

TIBCO Spotfire® Lead Discovery 4.5 User's Manual

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Other patent(s) pending. TIBCO Software Inc. Confidential Information

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1 Introduction

1.1 Introduction

These additional help topics provide a description of the structure display and search functionality available in TIBCO Spotfire Lead Discovery. TIBCO Spotfire Lead Discovery allows you to:

- Open an SDF file and view its fields in the table visualization, including the molecular structures.
- View SMILES strings as chemical structures in a table visualization or the Structure Viewer.
- Load chemical structures from a database.
- Export data to an SDF file.
- Use the Structure Viewer to view chemical structures, and to create, export, and import ID lists.
- Search on structures in a database using similarity and substructure search.

2 Loading Data

2.1 Opening an SDFFile

You can open an SDFFile and view it in the TIBCO Spotfire table visualization.

► **To open an SDFFile:**

1. Click on the Open button on the toolbar, or select **File > Open....**
2. Browse to the SDFFile of interest and click **Open**.
Response: You will see an initial visualization using the fields of the SDFFile.
3. If your initial visualization is not a table, create a new Table visualization.
Response: You will see the table containing the fields of the SDFFile, including the chemical structures.

As with any table visualization in TIBCO Spotfire, you can:

- Save this analysis to file or library (see the "Saving an Analysis file in the Library" topic of the TIBCO Spotfire online help).
- Change the column order, column width, or row height; add, remove, sort, or mark rows (see the "How to Use the Table" topic of the TIBCO Spotfire online help).
- Change the table appearance and settings using the Table Properties Dialog.

Once your analysis in TIBCO Spotfire Lead Discovery is done, you can also export the contents of a table visualization to an SDFFile.

Tip: If your main purpose with TIBCO Spotfire is to view data containing structures, you can change the default row height in the table visualization by selecting **Tools > Options** and go to the **Table** page. There, change the Data row height to a suitable number. You can also change the default initial visualization to be a table by going to the **Document** page, and changing the Initial visualization when loading data to Table.

3 Exporting Data

3.1 Exporting Data to an SDFFile

You can export data from TIBCO Spotfire Lead Discovery to an SDFFile.

► **To export data from a visualization to an SDFFile:**

1. Right-click on the table and select **Export to SDFFile...**
2. Select whether to export all rows, marked rows or filtered rows only:
All rows - exports every row in the data table regardless of filtering.
Marked rows - exports the marked rows of the table only.
Filtered rows - exports the rows remaining after filtering only.
3. Select the **Molfile structure column** from the drop-down list.
Comment: The SDFFile format supports only one structure per record. You may select any column in the table that contains Molfile structures. The first column containing structures is displayed as the default choice.
4. Use the **Add >**, **< Remove**, and **Remove All** buttons to select the columns to be exported with the structure.
5. Use the **Move Up** and **Move Down** buttons to specify the order of columns in the SDFFile.
6. Click **OK**.
7. In the **Save As** dialog, specify a filename, browse to the location where you want to save the file and click **Save**.

Tip: You can also export data to an SDFFile by selecting **File > Export > Data...** from the main menu and choosing Save as type: SDFFile (*.sd;*.sdf). However, you will not be able to change the columns to include in the export if you use this method.

► **To export data from the Structure Viewer to an SDFFile:**

1. Select the IDs you want to export in the List Content pane of the Structure Viewer panel or popover.
2. Right-click on any of the selected IDs and select **Export Selection to SDFFile....**
3. Select the **Molfile structure column** from the drop-down list.
Comment: The SDFFile format supports only one structure per record. You may select any column in the table that contains Molfile structures. The first column containing structures is displayed as the default choice.
4. Use the **Add >**, **< Remove**, and **Remove All** buttons to select the columns to be exported with the structure.
5. Use the **Move Up** and **Move Down** buttons to specify the order of columns in the SDFFile.
6. Click **OK**.
7. In the **Save As** dialog, specify a filename, browse to the location where you want to save the file and click **Save**.

