

## Creating a tool panel

**Required functionality and modules:** Discovery Studio Client.

**Required data files:** None.

**Time:** 20 minutes.

### Introduction

The Discovery Studio Client offers considerable flexibility for configuring and customizing the user interface. New toolbars and script commands can be easily created to provide easy access to commonly used features.

The most flexible parts of the interface for providing custom access to functionality are tool panels. The Discovery Studio Client provides a wide number of tool panels that host pre-configured functionality. Most of the tool panels contain features that can be used to perform advanced analysis tasks on different types of data.

However, you can easily create new tool panels designed to satisfy specific tasks. One use for this customizability is to create [Discovery Guides](#) that can aggregate all the steps required for a particular task and provides instructions to walk the user through the task. In the following tutorial you will create a tool panel that exposes all the steps necessary to generate a set of conformations, calculate their RMSDs relative to the starting molecule, and plot the results.

**Tip.** The tool panel that is generated in this tutorial is also available in the Samples | Customizations folder if you wish to view the completed version. The file is called `GenerateCompareConformations.panel`

In this tutorial you will learn how to:

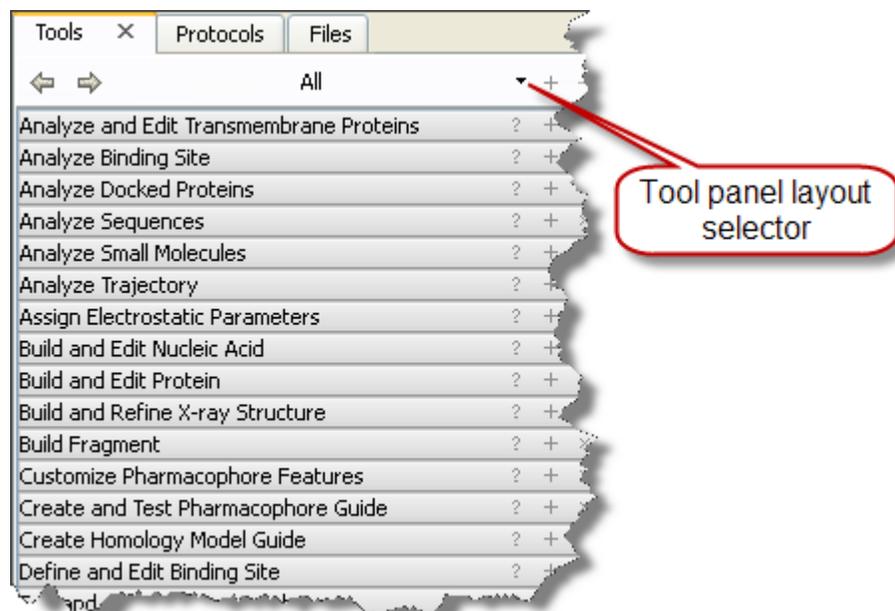
- [Create a new tool panel](#)
- [Add a tool panel to a specific layout](#)
- [Export a tool panel](#)

### Creating a new tool panel

Open the Tools Explorer.

If the Tools Explorer is not visible, turn it on by choosing **View | Explorers | Tools** from the menu bar.

Choose the **All** tool panel layout from the list at the top of the Tools Explorer.



It is not necessary to switch to the All layout to create tool panels. However, choosing All allows you to ensure that you do not add a layout using a name that already exists.

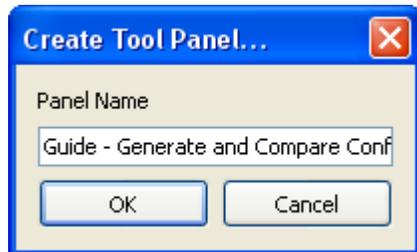
In the next step, you will create a new tool panel named "Guide - Generate and Compare Conformations".

