

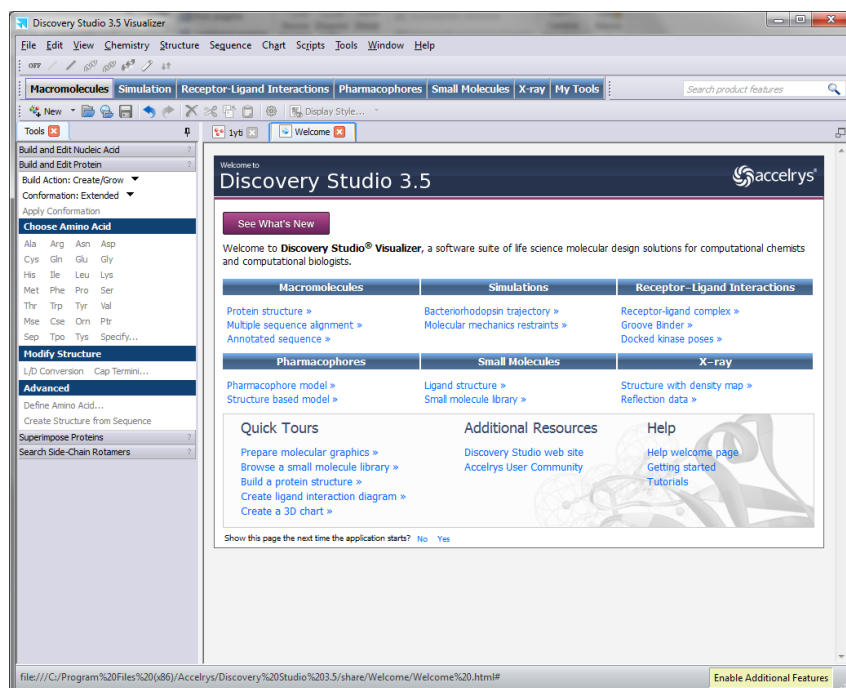
Introduction to the Discovery Studio Visualizer

Introduction

Discovery Studio is a comprehensive software suite for analyzing and modeling molecular structures, sequences, and other data of relevance to life science researchers. The product includes functionality for viewing and editing data along with tools for performing basic data analysis.

The Discovery Studio Visualizer is a free viewer that can be used to open data generated by other software in the Discovery Studio product line. It is designed to offer an interactive environment for viewing and editing molecular structures, sequences, X-ray reflection data, scripts, and other data. It also provides a rich set of viewers for displaying plots and other graphical representations of data. The application runs on Windows and Linux and is a fully integrated desktop environment that provides access to standard operating system features such as the file system, clipboard, and printing services.

This application starts by clicking on the icon on the Desktop.

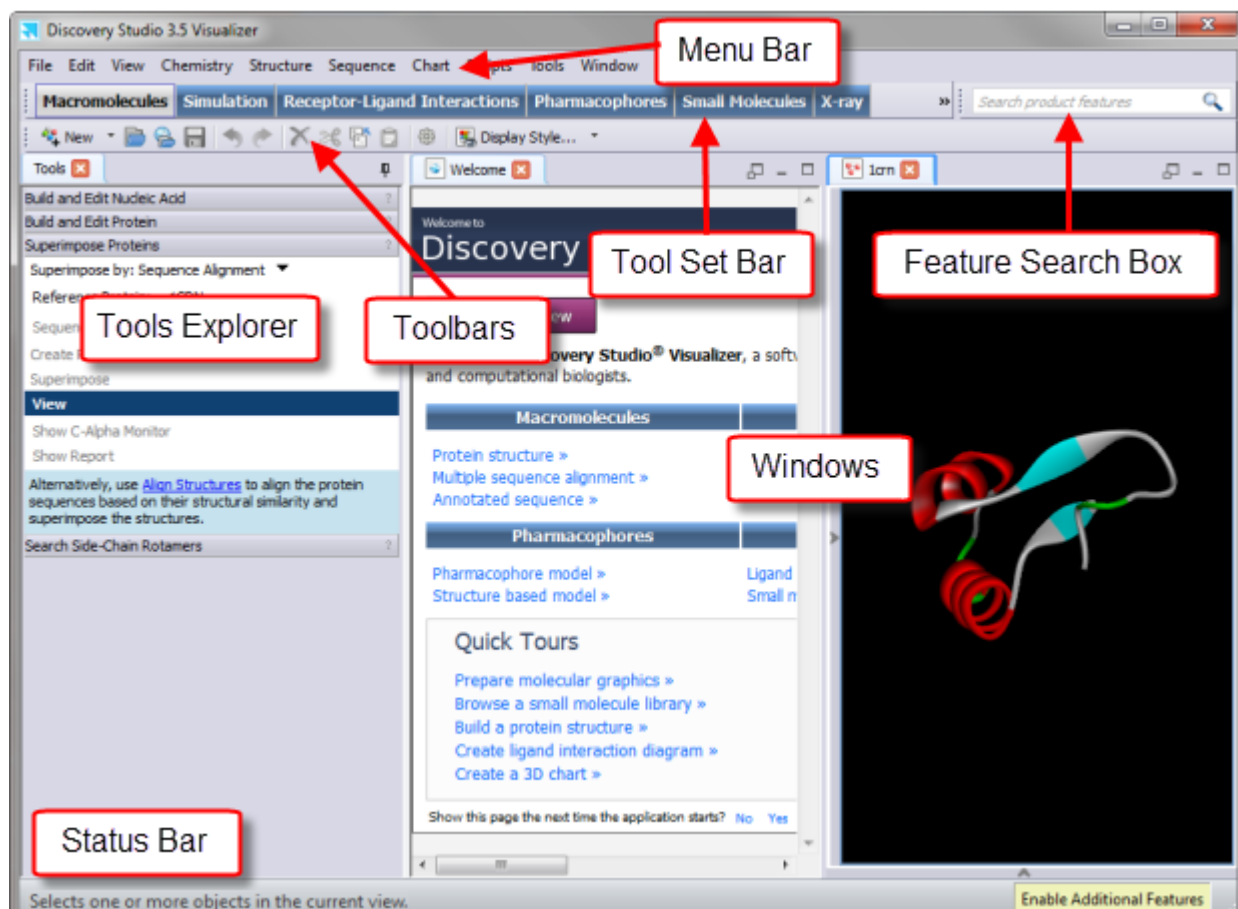


This tutorial covers some (but not all) topics of the program. If you like to know more you can access the Help system of the program where you can find all information you need and a lot of tutorials, also this one is taken in part from them. You should also consider that the free version of the program allows only the complete visualization of molecules and their properties but very limited possibility of computer chemistry calculations.

Application Workspace

The application workspace occupies the main screen area when the application is opened. By default, a Welcome page is displayed in this space when the application is first started. As

subsequent windows are opened they can be easily arranged to either tile them or arrange them on top of each other.




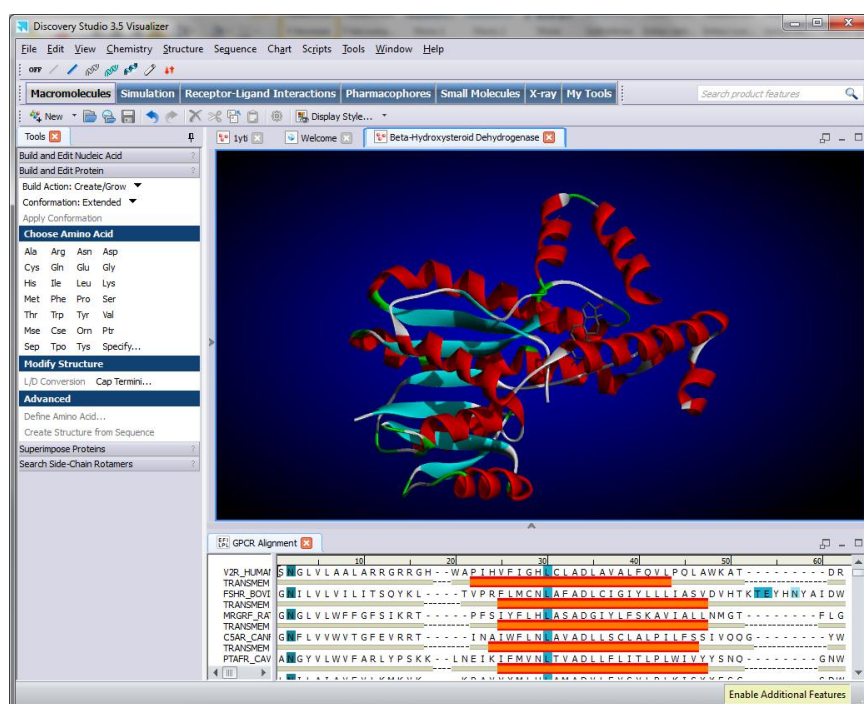
Discovery Studio Visualizer features


Feature	Description
Feature Search Box	Use this to search and open functionality.
Menu Bar	Select menu items to access commonly used tools, such as file access, editing, and viewing commands.
Toolbars	Click buttons to gain access to commonly used tools for viewing and editing data.
Tool Set Bar	Click buttons in the tool set bar to display different groups of related analysis tools in the Tools Explorer.
Windows	The Discovery Studio Visualizer allows you to work with data in a variety of windows, including: <ul style="list-style-type: none"> ▪ Molecule Window: Edit and view molecular structures and property data. ▪ Sequence Window: Edit and view sequences and sequence alignments. ▪ Script Window: Create, edit, and execute Perl scripts within the Visualizer.
Status Bar	Displays information about the current application activity.

Files Explorer

Explore the file system to locate and open data files.

The application offers several ways of organizing and switching between windows. You can move a Window by clicking and dragging its tab to the desired position. In this way you can arrange windows on top of each other or organize them to view them simultaneously. You can also open windows outside of the main application window by clicking on the Undock button on the right side of the window header. This feature is useful when working with multiple monitors. 



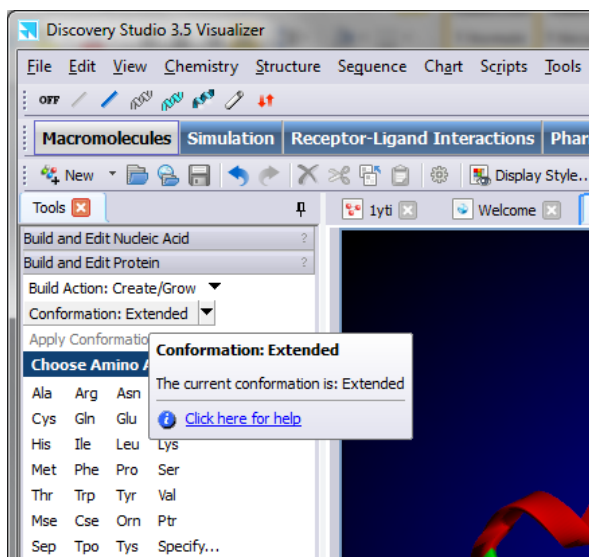
It is also possible to work with the explorer windows in autohide mode to increase the viewable area. To set this mode, click the Pushpin button at the top of an explorer dock. This causes the dock to collapse. 

When you subsequently click on the tab of an explorer, the window is temporarily revealed. If you want to restore the explorer window you should relick the Pushpin button.

