

Creating charts

Required functionality and modules: Discovery Studio Client.

Required data files: NCI Drug Sample.sd

Time: 10 minutes.

Introduction

The Molecule Window provides powerful features for visualizing 3D molecular structures and related property data. In addition to this, there is a range of viewers in which you can chart molecular data properties. The following types of charts are supported:

- Line Plots
- Point Plots
- 3D Point Plots
- Histogram
- Heat Map

All charts are fully interactive. You can select data in a chart, and the same data will be selected in other windows. As multiple charts are generated from a data set, selections in one chart update the parent data and any other dependent charts.

In this tutorial, you will use a sample set of drug molecules with precalculated properties to generate a Point Plot, 3D Point Plot, and Heat Map:

- [Create a simple Point Plot](#)
- [Create a 3D Point Plot](#)
- [Create a Heat Map](#)

Create a simple Point Plot

From the **Files Explorer**, open **Samples | Tutorials | Quick Start Tutorials | NCI Drug Sample.sd**.

This file contains a set of 2000 ligands, with several precalculated properties. In addition, a principal component analysis has been performed on the data, and the first eight principal components, explaining 75% of the variation in the molecules are included in the data file.

The data set will open in the Data Table View of the Molecule Window.

From the menu bar, choose **Chart | Point Plot**.

This opens the Choose Plot Axis dialog. This dialog allows you to select the variables to be plotted. The X-axis variable is selected with a radio button in the X axis. Multiple Y-axis variables can be selected using check boxes in the Y column. You can also select the two axes in the view before selecting the plot, and the plot will be generated directly.

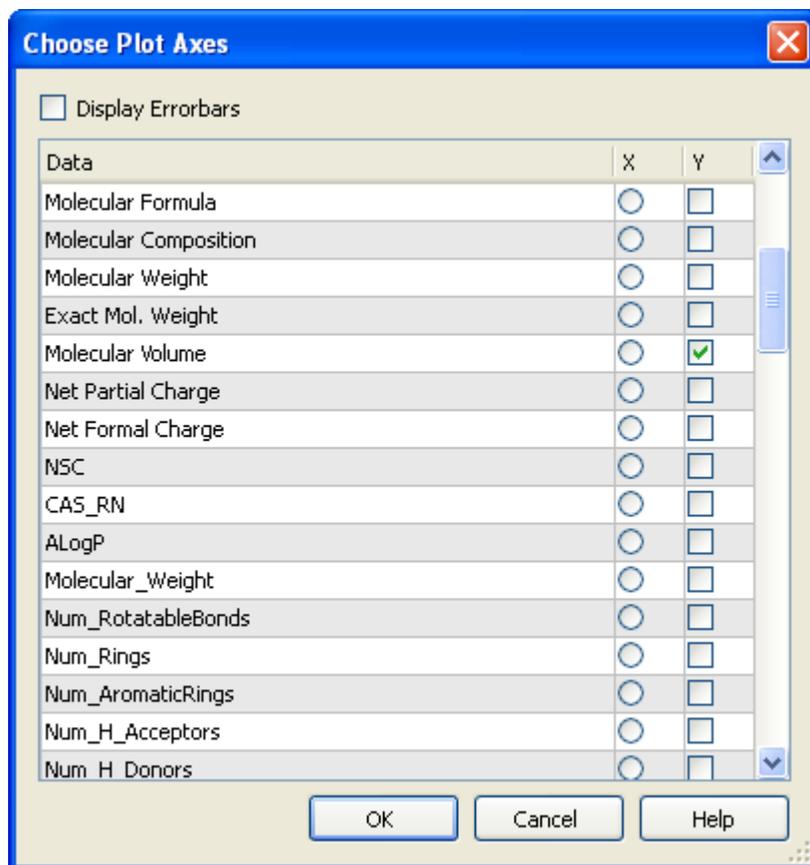
For **Choose Plot Axis** click the radio button in the X column next to the Minimized Energy row.

Select the Molecular Volume check box in the Y column.