Right-click on one of the tool panels and choose **Insert New Panel...**

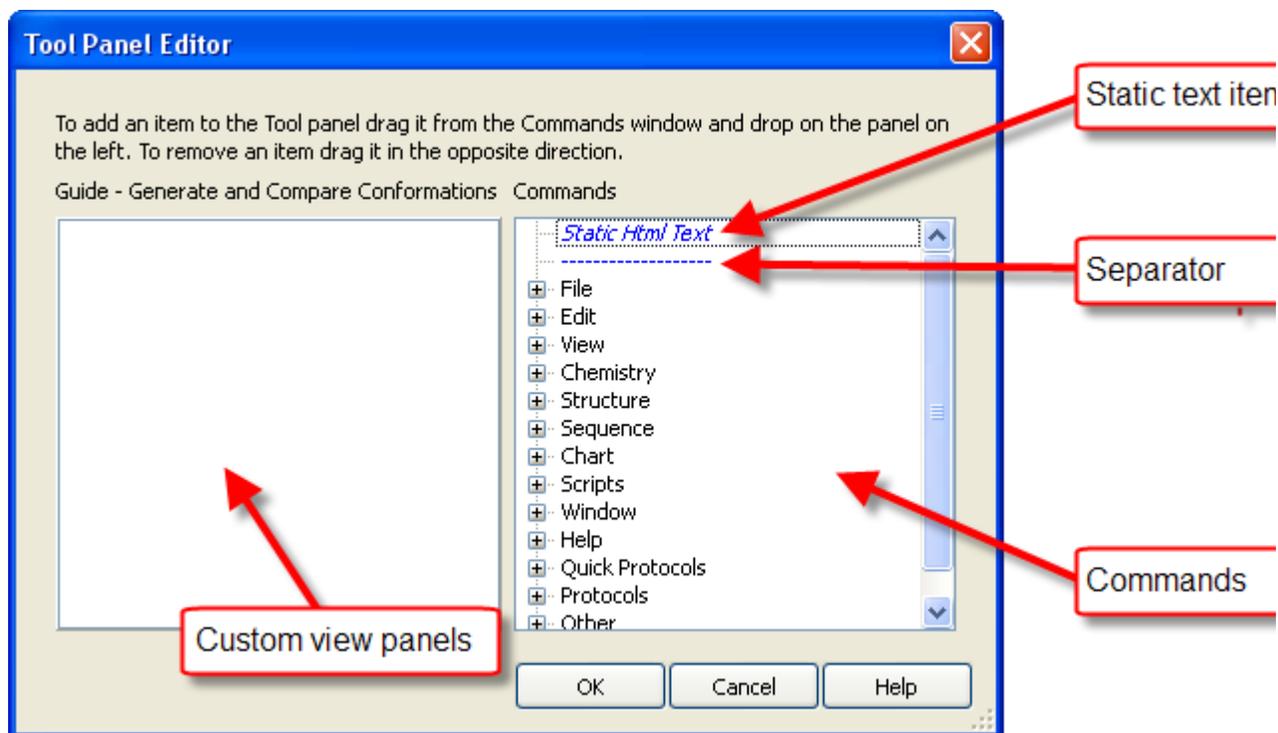
This opens the *Create Tool Panel...* dialog which will prompt you for a name.

In the *Create Tool Panels* dialog, type "Guide - Generate and Compare Conformations" for the name.

The prefix "Guide" is not mandatory, but it helps to distinguish it from regular tool panels.



Once you create the new tool panel, the Tool Panel Editor dialog will automatically open, allowing you to add tools and text.



In this tutorial, you will create a guide that can be used to generate a set of conformations and then compare the reference molecule with the conformations by computing the RMSDs:

1. Generate conformations
2. Visualize conformations
3. Calculate RMSDs
4. Display RMSDs in a chart

Create a tool group and help text for the conformation generation.

In the *Tool Panel Editor* dialog, click **Separator** in the **Commands** list box and drag it to the Custom view panels preview.

This inserts an html text item that inserts a separator. For this tutorial, you will add a header to the separator to emphasize that it is a one step in a sequence of steps.