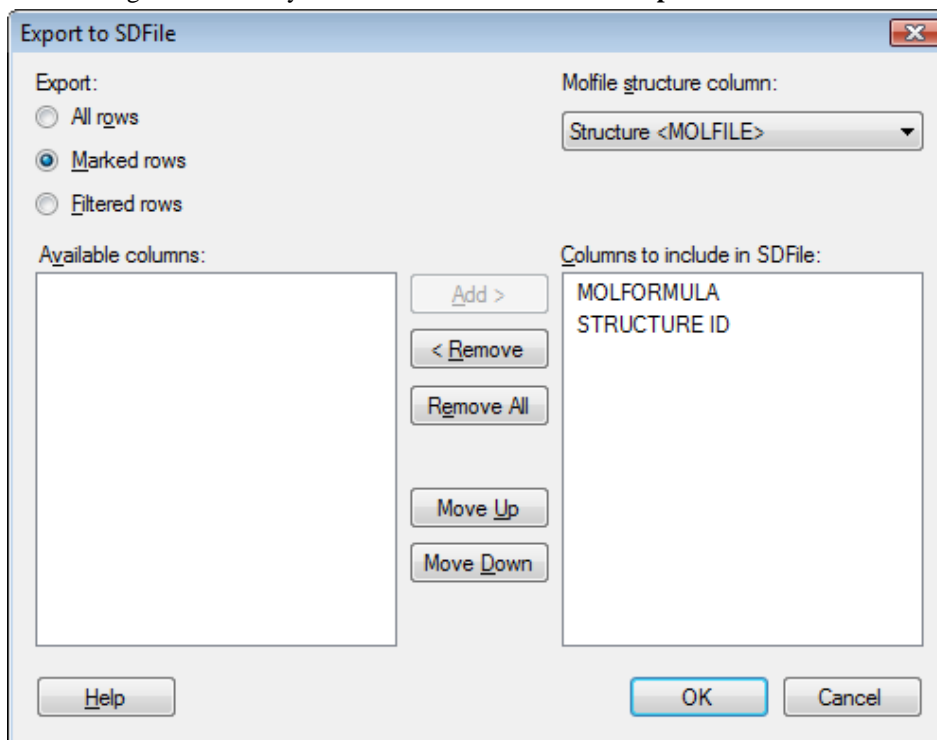
3.2 Details on Export to SDFFile

► **To reach the Export to SDFFile dialog:**

1. Right-click on the table and select **Export to SDFFile...**
Comment: If the table does not contain any structures, the **Export to SDFFile...** menu item will be unavailable.
OR

Select the IDs you want to export in the List Content pane of the Structure Viewer panel or popover.

Right-click on any of the selected IDs and select **Export Selection to SDFFile....**



Option	Description
Export	Note: If you exported data from the Structure Viewer, these options will not be available since you have already selected which rows to export.
All rows	Exports all rows in the selected data table.
Marked rows	Exports data for the marked rows only.
Filtered rows	Exports data for the filtered rows only.
Molfile structure column	Specify the column in the data table that contains molecular structures. Displays the available structure columns. Select the one you wish to export. If no structure column is available in the actual data set (for example, if structures are shown in a virtual column) you will not be able to export the structures using this tool.
Available columns	Lists the columns of the data table that are currently not selected for exporting to the SDFFile.
Columns to include in SDFFile	Lists the columns of the table that are currently selected for exporting to the SDFFile.
Add >	Adds the selected column to the list of columns to include in the SDFFile.

< Remove	Removes the selected column from the list of columns to include in the SDFFile and returns it to the list of available columns.
Remove All	Removes all columns from the list of columns to include in the SDFFile and returns them to the list of available columns.
Move Up	Moves the selected items in the Columns to include in SDFFile list up one step. The order of the columns in this list determines the order of the columns in the resulting SDFFile.
Move Down	Moves the selected items in the Columns to include in SDFFile list down one step. The order of the columns in this list determines the order of the columns in the resulting SDFFile.