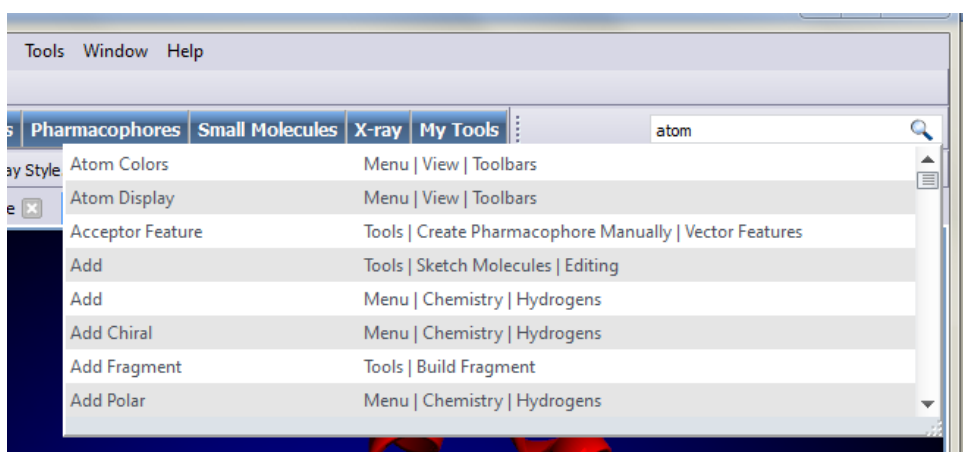
Tools

Discovery Studio offers a wide variety of tools for working with and visualizing data. Tools can be accessed from menus, toolbars and tool panels. In addition you can create you own tools using scripting and expose them anywhere in the application. Of all of the methods for accessing the tools, tool panels are the most flexible. Tool panels group tools based on specific tasks you want to perform. Furthermore, tool panels are groups into large sets for working in areas such as Pharmacophores and Receptor-Ligand Interactions.

A useful feature for most buttons and menu items is the tool tip. Hover your cursor over a feature to display a small note that offers basic information about it. In many cases, the tool tip includes a link to more detailed help or related functionality such as preferences.



Another valuable resource for finding information about the application is the Feature Search Box in the toolbar. To locate a feature, begin typing its name, or some term that relates to its functionality. A list of associated features appears in a dropdown list. The Feature Search Box matches text in the short descriptions of features so matches are obtained even if you do not specify the precise name of a tool. Click on it in the list to present the corresponding menu item, toolbar button, or tool panel.



Menus

The main menu of the application window provides access to basic tools for accessing, editing, and viewing data. The following menus provide access to related sets of functionality:

- File
- Edit
- Menu
- View
- Chemistry
- Structure
- Sequence
- Charts
- Scripts
- Tools
- Windows

- Help

Individual menu items are enabled and disabled depending on the data being viewed. The status bar provides information about what type of data is needed to enable a command, but detailed help for the tool can be opened by hovering over the tool and pressing F1.

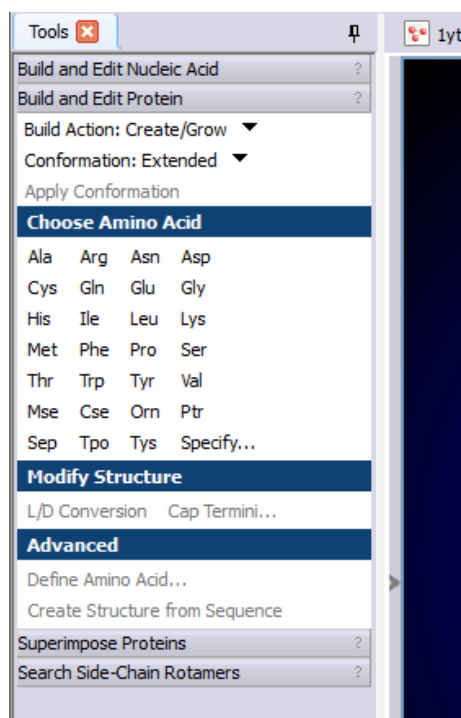
Toolbars

Toolbars are useful for providing quick access to commonly used, quick-running tools. A large set of toolbars are provided, which can be shown or hidden depending on the current task. By default, a set of general purpose toolbars such as Standard and Display are shown when you start the application for the first time. However, as you start to work with the application you can add additional toolbars by right clicking on an existing toolbar and selecting from a drop down list.

Tool Panels

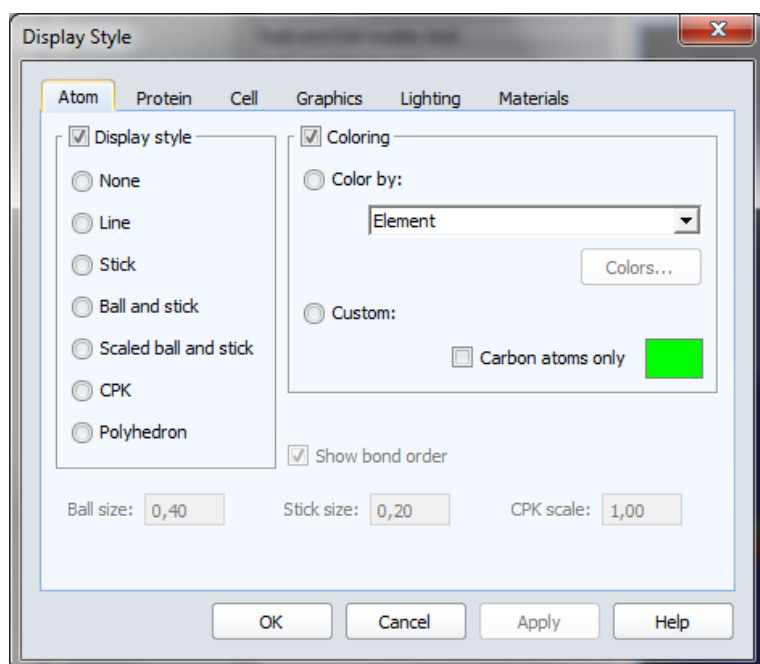
Tool panels are another way of invoking tools to analyze data. Tool panels are graphical palettes that contain buttons, dropdowns and other controls that provide access to related sets of functionality. The tools exposed on tool panels typically operate directly on a selected object in the current window, and like other tools, are enabled and disabled depending on whether the appropriate data is selected.

Tool Panels are located in the Tools Explorer. Custom tool panels can be created from the Tools Explorer or using the Tool Panels preferences page.



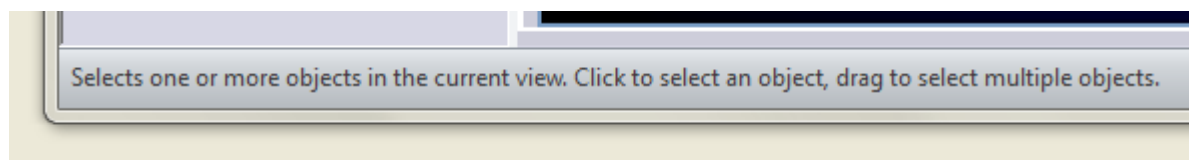
Display Style Dialog

The Display Style dialog is used to change the settings that affect the appearance and behavior of specific data opened in different windows. When data is opened in the application, you can access this dialog by right-clicking the view or from the View menu. This dialog provides access to settings that control particular aspects of the appearance of data or the way the display is configured. Any changes made in the display style dialog are stored with the data if it is saved in a Discovery Studio file format (.dsv).



Status Bar

The Status Bar at the bottom of the application window displays useful information relating to your current activity in the Visualizer. During the execution of some operations, it will display a *Progress Bar* that shows status of the current operations. Clicking the *Close* icon stops the operation. In addition, when working with molecules or sequences, the Status Bar often displays information about the state of the selected object.



Mouse and keyboard actions

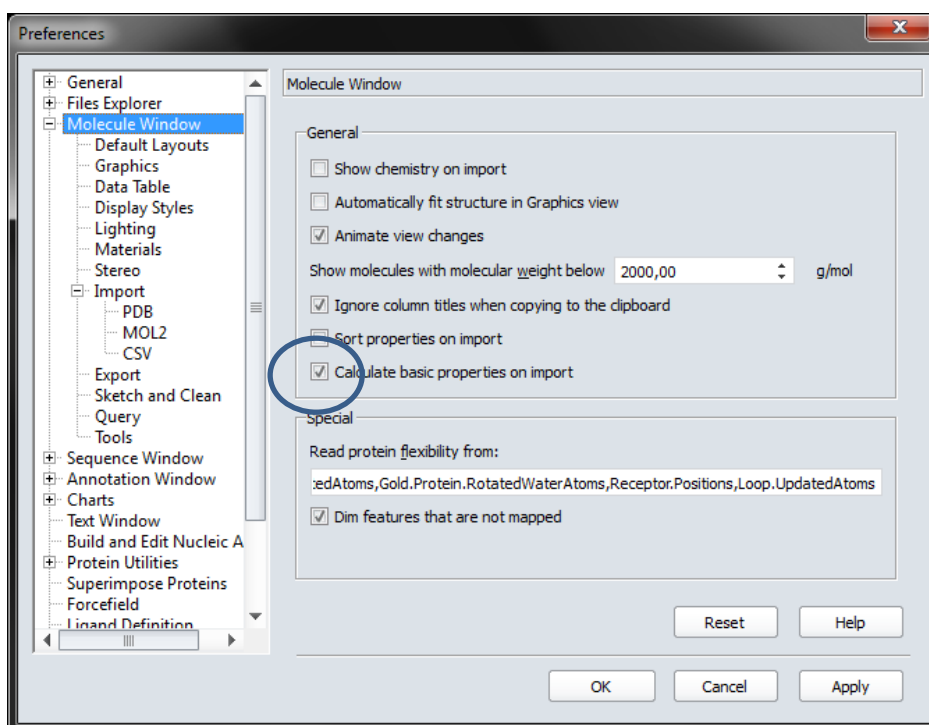
Open Discovery Studio Visualizer. In the Welcome windows click on **Small molecule library** under **Small Molecules** menu. The hydrazide of the furoic acid, the first molecule of the Data Table (on the bottom of the screen, is shown in the workspace. This is the default visualization: molecule is represented as “Stick” corresponding to bonds; the bond order is shown (double bond are represented by two parallel sticks), the atoms are colored according to their type: carbon are grey, oxygen red, nitrogen blue, sulfur yellow, phosphorous violet and so on; hydrogens are not shown.

The Data Table can be hidden and shown by pressing CTRL+T.

The Data Table can show some molecular properties, but it is necessary to modify the default options of the program.

From the menu bar, choose **Edit | Preferences** to open the Preferences dialog.

In the navigation panel click **Molecule Window**. Ensure that the **Calculate properties on import** checkbox is checked.