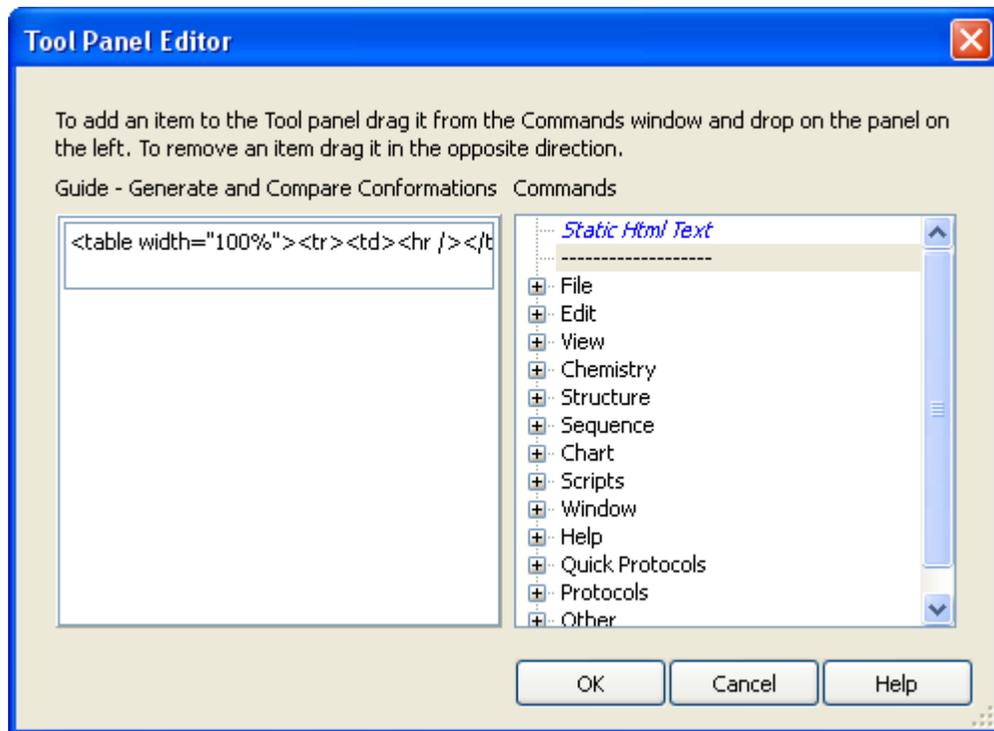
Insert the following html snippet:

```

<table width="100%">
<tr>
<td><font color="blue">1. Generate Conformations</font></td>
<td><hr /></td>
</tr></table>

```

This fragment uses the <hr> tag to insert a header and formats the header using html table <td> tags. Note that the text is colored blue using the <font color="blue"> tag.



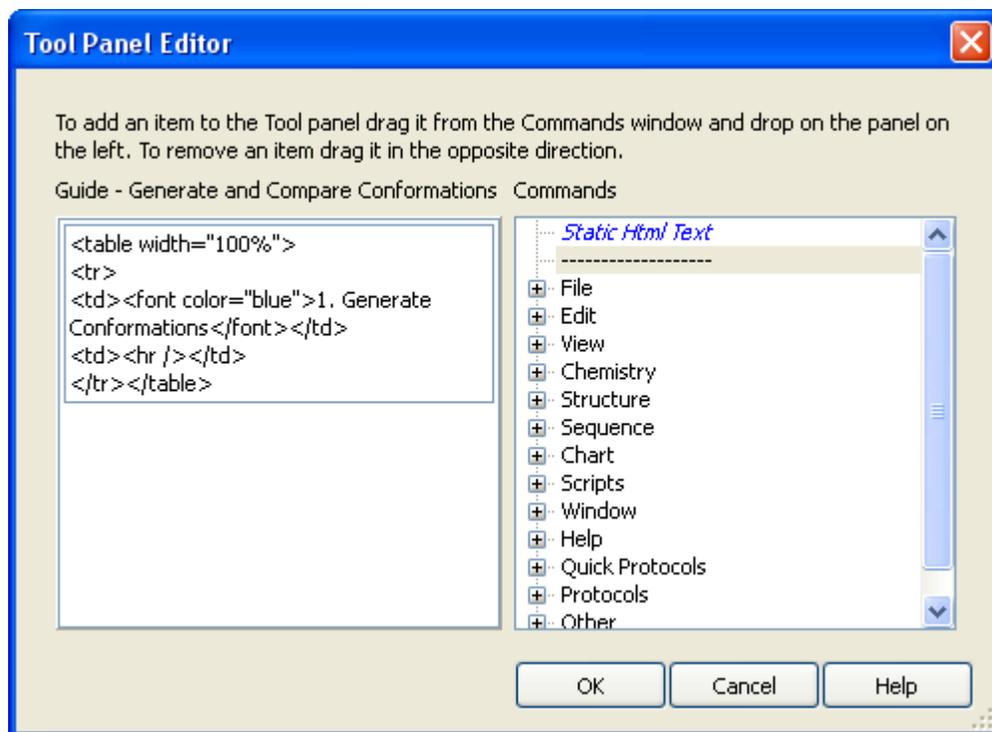
Enter some additional text to explain the purpose of the step.

Double-click **Static Html Text** in the Commands list and drag it to the Tool panel preview view. Delete the text and insert the following html snippet:

```

<html>Select a conformational search method<br>
and then select Generate Conformations<br>
to start search.</html>

```

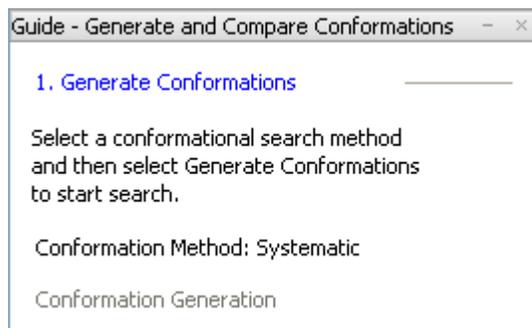


Now add two commands to choose the Conformation Method and the Conformation Search items. Note that these commands are located in the *ConformationSearchPlugin* node of the *Other* node. The various commands that appear in different tool panels are arranged on the basis of the library they are stored in rather than by the tool panel.

