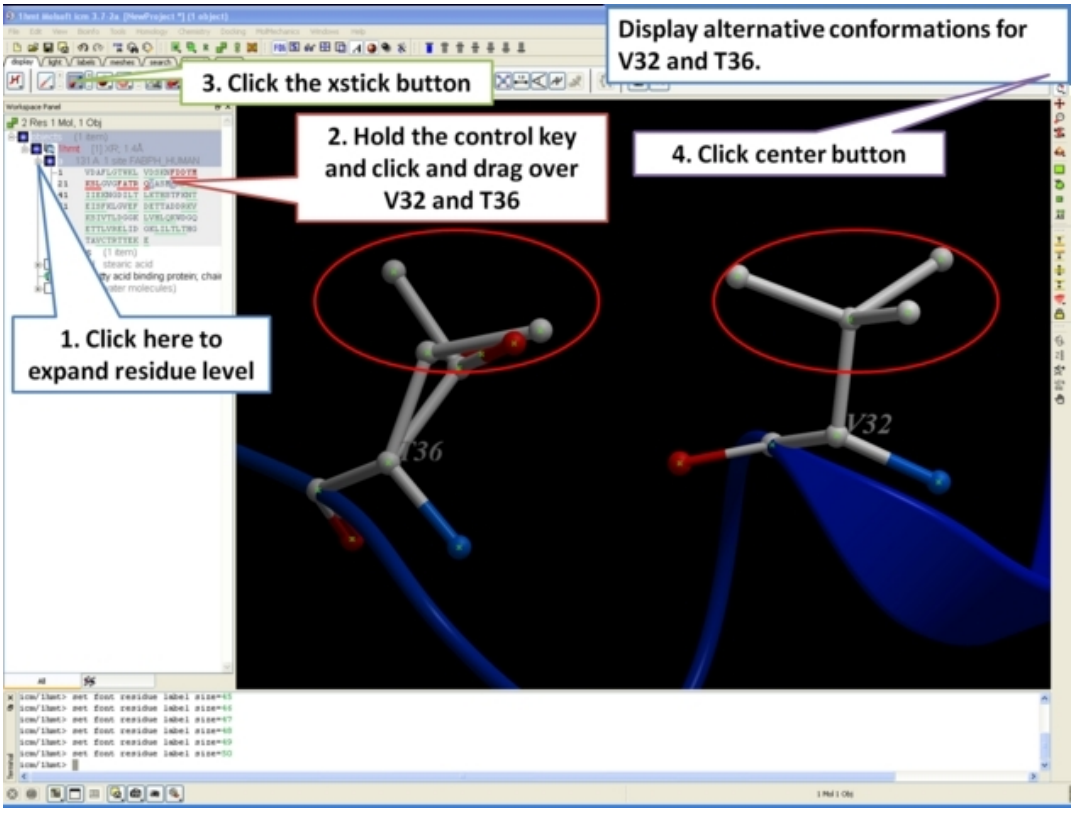
Residues with high B-Factor are colored red

8.3.7 PDB Preparation - Residue Alternative Orientation

For some very high resolution structures two alternative conformations for a residue are provided. Therefore for docking you need to decide to use one conformation of the residue or generate seveal separate docking models. This could be performed using multiple receptor conformation docking.

Here is an example of alternative residue orientations found in a crystal structure of a Fatty Acid Binding protein in complex with stearic acid.





8.3.8 Biomolecule Generator

Objective

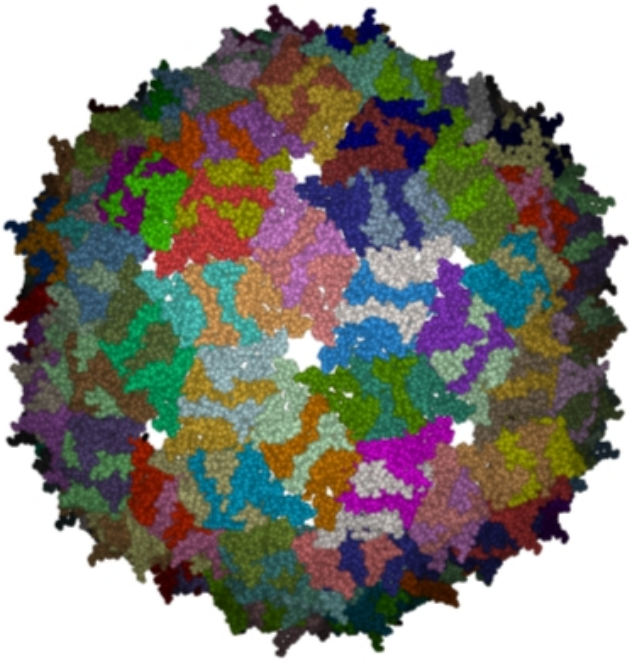
Here we will investigate the biological environment of a virus protein . PDB code 1DWN.

Background

It is very useful to know how a protein from the PDB may look in a biological environment. The PDB entries solved by X-ray crystallography and deposited in the PDB contain the information about the crystal structure rather than the biologically relevant structure. For example, for a viral capsid only one instance of capsid protein complex will be deposited and only one or two molecules of haemoglobin that is a tetramer in solution maybe deposited. In some other cases the asymmetric unit may contain more than one copy of a biologically monomeric protein. ICM reads the biological unit information and has a tool to generate a biological unit. Not every PDB entry has the biological unit information.

Instructions

- Read and load the PDB file 1DWN
- Tools/Xray/Biomolecule Generator
- Tick the makeAllBiomolecules box (Warning this may take a few minutes to generate)
- The generated molecules will be listed in the ICM Workspace. Each one can be selected and displayed. The biomolecule is shown below.



NOTE: Please note that right clicking on a PDB file in the ICM Workspace will tell you whether there is any **Biomolecule** information available for the structure. If this information is not present then the option will be greyed out.

Manual References (Web Links)

`Biomolecule Generator`

Index