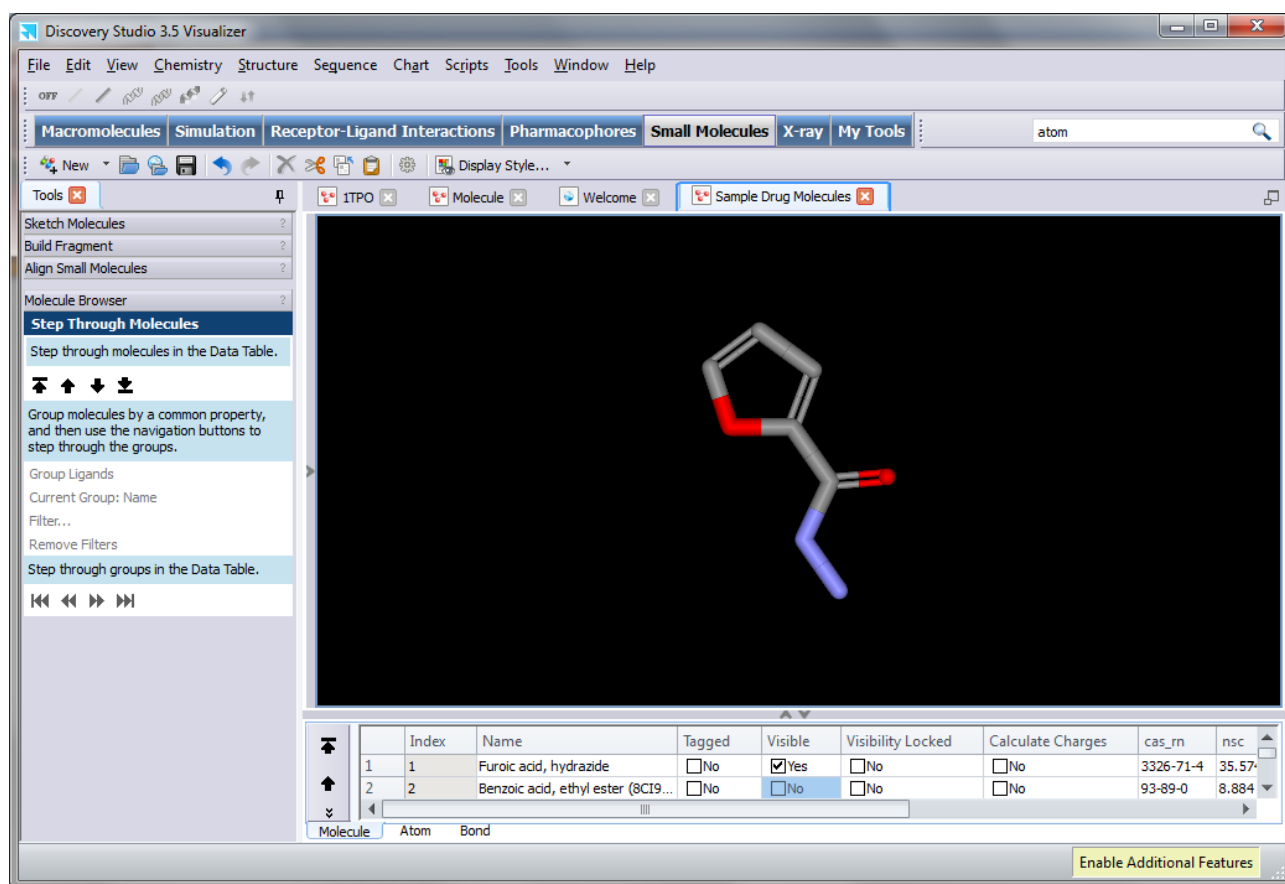


Click **OK** to close the dialog.

When files are opened, the properties will now be calculated and displayed automatically.

Close both the Graphic and the Data Table windows and reopen from the Welcome windows the **Small molecule library**.

Click on the “Atom” and “Bond” tabs at the bottom of the Data Table to see the properties of atoms and bonds of the selected molecule.



Now try to manipulate the molecule.

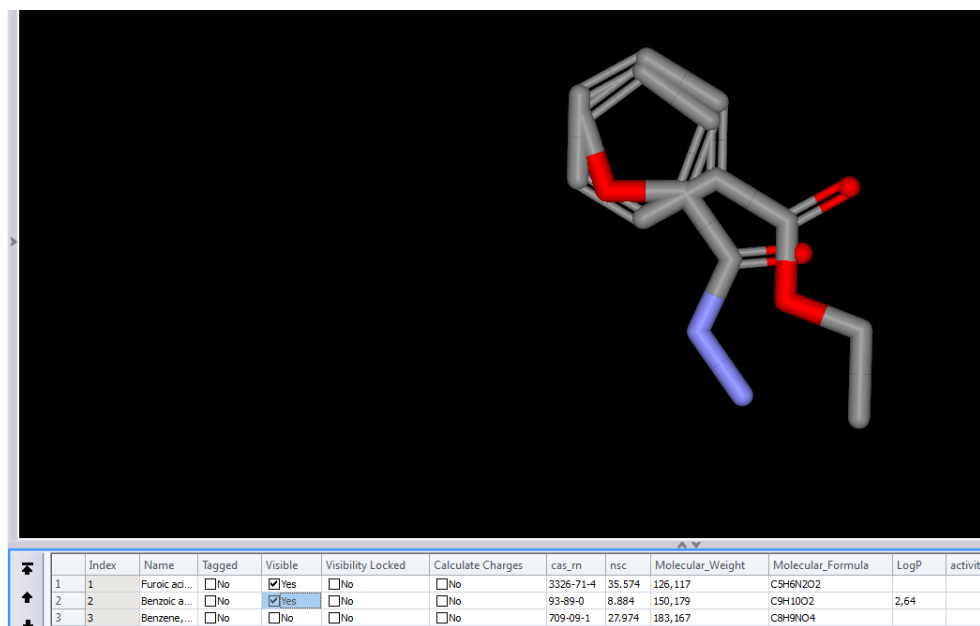
Try to rotate the molecule about x and y axes: **Right-click and drag**

and about z axis: **SHIFT+right-click and drag**

Then try to translate in xy-plane: **Middle-click and drag**

and along the z direction: **SHIFT+middle-click and drag left or right**

Now make visible the second molecule of the library, the ethyl ester of the benzoic acid, by clicking on its “Visible” option on the molecular list. The two molecules are superimposed on the screen.



You can try again the previous commands: they act on both molecules together.

If you click on an atom or in the middle of a bond you can select that atom or that bond respectively: the selected atom/bond appears colored in yellow.

If you double click on any atom the whole molecule is selected: the whole molecule appears colored in yellow. Now you can operate only on the selected molecule by using the same commands already used, but while you **press the CTRL key**, therefore:

Try to rotate the selected molecule about x and y axes: **CTRL+Right-click and drag**

and about z axis: **CTRL+SHIFT+right-click and drag**

Then try to translate in xy-plane: **CTRL+Middle-click and drag**

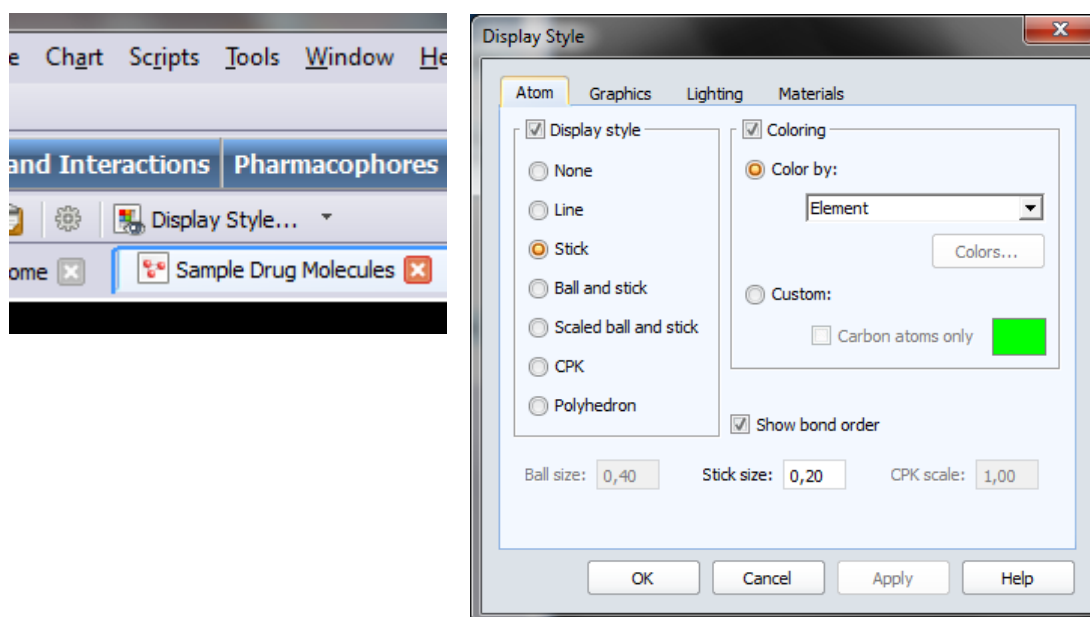
and along the z direction: **CTRL+SHIFT+middle-click and drag up or down**

A selection can be canceled by clicking on a empty region of the workspace. Normally making a selection cancels the previous ones: If you want to add a selection you need to select while you are pressing the SHIFT key. For a multiple section click and drag.

Other mouse and keyboard actions are specific to particular tool modes and may behave differently between modes.

Display Styles

Click on “Display Style...” and graphic menu appears:



Explore the possible styles to represent a molecule: select a display style and click on “Apply”.

If there is some selection (some atoms or some molecule) the display style is applied only to the selection.

You can also explore the graphic possibilities offered by the computer by exploring the other menus (Graphics, Lighting, Materials)

Now load a protein in another window (it would be better if you close the window with the till here considered small molecules. (File/Close)

Working with protein structures and sequences

Introduction

Discovery Studio provides a range of viewers for working with molecular structures and properties. When working with proteins, the Molecule and Sequence Windows are of most value and can be used very effectively to explore different aspects of a molecule and make inferences about its functionality. For example, protein secondary structure predictions can be made on the sequences, and highlight the corresponding regions in the Molecule Window.

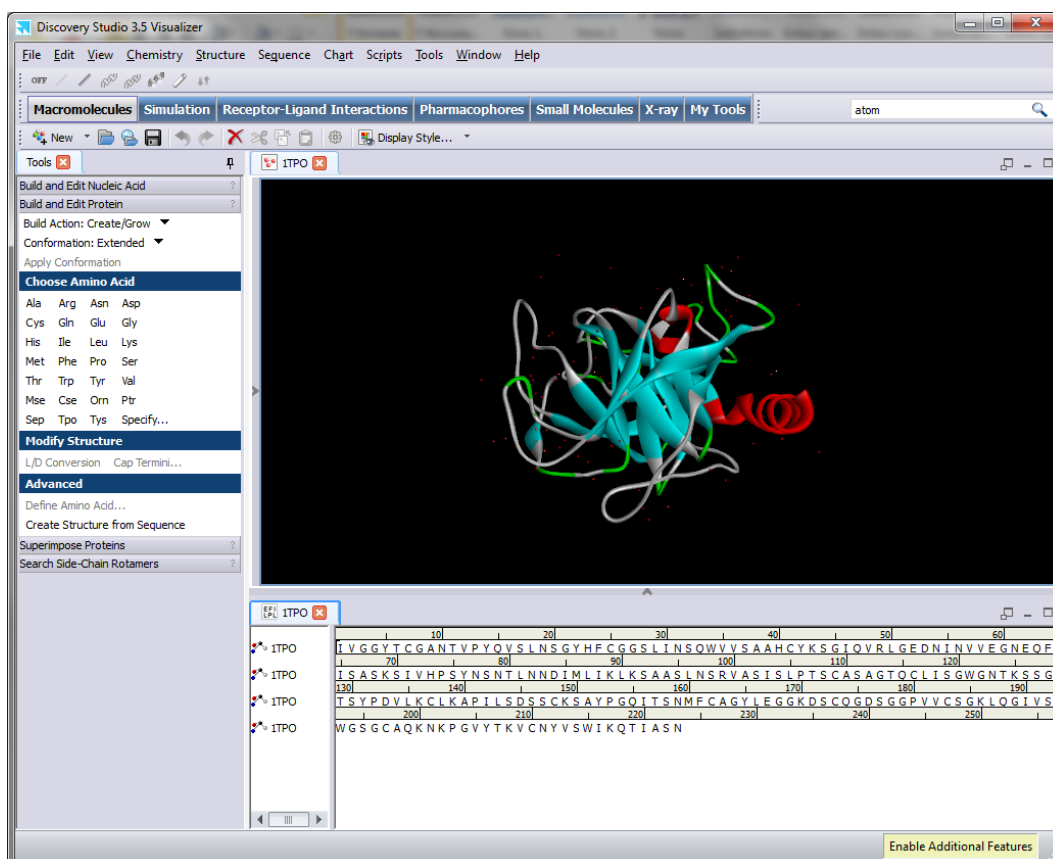
Opening and viewing a protein molecule and its sequence

Choose **File | Open...** from the menu bar and open **Samples | Tutorials | Quick Start Tutorials | 1TPO.pdb**.