Double-click on the **Other** node and then click on the **ConformationSearchPlugin** node. Drag the **Conformation Method: Systematic** and **Conformation Generation** commands to the Tool panel preview view.

Click **OK**.

The new tool panel appears:



Next you will reopen the Tool Panel Editor dialog and add two additional groups to view and analyze the conformations.

In the Tool Panel, right-click and choose **Edit...**

This opens the Tool Panel Editor dialog.

Double-click **Separator**, drag it to the Tool panel preview view, and then replace the text with the following:

```
<table width="100%">
<tr>
<td><font color="blue">2. View Conformations</font></td>
<td><hr /></td>
</tr></table>
```

**Tip.** To simplify this task, copy the html from the first separator and paste it to the new separator. Double-click in the

first separator and press CTRL+A to select all the text. Press CTRL+C to copy the text to the clipboard, and then double-click in the second separator and press CTRL+A to select the text. Press CTRL+V to paste the formatted html. Now you can replace the text with the replacement text.

Double-click **Static Html Text** item in the Commands list and drag it to the Tool panel preview view. Delete the text and insert the following html snippet:

```
<html>Select Show All to make all<br>
conformations visible. Select Tile<br>
Molecules in View to arrange the <br>
molecules and compare them.</html>
```

Double-click the **View** node, and then click **Visibility** node. Drag the **Show All** command to the Tool panel preview view. Repeat this for **Tile Molecules in View**.

Repeat the previous steps to add a group for calculating the RMSD.

Double-click **Separator**, drag it to the Tool panel preview view, and then insert the following:

```
<table width="100%">
<tr>
<td><font color="blue">3. Calculate RMSD</font></td>
<td><hr /></td>
</tr></table>
```

Double-click **Static Html Text** and drag it to the Tool panel preview view. Delete the text and insert the following html snippet:

```
<html>Select the original molecule and<br>
choose Set Reference. Select All<br>
Atoms to compute RMSDs.</html>
```

Repeat the previous steps to add a group for plotting the data.

Double-click **Separator**, drag it to the Tool panel preview view, and then replace the text with the following:

```
<table width="100%">
<tr>
<td><font color="blue">4. Plot Data</font></td>
<td><hr /></td>
</tr></table>
```

Double-click **Static Html Text** in the Commands list, drag it to the Tool panel preview view, and then insert the following:

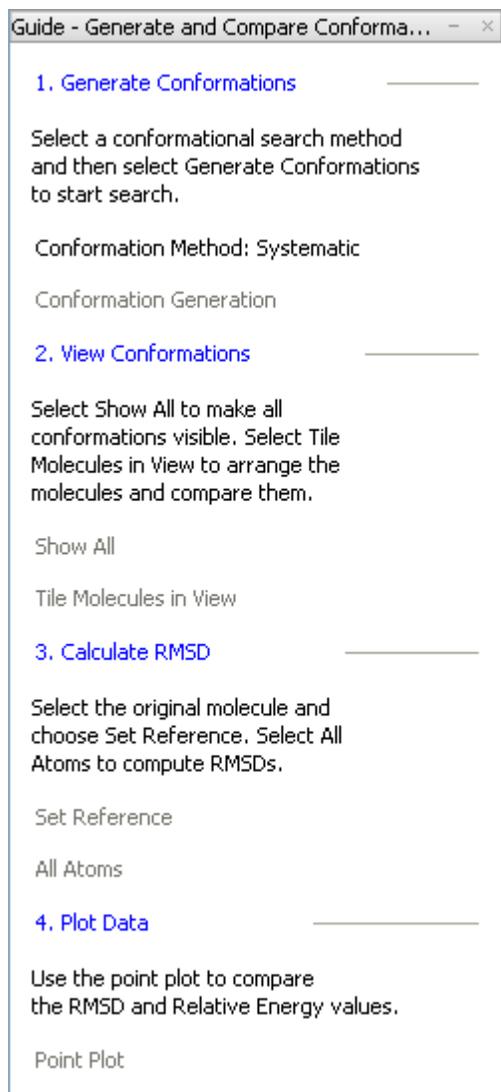
```
<html>Use the point plot to compare<br>
the RMSD and Relative Energy values.</html>
```