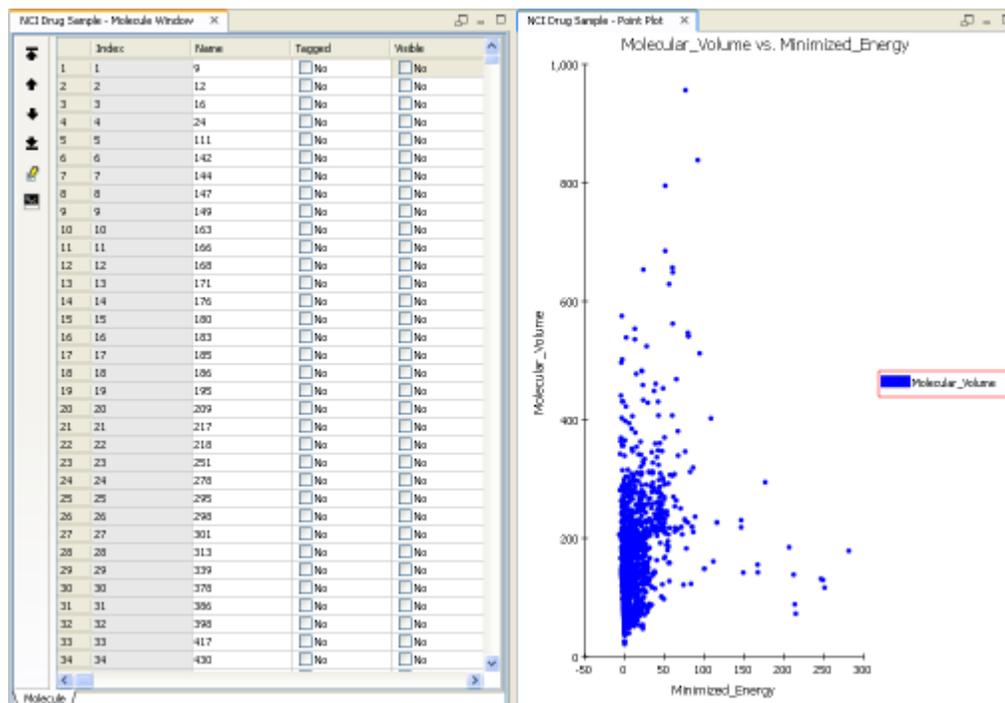
Click **OK**.

A new window is created containing the point plot.

Choose Plot Axis Dialog



Drag the plot window tab to the right side of the application workspace so that it displays next to the Molecule Window.



All of the standard viewing controls can now be used to interact with the plot. For example, you can zoom in and out by turning the mouse wheel. Alternatively, to translate the plot, press the wheel and drag the plot within the axes.

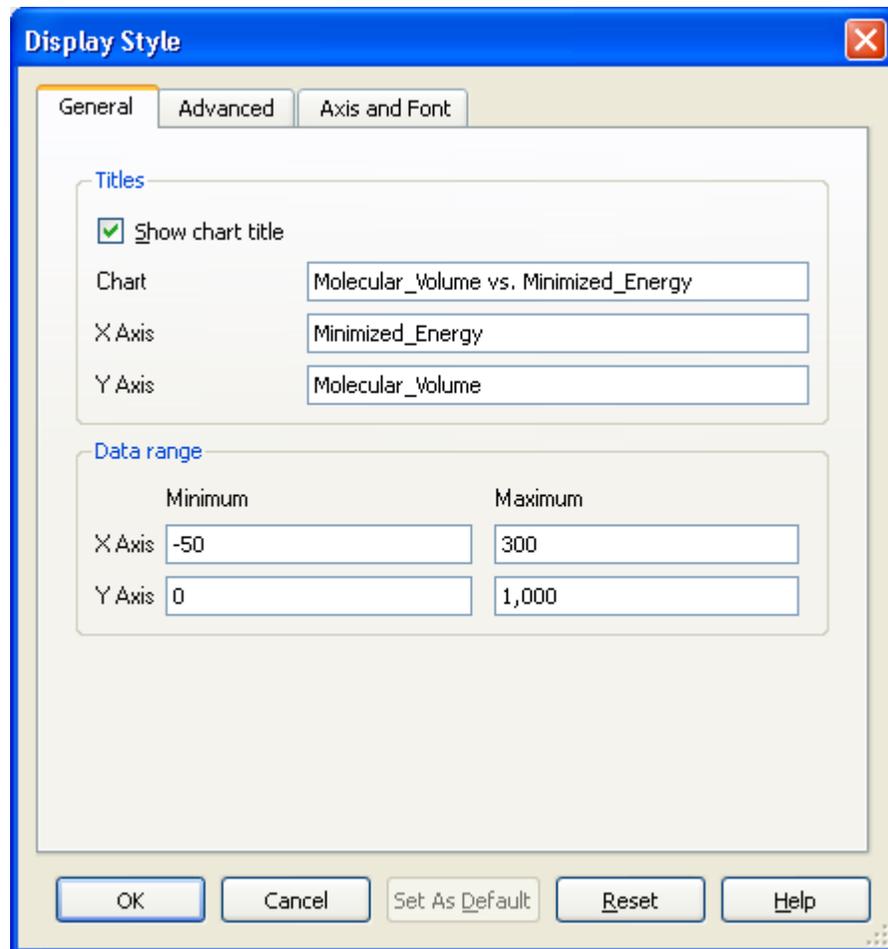
Tip. Alternatively, if you do not have a mouse wheel, use the tools on the **View** toolbar to perform these actions.