The protein structure is shown as a ribbon following the backbone of the protein. Where there are secondary structure features the ribbon is more fat and colored (in light blue for barrels and red for helices). This kind of visualization clearly show the secondary and tertiary structure of the protein but completely hide atoms and in particular the side chain ones.

From the menu bar, choose **Sequence | Show Sequence** to view the sequence of the molecule.

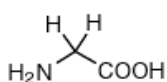
This opens a new Sequence Window that allows you to visualize and manipulate the amino acid sequence and the corresponding 3D structure simultaneously.



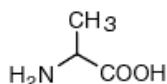
Tip. You can easily adjust window layouts to suit the task at hand. Windows can be tabbed, set side-by-side, or hidden from view. You configure different window layouts by dragging window tabs to desired positions. You can also choose a preset window layout by choosing [Window | Arrange windows](#) from the menu bar. For example, the Macromolecules layout arranges structure windows in the top left, sequence windows along the bottom of the application workspace, and all other windows in the top right. In addition, you can adjust the interface using the actions of the *View* menu and its associated shortcut keys.

The amino acids are indicated with the one-letter code:

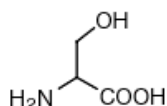
Small



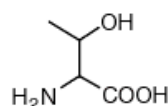
Glycine (Gly, G)
MW: 57.05



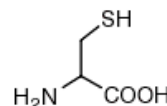
Alanine (Ala, A)
MW: 71.09



Serine (Ser, S)
MW: 87.08, pK_a ~ 16

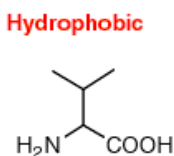


Threonine (Thr, T)
MW: 101.11, pK_a ~ 16

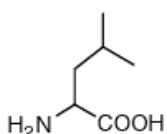


Cysteine (Cys, C)
MW: 103.15, pK_a = 8.35

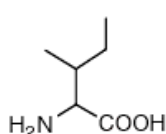
Nucleophilic



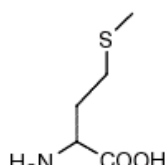
Valine (Val, V)
MW: 99.14



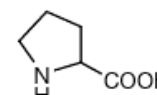
Leucine (Leu, L)
MW: 113.16



Isoleucine (Ile, I)
MW: 113.16

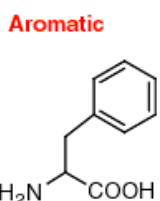


Methionine (Met, M)
MW: 131.19

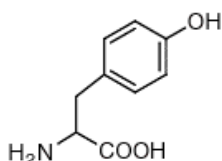


Proline (Pro, P)
MW: 97.12

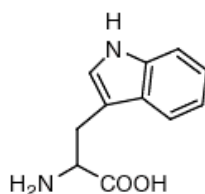
Hydrophobic



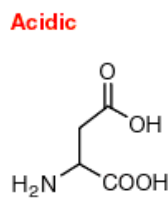
Phenylalanine (Phe, F)
MW: 147.18



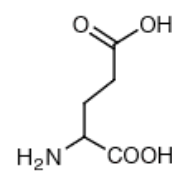
Tyrosine (Tyr, Y)
MW: 163.18



Tryptophan (Trp, W)
MW: 186.21

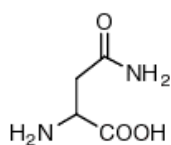


Aspartic Acid (Asp, D)
MW: 115.09, pK_a = 3.9

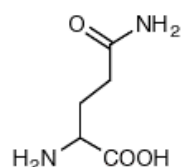


Glutamic Acid (Glu, E)
MW: 129.12, pK_a = 4.07

Amide

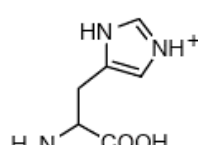


Asparagine (Asn, N)
MW: 114.11

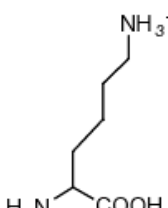


Glutamine (Gln, Q)
MW: 128.14

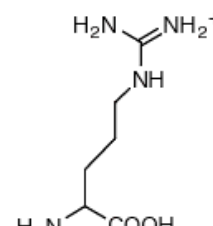
Basic



Histidine (His, H)
MW: 137.14, pK_a = 6.04



Lysine (Lys, K)
MW: 128.17, pK_a = 10.79

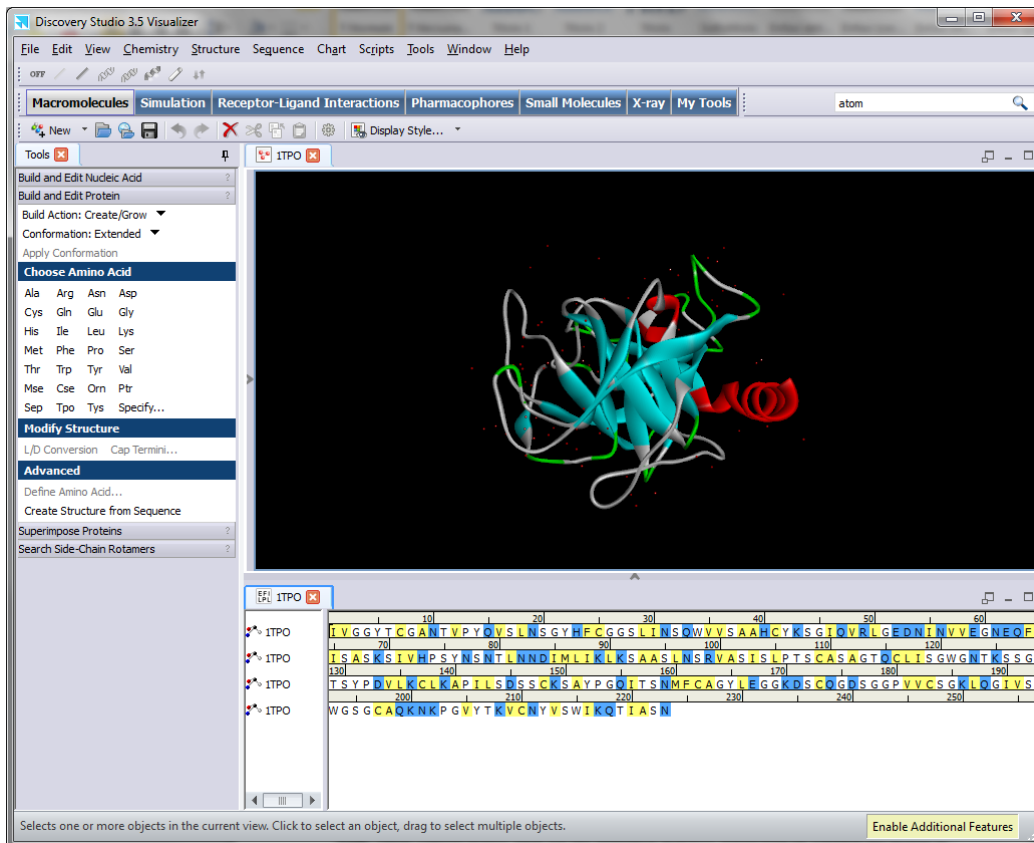
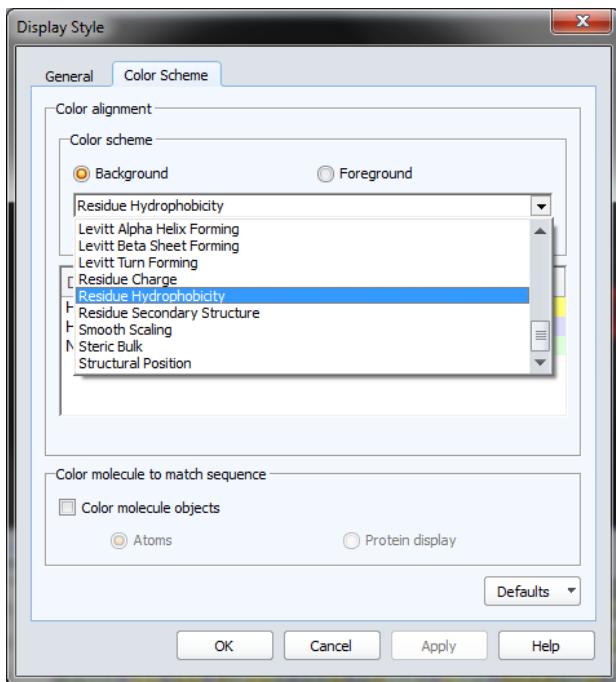


Arginine (Arg, R)
MW: 156.19, pK_a = 12.48

Click the **1TPO** Sequence Window tab to make it active.

Click on the arrow to the right of the Display Style button on the View toolbar and choose **Color by Residue Hydrophobicity**.

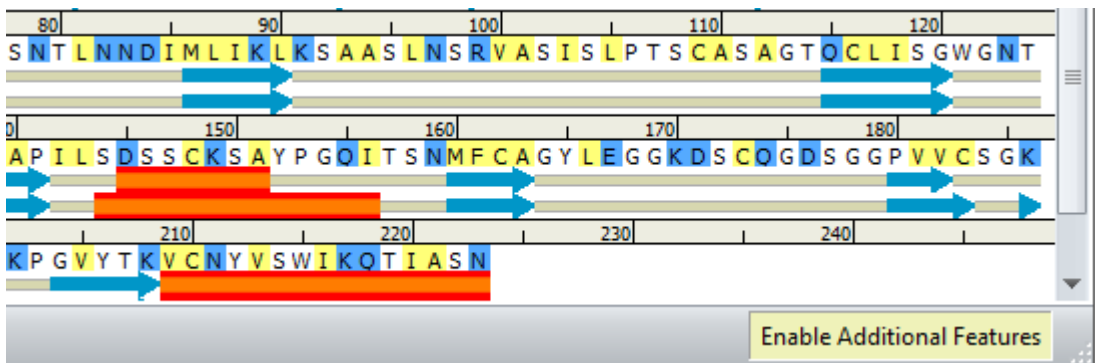
This changes the residue background colors in the Sequence Window based on hydrophobicity of the residue type.



Place the mouse over residues, and then right-click in the Sequence Window and click the **Secondary Structure Cartoon** button.



This displays the PDB and Kabsch-Sander secondary structure cartoon. The blue arrows represent beta strands and the solid red cylinders represent alpha helices.

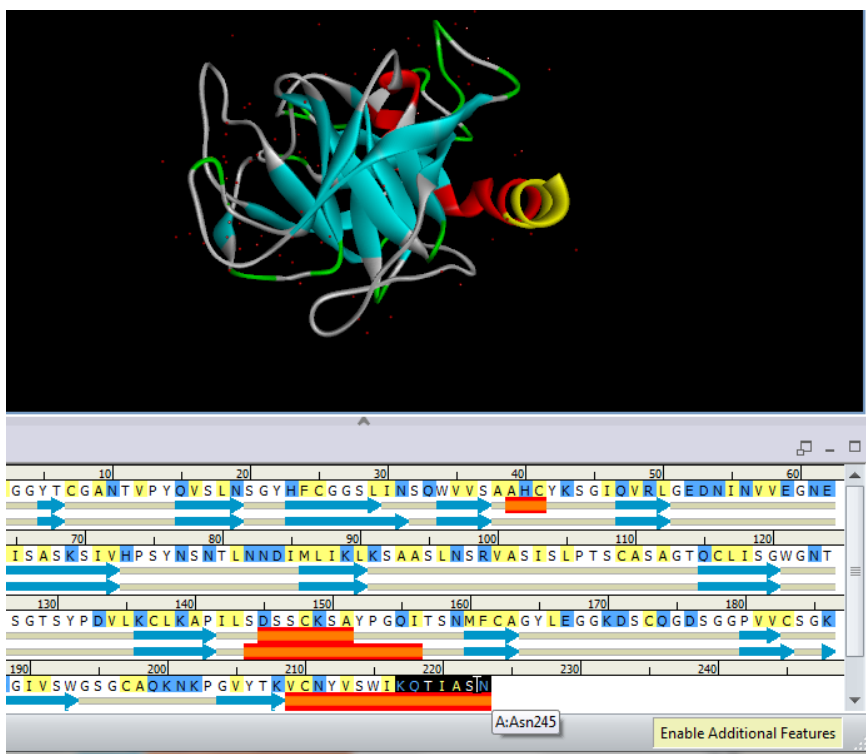


Note. You can also control the secondary structure cartoon display by choosing **Sequence | Secondary Structure | Visibility...** from the menu bar.