**Tip.** You can increase the size of the Tool Panel Editor dialog by clicking and dragging the bottom-right corner.

At this point, the Tool Panel Editor dialog appear as follows:



Close the dialog and review the Tool Panel



## Add a tool panel to a specific layout

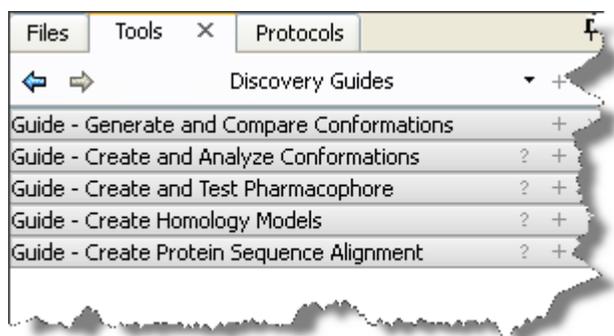
If you have a large number of tool panels installed, it may be useful to add them to particular layouts to make it easier to access them. The tool panel that you created is intended as a guide and so is usefully added to the Discovery Guides layout:

In the Tools Explorer, right-click **Layout dropdown** at the top of the Explorer Window.

A list is displayed that shows all the available layouts.

Select **Discovery Guides**.

Right-click the Tools Explorer tab and choose **Guide - Generate and Compare Conformations**.



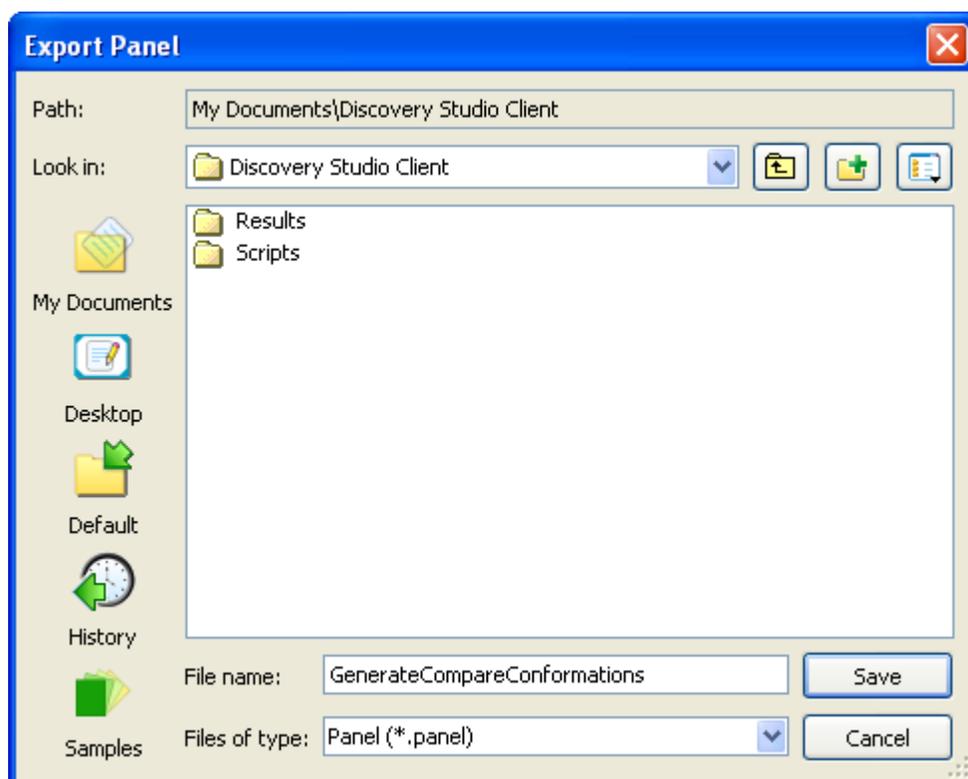
## Export a tool panel

It is possible to share your new tool panel with other users by exporting it to a `.panel` file that they can import.

In the Tools Explorer, open **Guide - Generate and Compare Conformations**.

Right-click and choose **Export....**

This opens the Export Panel dialog.



The `.panel` file will be saved in Discovery Studio Client folder in your home directory.

Click the **My Documents** shortcut on the left side of the dialog.

Double-click the **Discovery Studio Client** folder.

In the **File name:** input box type **GenerateCompareConformations**.

Press **Save**.

The `.panel` file is now saved in the Discovery Studio Client folder and can be shared with other users.