Once a chart is generated, the appearance is easily customized using the Display Style dialog.

From the toolbar, click **Display Style**.

Tip. Press CTRL+D or right-click in the Point Plot Window and select *Display Style...* from the context menu.

Point Plot Window Display Style Dialog

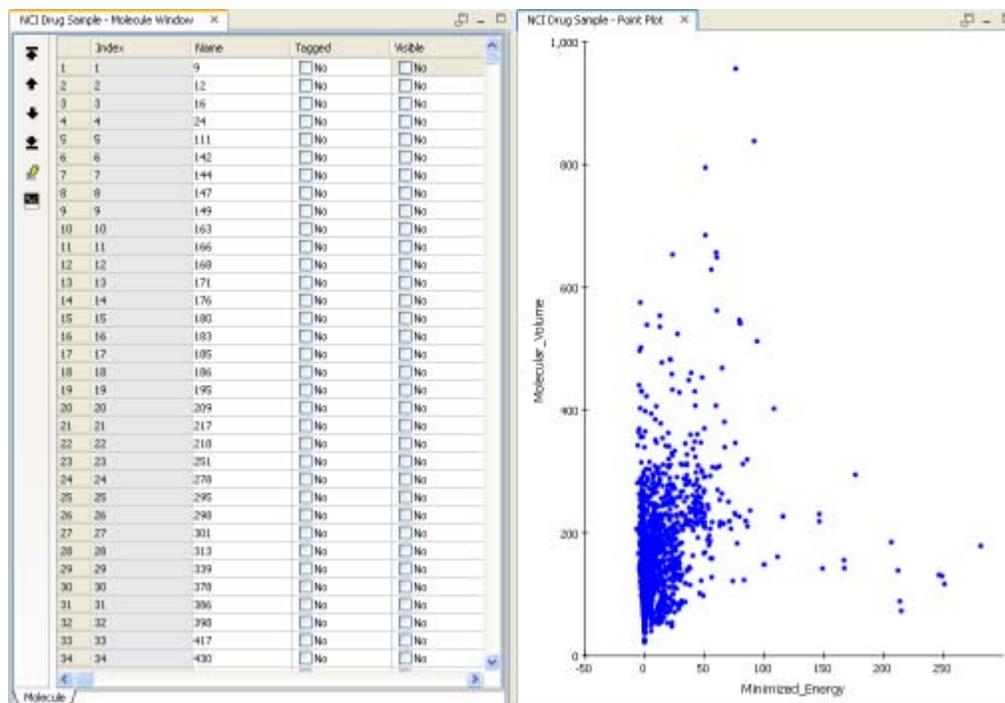


On the Display Style dialog, click the **General** tab and check the **Show Chart Title** check box to turn it off. Click the **Advanced** tab and select the Circle shape from the **Point marker** list.

Click the **Axis and Font** tab and uncheck the **Show legend** check box to turn it off.

Click **OK** to update the display.

The chart now shows the point plot without title or legend, and hollow circles for shapes.



A common use of the charts is to identify specific points of interest in the original data (e.g., clusters of related properties or individual outliers). Selections made in the plot are also reflected in the Molecule Window, and vice versa. Once the selection has been made, the corresponding molecule can be quickly located using the filtering functionality in the Molecule Window.

Locate the outlier data point at the top of the plot with a molecular volume of ~950. Hover over the point to get more information about its value.

Select the point using the  **Select** tool.

Select the **Molecule Window**.