Note. Three context menus exist for the Sequence Window depending on whether the mouse is in the sequence name pane, ruler display, or residues area.

Selecting residues

Discovery Studio Visualizer offers numerous methods for selecting specific residues or other objects. Windows displaying the same data are interactive. If you make a selection in a Sequence Window, the same selection is made in the corresponding Molecule Window. Different views of the data in the Molecule Window can also be used to make selections.



The selected residues are coloured in yellow in the structure and are backgrounded in black in the sequence

Hover the cursor over any **residue** in the Sequence Window.

The residue ID is reported in a tooltip (A:Asn245).

With the mouse over the ruler area of the Sequence Window, right-click and choose **Residue ID** to display the residue IDs for the first (and in this case, the only) sequence. Find and select the three residues of the Catalytic Triad - **HIS57**, **ASP102**, and **SER195**.

```

167 168 169 170 171 172 173 174 175 176 177 178 179 180 181
I V G G Y T C G A N T V P Y O V S L N S G Y H F C G G S L I N S Q W V V S A A H C Y K S G I Q V R L G E D N I N V V E G N E O F
139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171
S G W G N T K S S G T S Y P D V L K C L K A P I L S D S S C K S A Y P G Q I T S N M F C A G Y L E G G K D S C Q G D S G G P V

```

If you make a mistake when selecting a residue, you can undo that selection action by choosing *Edit / Undo* from the menu bar, or by pressing CTRL+Z.

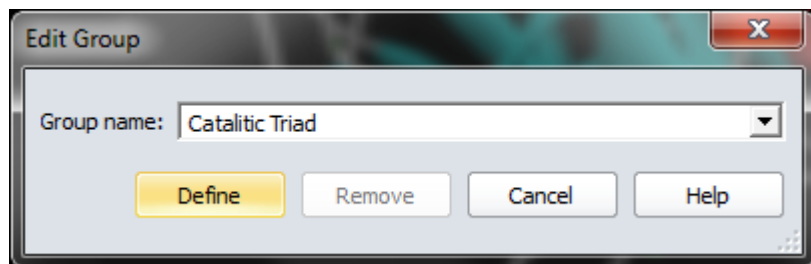
Tip. You can also use the Hierarchy View or Data Table View to select the residues. Use CTRL+H and CTRL+T to control the display of these views.

At this point it is useful to be able to save the current selection in the structure and restore it later. Discovery Studio Visualizer supports the creation of *Groups* to provide this functionality. Groups can be created from any combination of objects that are selected in the Molecule Window. Once created, they are displayed in the Hierarchy View. Any groups that you have created are saved in the [.dsv](#) format. This is a proprietary format which saves all is in the workspace including all selections and rendering.

Click the **1TPO - Molecule Window** tab to make it active.

With the Catalytic Triad residues selected, from the menu bar, choose **Edit | Group...** to open the Edit Group dialog.

Enter **Catalytic Triad** as the **Group Name** and click **Define**.

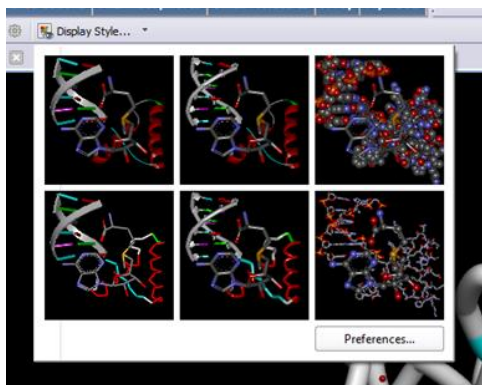


Select **View | Transform | Fit To Screen**, or click **Fit To Screen** on the **View** toolbar to center and zoom over the Triad.

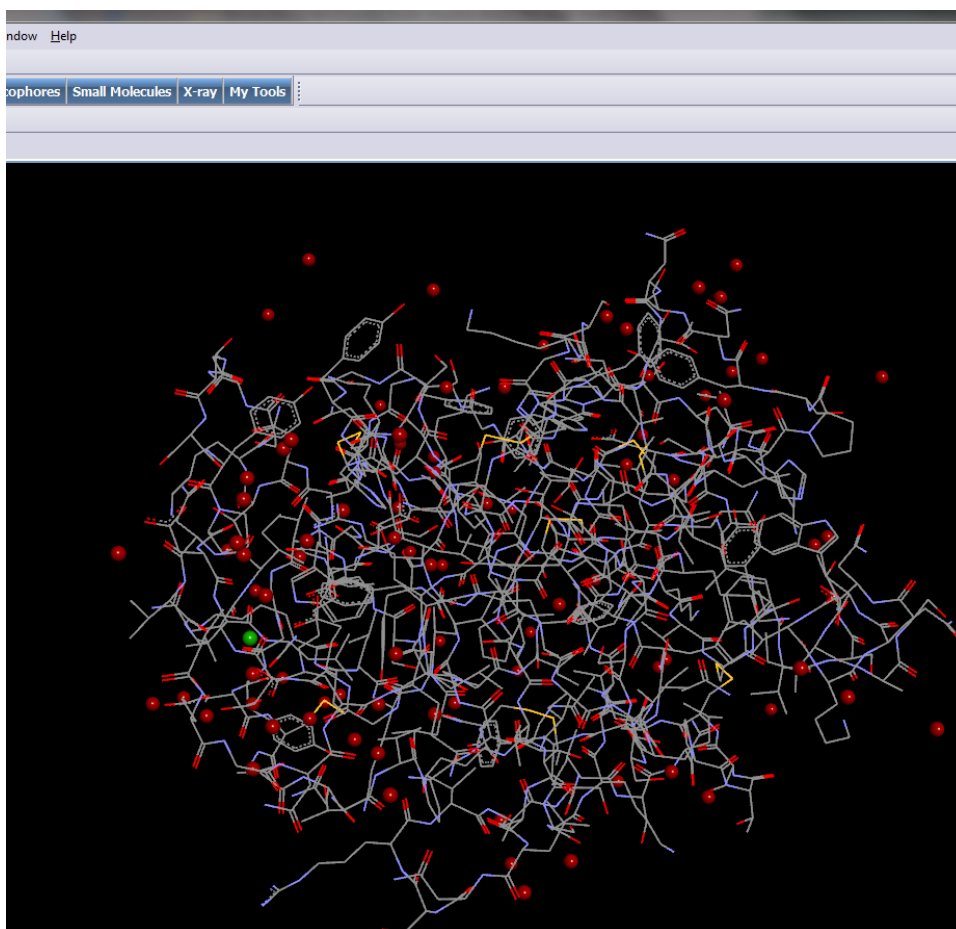
Note. The Catalytic Triad group is added to the Hierarchy View (at the bottom) and Data Table View (Group tab).

To view the individual residues more easily it is useful to change the display style of the structure to an atomistic representation. To do this you can use the Display Style control on the View toolbar.

Click on the arrow to the right of the Display Style button on the View toolbar and select one of the styles of the preview page: click on line mode display (the bottom right style).

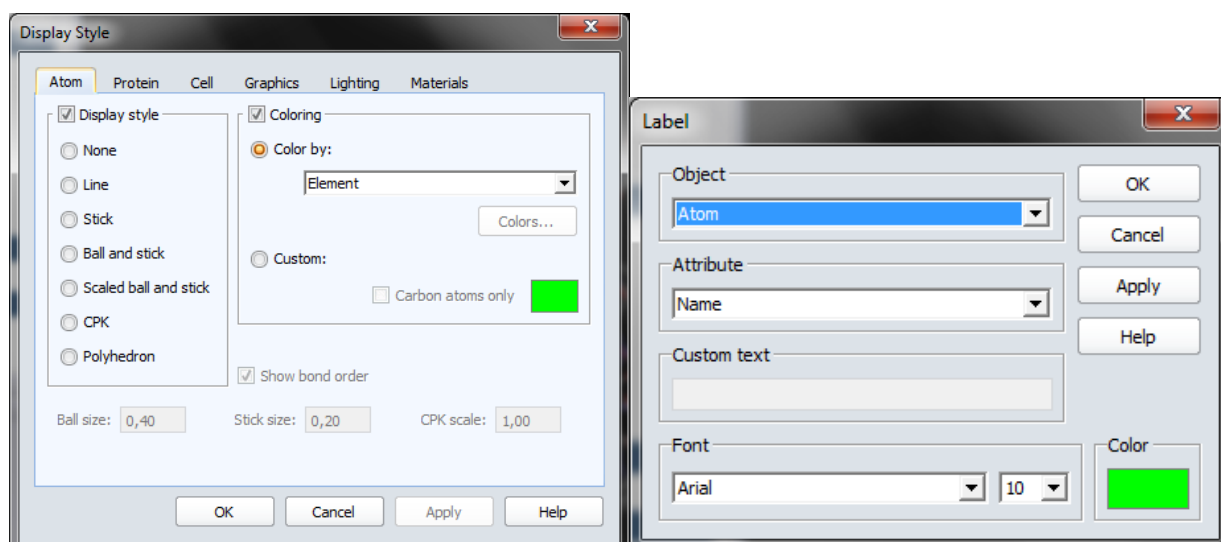


The appearance of the structure is now updated to show the atoms in line mode.



Alternatively you can open the “**Display style**” windows and select the way of appearance for atoms, protein, etc. or you can insert labels giving **Structure | Labels | Add**.

Remember that all this display changes will be applied only to the active selection or, if there are not any active selection, to all the molecules in Workspace.



Customizing the appearance of the protein structure

Click an empty area of the window to cancel the selection.

Select **View | Display Style...** from the menu bar.

On the **Atom** tab of the Graphics View Display Style dialog, set the **Display style** to **None**.

Click the **Protein** tab and set the **Display style** to **Solid Ribbon**.

Click the **Color by:** radio button in the **Coloring** group and set the value to **Secondary Type**.

Click **OK**.

Choose **View | Transform | Fit To Screen** from the menu bar, or click **Fit To Screen** on the **View** toolbar to display the entire molecule.

This will remove all the atom-based rendering and only display the solid ribbon rendering.

From the Hierarchy View, select the **Catalytic Triad** group. Open the Display Style dialog and select **Stick** on the **Atom** tab. Click **OK**. Select **View | Transform | Fit To Screen** from the menu bar, or click **Fit To Screen** on the **View** toolbar to focus on the triad again.

In the Graphics View, notice that only residues HIS57, ASP102, and SER195 are displayed as stick models, and the remainder of the protein is rendered as a ribbon. By only allowing a subset of residues to be visible on the Graphics View, you have a more focused view of the residues of interest, a simplified view of the Catalytic Triad in this case.

Tip. Saving files in [.dsy](#) format will retain the active view, the rendering, the labels, or any other annotations that you have made. [.dsy](#) files provide an efficient medium for sharing information with colleagues.

From the menu bar, choose **Window | Close All** to prepare for the next section of the tutorial. There is no need to save any files, so select **No** in the dialog that appears.

Exploring interactivity between the Molecule Window and the Sequence Window

The previous section illustrated interactivity between windows by describing residue selection in the Sequence Window and display style changes in the Molecule Window. In this section, you will continue to explore examples of window interactivity and see additional examples that illustrate the value of window-to-window interactivity.

Choose **File | Open...** from the menu bar and open **Samples | Tutorials | Quick Start Tutorials | 1BVN.pdb**.

From the menu bar, choose **Sequence | Show Sequence** or press **CTRL+Q** to open the Sequence Window.

Press **CTRL+H** to open the Hierarchy View if it is not already displayed. Notice three chains in the Hierarchy View named P, T, and P. Click the first **P** chain to select it.

A selection will be made in the Graphics View and also in the Sequence Window. If you select residues in the Sequence Window, they are also selected in the Graphics View, the Hierarchy View, and the Data Table.

On the **Sequence Window**, slowly click and drag from left to right starting from residue 1 in the ruler.

In the Sequence Window, the selection will have a black background. The selection in the Hierarchy View and the Graphics View is highlighted in yellow. A selection is also made in the Data Table.

Use the **Select** tool to select a region of the structure in the Graphics View.

Notice that residues in the Sequence Window are highlighted as well.

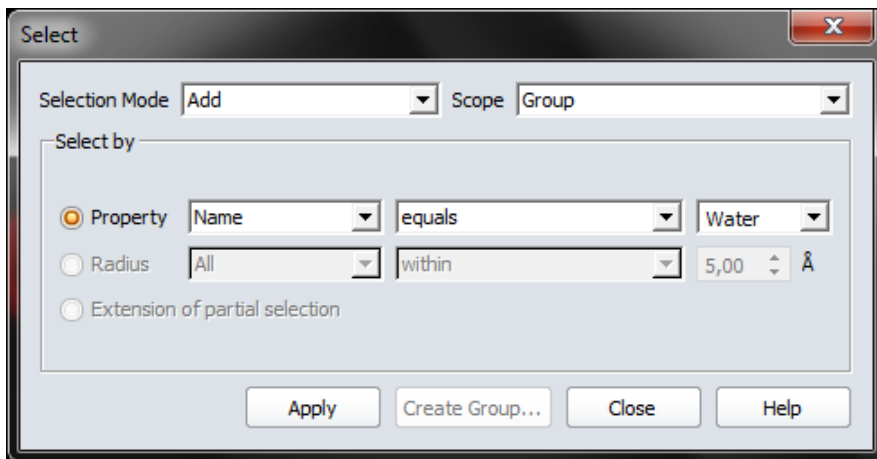
From the menu bar, choose **Window | Close All** to prepare for the next section of the tutorial. There is no need to save any files, so select **No** in the dialog that appears.

Editing a protein structure

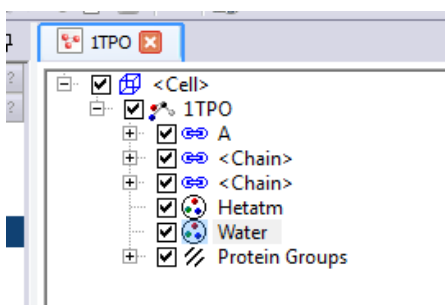
Choose **File | Open...** from the menu bar and open **Samples | Tutorials | Quick Start Tutorials | 1TPO.pdb**.

The structures archived into Protein Data Bank are saved as **.pdb** file. This file generally does not consider hydrogen atoms, moreover they are structures obtained from X-ray crystallography performed on proteins crystallized from aqueous solutions and therefore they contain crystallization water molecules which are shown here as red little spheres.

In order to delete water molecules they need to be selected in one of these ways: **Edit | Select** then in the Select windows choose Add – Group – Name equals Water,



Alternatively, you can open the Hierarchical windows (**Ctrl+H**) and click on Water,



or open the Group Table windows (**Ctrl+T**), click on Group (bottom right) and on the number 2 corresponding to the group Water.

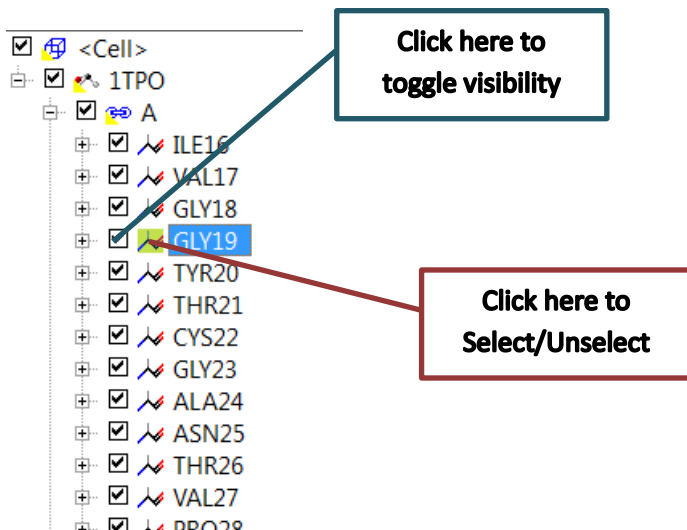
	Name	ID	Visible	Parent	Size
1	Hetatm	0	<input checked="" type="checkbox"/> Yes	1TPO	85
2	Water	0	<input checked="" type="checkbox"/> Yes	1TPO	84
3	Disulfide ...	0	<input checked="" type="checkbox"/> Yes	Protein Gr...	12
4	Backbone	0	<input checked="" type="checkbox"/> Yes	Protein Gr...	893
5	Sidechain	0	<input checked="" type="checkbox"/> Yes	Protein Gr...	736
6	Hydropho...	0	<input checked="" type="checkbox"/> Yes	Protein Gr...	77

Molecule Cell AminoAcidChain AminoAcid Atom Chain Residue Bond Group

In all cases all the water molecules should be selected (colored in yellow) and you can delete them by pressing the Del key.

Select/Unselect, Show/Hide in Hierarchical Table

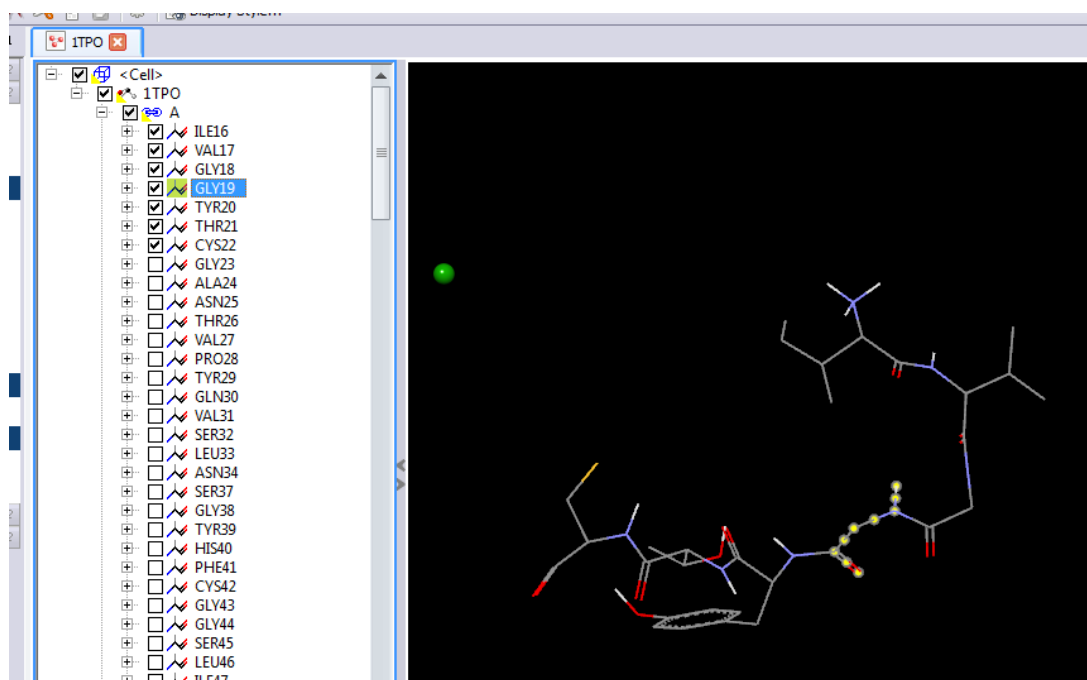
Clicking on you can expand Cell→Structure→Chains→Residues→Atoms. Clicking on you can compress the Table. Clicking on the Table you can Toggle the visibility or Select/Unselect. If you need to select a series of residues (or atoms) in sequence you can click on the first and then click on the last while you maintain pressed the Shift key.



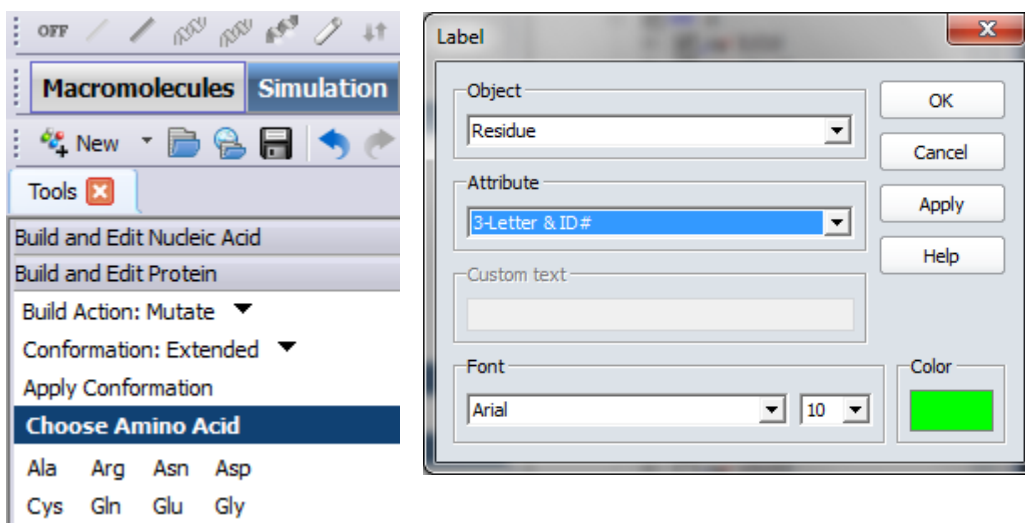
The missing hydrogens can be easily added. Select line mode display. Choose **Chemistry | Hydrogen | Add**. For simplifying the display now hide all hydrogens (**Chemistry | Hydrogen | Hide**) and show only the polar ones, i.e. those linked to heteroatoms (**Chemistry | Hydrogen | Show Polar**). Only polar hydrogens can give H-bond.

You can mutate a residue. This can be very useful if the pdb structure has some unresolved residues that appears as alanines, i.e. with only a methyl in the side chain.

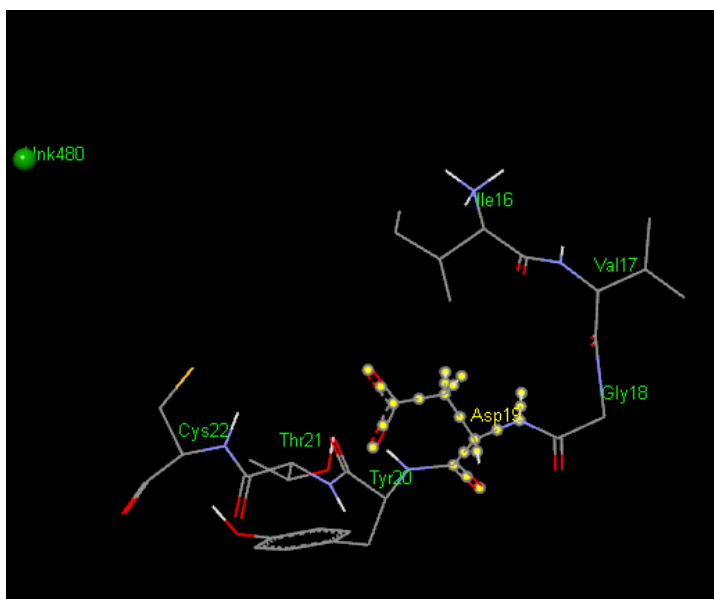
Mutate residue Gly19 into an aspartate. Firstly simplify the display showing only the first 7 residue, while all others are hidden (not canceled) and select the residue Gly19. In the hierarchical window deselect the A chain, then select the first 7 residues and click on the structure symbol of Gly19. The green sphere is a Ca ion contained in the structure.