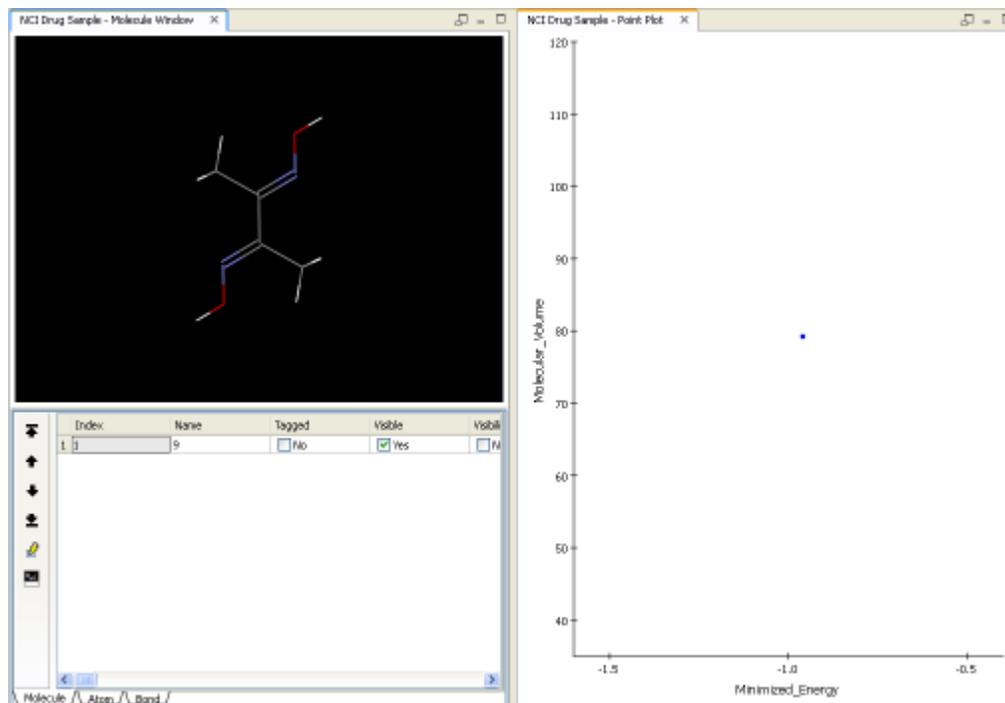
Right-click the **Data Table View** and choose **List Only Visible Objects**.

The Data Table View is now filtered and only the single selected molecule is shown. At this point it is easy to inspect properties or view the molecular structure in the Graphics View.

In the **Data Table View**, click the **Visibility** check box for the filtered molecule.

Right-click and choose **View | Graphics** to open the Graphics View.

The 3D structure is now displayed in the Graphics View.



Create a 3D Point Plot

The range of chart types supported in the application makes it possible to view different sets of variables simultaneously. In this tutorial's data set, a principal component analysis has been performed, and the eigenvalues for the different eigenvectors are stored in the file.

Turn off the filter in the Data Table from the previous step to ensure all molecules are listed.

Click the **Molecule Window**.

In the **Data Table View**, right-click and de-select **List Only Visible Objects**.

All molecules are now be listed in the Data Table View.

From the menu bar, select **Chart | 3D Point Plot**.

This opens the Choose Plot Axis dialog.

In the **Choose Plot Axis** dialog, choose **PCATempModel_PC1** for the X axis and **PCATempModel_PC2** for the Y axis.

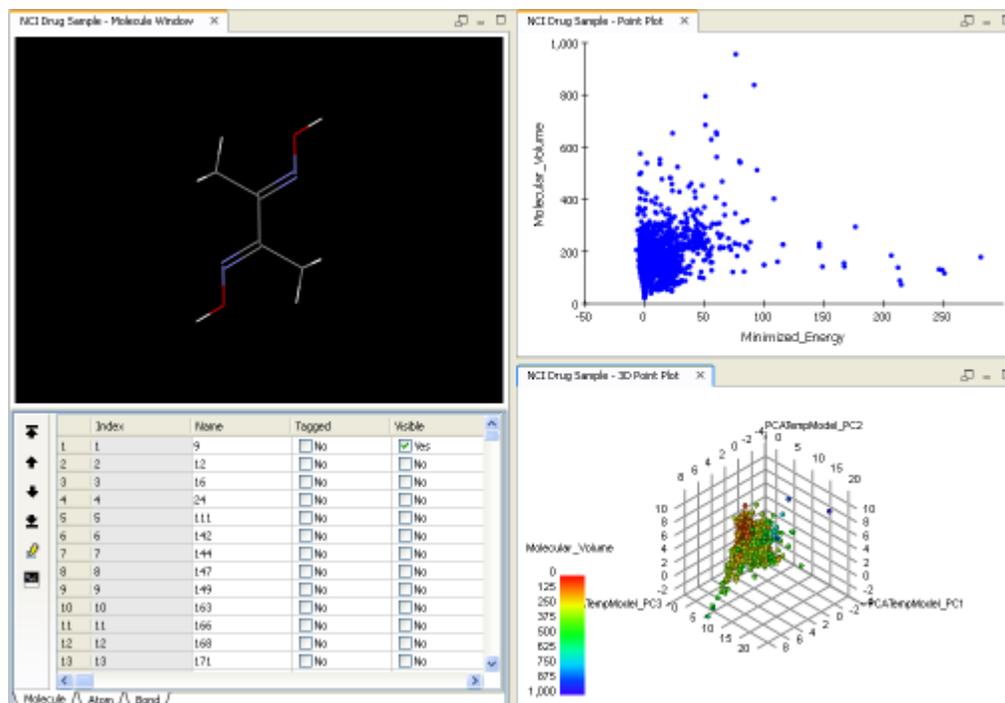
For the Z axis, choose **PCATempModel_PC3** and select **Molecule_Volume** for the Color.

Click **OK**.

A 3D point plot is generated and displayed in a new window. This plot is fully interactive with the original data and with the previously generated Point Plot.

Drag the **3D Point Plot Window** tab beneath the Point Plot window.

Locate the outlier point in the corner opposite the origin. Hold the mouse over the point, the status bar indicates "22.2606 : 11.9444 : -0.0001"; select it.



Create a Heat Map

Another useful chart type provided in Discovery Studio is the Heat Map. Heat maps are a valuable way of inspecting multiple sets of variables to identify patterns. Any set of tabular data can be plotted as a heat map whether it comes from a molecule file or a comma separated value file.

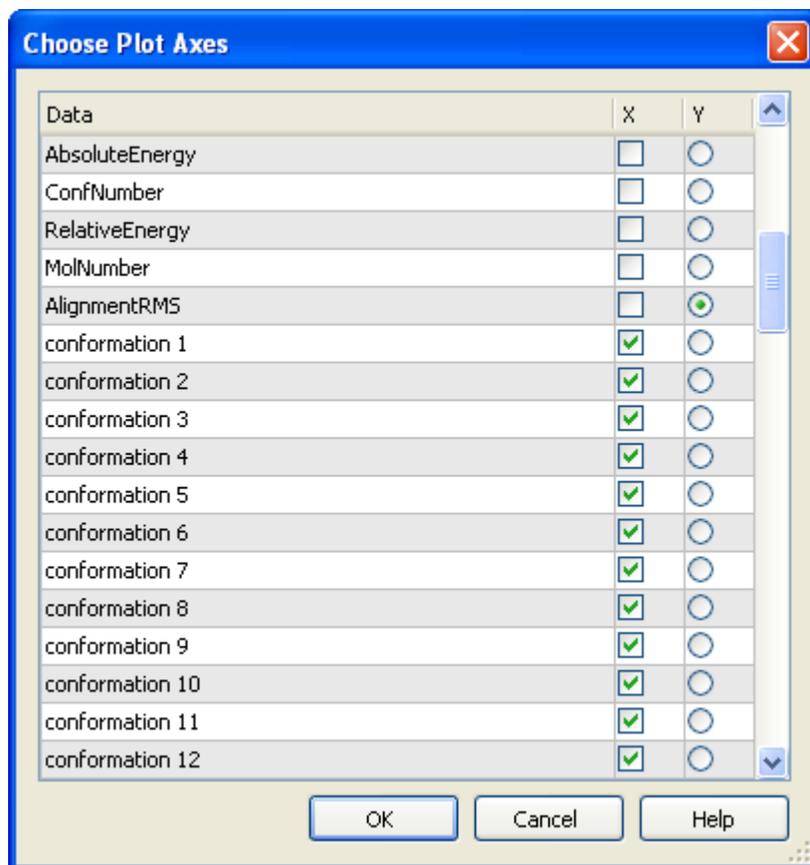
From the menu bar, choose **Window | Close All**.

From the **File Explorer**, open **Samples | Tutorials | Quick Start Tutorials | 1fvv_conformations.sd**.

This file contains a set of conformations and associated RMSD values for the conformations relative to the original ligand structure.

From the menu bar, choose **Chart | Heat Map**.

This opens the Choose Plot Axis dialog.



You will generate a heat map will be generated to show the different RMSD values for the conformations.

In the **Choose Plot Axis**, click select conformation 1 for the X axis. Scroll down the list and click the check box for conformation 78 while pressing SHIFT. For the Y axis, select the AlignmentRMS variable.

Click **OK**.

Click on individual cells to select the corresponding molecules in the Molecule Window.

AlignmentRMS vs. Properties