Alternatively you can select a residue by clicking twice on an atom of it. In this case is convenient to label the residues with name and number: choose **Structure | Labels | Add** then **Residue and 3-Letter & ID#**

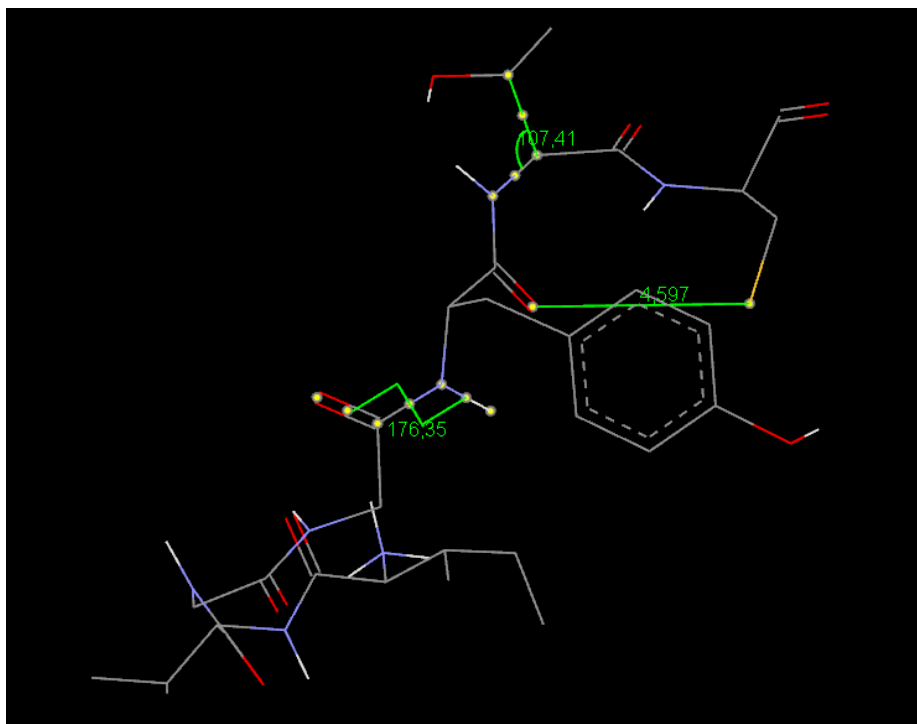


When the residue Gly19 is selected (it is colored in yellow) in the tool explorer (it should be selected the Macromolecule tool) open the Build and Edit Protein menu and select Mutate, then click on Asp and Gly19 now is Asp19.

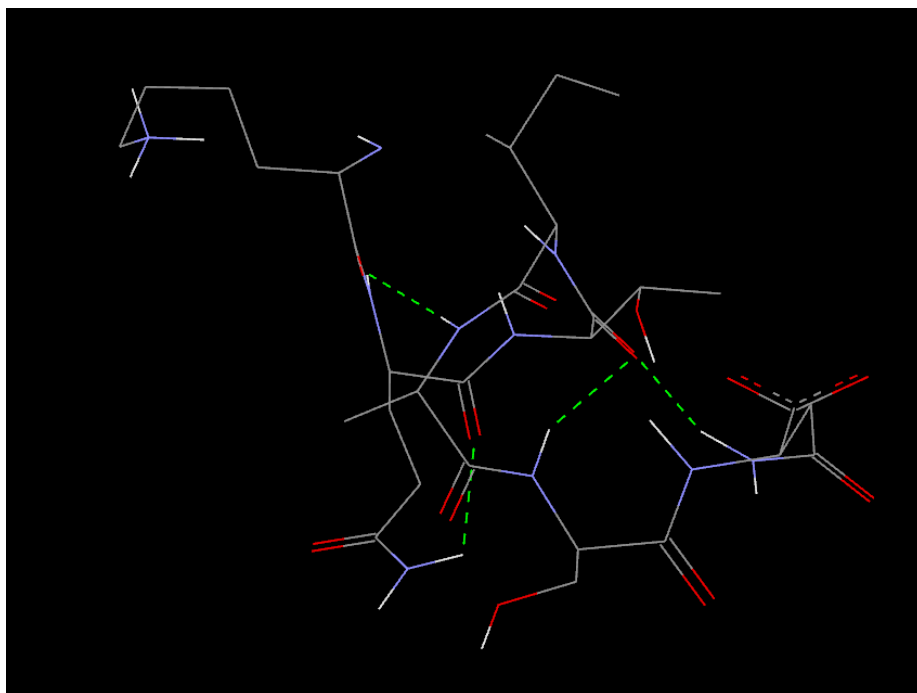


It is possible to measure distance and angles and show intermolecular H-bond.

For measuring distance select two atoms at the same time by clicking once on both (remember that it is necessary to maintain pressed the Shift key while clicking if you want to add selection) then choose **Structure | Monitor | Distance**. For angle select three atoms then **Structure | Monitor | Angle**, for torsion select four atoms then **Structure | Monitor | Torsion**.

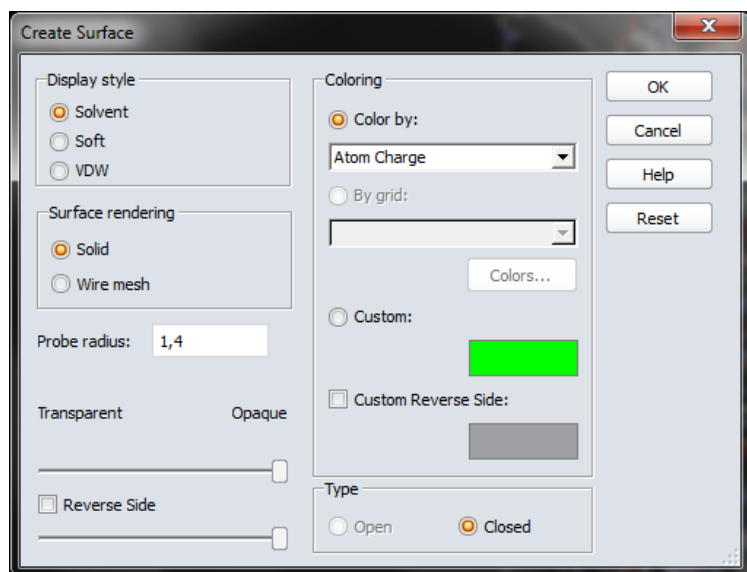


For showing H-bond choose **Structure | Monitor | HBonds**, however if you are seeing the first 7 residues you cannot see any H-bond because there are not. You need to make visible all the molecule or the last 7 or more residues where there are H-bonds. To do this use the hierarchical window as previously explained.

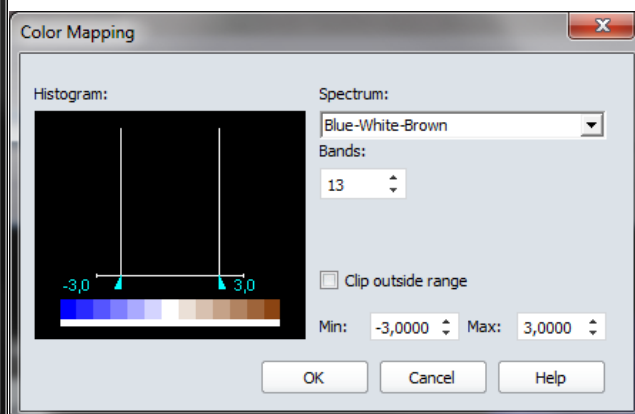
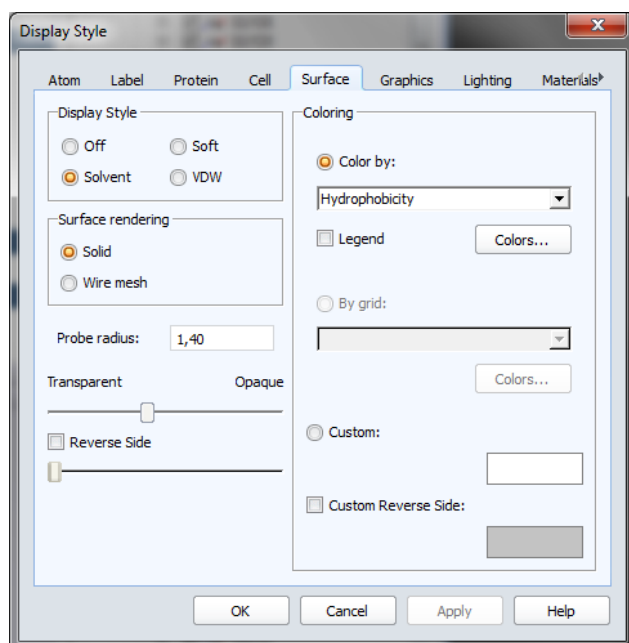


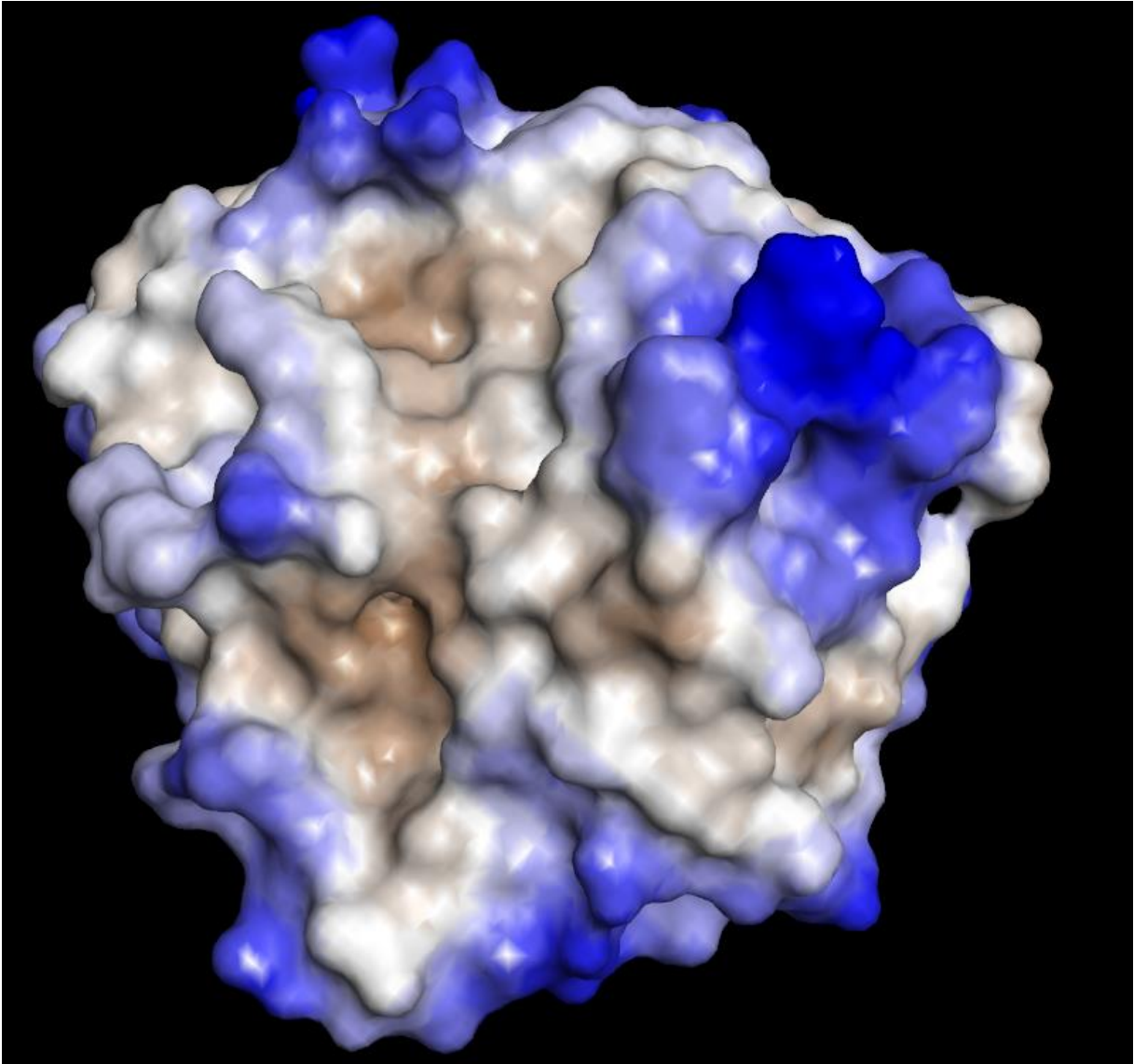
A very useful tool for analyzing the molecular properties is that to draw the molecular surface and color it according to the value of certain properties.

To draw a molecular surface firstly make visible the whole protein through the hierarchical window then choose **Structure | Surface | Add** and in the Create Surface windows choose Display style Solvent (draw the surface exposed to solvent), Surface rendering Solid and press OK



You can change the surface: open the Display Stule window and select Surface. You can change the kind of style and rendering, the transparency, and the color method. For example if you wanto to analyze the hydrophobic properties of the protein choose Color by Hydrophobicity; by pressing Colors... button you can select the color spectrum: the default spectrum colors the hydrophobic region in brown and the lipophilic ones in blue. You can explore other styles, properties and colors.





Appendix A.

Default mouse and keyboard actions

To	Press
Select single object	Left-click the object
Select an object's parent in the Graphics View	Double-click the object to continue selecting the object's ancestry. For example, double-clicking a selected atom that has a residue as its parent will select the whole residue. If that residue has a chain as its parent, double-clicking the atom again will select the whole chain. By continuing this action, the molecule, cell, and root object (all objects) can be selected if the hierarchy exists.
Translate view in xy-plane	Middle-click and drag
Translate selected object in xy-plane	CTRL+middle-click and drag
Translate view along z-axis	SHIFT+middle-click and drag left or right*
Translate selected object along z-axis	CTRL+SHIFT+middle-click and drag up or down*
Rotate view about x- and y-axes	Right-click and drag**
Rotate selected object about x- and y-axes	CTRL+right-click and drag
Rotate view about z-axis	SHIFT+right-click and drag
Rotate selected object about z-axis	CTRL+SHIFT+right-click and drag
View from the right (end of x-axis)	X
View from the top (end of y-axis)	Y

View from the front (end of z-axis)	Z
Zoom in	Mouse wheel roll forward
Zoom out	Mouse wheel roll backward
Back clipping plane	SHIFT+mouse wheel
Front clipping plane	CTRL+mouse wheel
Both clipping planes	CTRL+SHIFT+mouse wheel
Context menu	Right-click

Keyboard controls

To	Press
Open the Graphics View	CTRL+G
Open the Hierarchy View	CTRL+H
Open the Data Table View	CTRL+T
Select all	CTRL+A
View full screen	F11
Cut	CTRL+X
Copy	CTRL+C
Paste	CTRL+V
Find	CTRL+F
Delete selected objects	DELETE
Zoom in	CTRL+(plus)
Zoom out	CTRL+(minus)
Capture a scene	INSERT
Return to the first scene	CTRL+HOME
Toggle visibility of all Explorer Windows	CTRL+1
Toggle visibility of left-docked Explorer Windows	CTRL+2
Toggle visibility of horizontally-docked Explorer Windows	CTRL+3
Toggle visibility of right-docked Explorer Windows	CTRL+4

Toggle visibility of the Jobs Explorer	CTRL+J
Choose window	CTRL+TAB
Rotate view left on y-axis	Left arrow
Rotate view right on y-axis	Right arrow
Rotate view forward on x-axis	Up arrow
Rotate view backward on x-axis	Down arrow
Reset to original orientation	HOME
Stop current action	END
Change element type of selected atoms	C, H, O, N, P, S, F
Change bond order of selected bonds to single/double/triple/aromatic	1, 2, 3, or 4
Change hybridization of selected atoms (if no bonds are selected) to sp/sp ² /sp ³	1, 2, 3
Tile molecules in view	CTRL+L
Show next molecule	CTRL+Down arrow
Show previous molecule	CTRL+Up arrow
Show sequence	CTRL+Q

Tool-specific actions

Select tool

To	Press
Multiple selection	Left-click and drag
Select multiple items individually	SHIFT+left-click

Rotate tool

To	Press
Rotate view about x- and y-axes	Left-click and drag**
Rotate selected object about x- and y-axes	CTRL+left-click and drag
Rotate view about z-axis	SHIFT+left-click and drag
Rotate selected object about z-axis	CTRL+SHIFT+left-click and drag

Translate tool

To	Press
Translate view in xy-plane	Left-click and drag
Translate selected object in xy-plane	CTRL+left-click and drag
Translate view along z-axis	SHIFT+left-click and drag*
Translate selected object along z-axis	CTRL+SHIFT+left-click and drag*

Zoom tool

To	Press
Zoom in	Left-click and drag up
Zoom out	Left-click and drag down

Torsion tool

To	Press
Rotate torsion	Left-click bond and drag horizontally
Rotate opposite end of torsion	SHIFT+left-click bond and drag horizontally
Rotate peptide plane	CTRL+left-click and drag horizontally on amide bond
Rotate omega	CTRL+SHIFT+left-click and drag horizontally on amide bond

Sketching tool

Sketch mode

To	Press
Add carbon atom	Left-click in Molecule Window (drag + left-click attaches additional carbon atom)
Change single bond to double bond	Left-click the previously created atom
Add bond between atoms	Left-click a previously created atom, but not the most recently created (i.e., currently selected) atom
Stop sketching	Left-double-click or move cursor outside Molecule Window

Chain mode

To	Press
Create 2-carbon chain	Left-click in Molecule Window
Create chain of more than 2 carbons	Left-click and drag
Reflect chain by 180°	CTRL while left mouse button is still pressed following previous sketching action
Attach carbon chain to existing chain	Left-click and drag on existing atom

Ring mode

To	Press
Create 6-carbon ring	Left-click in Molecule Window
Create aromatic 6-carbon ring	CTRL+left-click
Create ring of more than or fewer than 6 carbons	Left-click and drag
Create aromatic ring of more than or fewer than 6 carbons	CTRL+left-click and drag
Attach 6-carbon ring to existing ring	Left-click atom in existing ring
Attach aromatic 6-carbon ring to existing ring	CTRL+left-click atom in existing ring
Attach ring of more than or fewer than 6 carbons to existing ring	Left-click and drag on atom in existing ring
Attach aromatic ring of more than or fewer than 6 carbons to existing ring	CTRL+left-click and drag on atom in existing ring
Fuse 6-carbon ring to bond in existing ring	Left-click bond in existing ring

Fuse aromatic 6-carbon ring to bond in existing ring	CTRL+left-click bond in existing ring
Fuse ring of more than or fewer than 6 carbons to bond in existing ring	Left-click and drag on bond in existing ring
Fuse aromatic ring of more than or fewer than 6 carbons to bond in existing ring	CTRL+left-click and drag on bond in existing ring

Text mode

Mode	To	Press
Annotation	Create text annotation	Left-click, then enter text in Annotation Text dialog.
Boxed	Create boxed text	Left-click, then enter text in Annotation Text dialog.
Callout	Create boxed text as callout	Left-click object, then left-click to place boxed text.

Note. To change the size of boxed or callout text, use *Select* to left-click and drag the small square on the corner of the box.

Display mode

To	Press
Display particular object type only	Left-click object name in Hierarchy View
Display range of objects	SHIFT+left-click objects defining range in Hierarchy View
Toggle display of object	Left-click object in Molecule Window

Sequence Window

To	Press
Show Annotations	Double-click the sequence name
Select residues	Left-click and drag
Select residues by secondary structure domain	Left-click secondary structure cartoon
Select block	Left-click and drag over
Select sequence	Left-click the sequence name or left-double-click residues
Extend residue selection	SHIFT+left-click
Add residue(s)	Left-click and drag over
Add/subtract single residue (toggle)	CTRL+left-click
Add/subtract sequence selection (toggle)	CTRL+left-click sequence name
Extend sequence selection	SHIFT+left-click sequence name

Add gap	Position the cursor at the desired location and press SPACE BAR
Remove gap	Position the cursor at the desired location and press DELETE or BACKSPACE
Add a chain break	Position the cursor at the desired location and press the / key
Shift a block	Select the block and left-click and ALT-drag or SHIFT-CTRL-drag
Shift an aligned block	Select the aligned block and left-click and ALT-CTRL-drag
Move a block of residues	Linux - First left-click , then press ALT Windows - Left-click, press ALT
Activate the linked molecule window	Double-click the link icon

Note. A block of residues is defined as a range of residues surrounded by gaps at both ends.

Annotation Window

To	Press
Scroll through the window when there are features outside of the view limit	Up arrow and down arrow
Move from one end of a sequence to the other	In Zoom mode, left arrow and right arrow
Copy the selection to the clipboard.	CTRL+C
Insert the contents of the clipboard in the current document. Requires that compatible data has been copied to the clipboard.	CTRL+V
Delete the selected sequence features.	DEL
Toggle the visibility of the Graphics View in the current window.	CTRL+G
Toggle the visibility of the Hierarchy View in the current window.	CTRL+H
Toggle the visibility of the Data Table View in the current window.	CTRL+T
Change the display style of the selected items. If nothing is selected the display style of all visible items is changed.	CTRL+D
Decrease/increase the magnification for the current view.	CTRL+/-/+
Reset the magnification in the current view to its original level.	CTRL+O
Reset the magnification level and orientation of data in the current view to their original settings.	HOME
Select all items in the current view.	CTRL+A

Charts

2 Dimensional

To	Press
Translate right	Right arrow
Translate right faster	CTRL+right arrow
Zoom	ALT+right arrow
Reposition	ALT+left arrow
Rotate	ALT+up arrow
Zoom out Y	ALT+down arrow

3 Dimensional

To	Press
Zoom	Roll mouse wheel
Reposition	Hold mouse wheel and drag
Rotate	arrows
Rotate slowly	SHIFT+arrow

* If you translate objects in the z-axis (which runs into and out of the screen) in orthographic mode, you will not see any apparent change in the display unless depth cueing is turned on or you are viewing with [perspective projection](#).

** These are preferences that can be set on the [Tools subpage](#) of the *Molecule Window* page of the Preferences dialog. *Track Surface* is the default setting and allows rotation about some combination of the x-and y-axes (or the z-axis if the SHIFT key is pressed as well) as the mouse is moved. The *Track Ball* setting uses the location of the cursor on the screen to determine the axis around which rotation occurs. If the cursor is in the middle of the screen, rotation around the x- and y-axes occurs. If the cursor is near the edge of the screen, rotation is around the z-axis.