4 Working with Structures

4.1 Structure Viewer

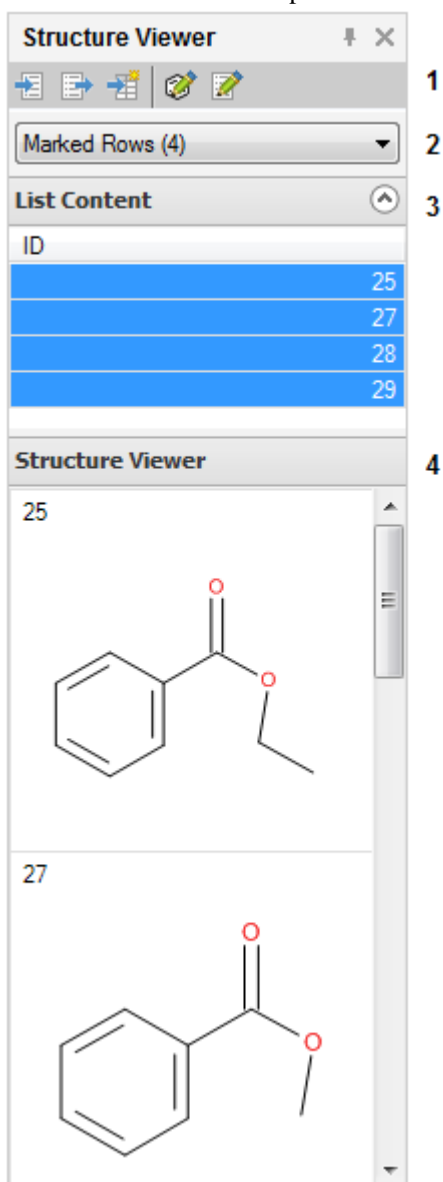
4.1.1 What is the Structure Viewer?

The Structure Viewer is used to:

- View the structures marked in the visualization or to display structure search results.
- View, create, import, and export ID lists.

The key elements of the Structure Viewer are:


- Toolbar and lists drop-down
- List Content pane
- Structure Viewer pane



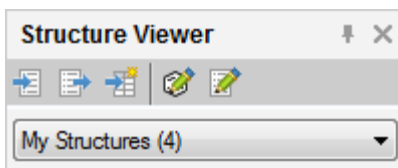
Option	Description
1. Toolbar	Contains the buttons that allow you to export, import, rename and delete ID lists, and to edit list settings.
2. Lists	<p>You can select an existing list in the Lists drop-down. The Structure Viewer maintains a dynamic list called Marked Rows that contains the marked rows in the active visualization.</p> <p>The number of items in each list is displayed within parentheses after the name of the list.</p>
3. List Content pane	Displays the list of identifiers for the list selected in the Lists drop-down. The values in this pane are taken from the ID column you selected when opening the Structure Viewer.
4. Structure Viewer pane	Displays the chemical structures for the list selected in the Lists drop-down. The structures in this pane are taken from the structure column you selected when opening the Structure Viewer, or from the results of a structure query.







4.1.2 How to Use the Structure Viewer

► To reach the Structure Viewer:

1. Open data in TIBCO Spotfire.
2. Click on the Structure Viewer button on the toolbar, .
 Comment: You can also select **View > Structure Viewer** from the menu.
 Response: The Configure Structure Connection dialog is displayed.
3. Select the columns in the visualization containing molecular structures and identifiers.
4. Click **OK**.
 Response: The Structure Viewer is displayed.
5. Mark or highlight compounds in a visualization.
 Response: When there are no marked rows, the structure from the currently highlighted row in the data table is displayed in the Structure Viewer pane of the Structure Viewer, and its identifier is displayed in the List Content pane. When there are marked rows, the structures from the marked rows are displayed in the Structure Viewer pane and their identifiers are displayed in the List Content pane. When you highlight a marked row, its corresponding identifier and structure will be highlighted in the Viewer and List Content panes.
Note: The Structure Viewer will also automatically become active when you perform a structure search.

4.1.3 Structure Viewer: Toolbar



Button / Control	Description
	Imports an ID list file to Structure Viewer.
	Exports the ID list currently selected in the Lists drop-down to an LST file.
	Displays the structures with the IDs from the active ID list in a separate data table visualization. Creates a new data table containing the structures and IDs from the current list. If additional data is available, it is included in the new table. Additional data may be drawn from the linked rows in the active data table or from an information link, depending on the source of the list.
	Opens the Structure Connection dialog where you can re-configure the mapping of ID and structure columns between data tables and Structure Viewer.
	Opens the Manage Lists dialog where you can change the name and description for previously created lists, as well as delete lists.
	Displays the name of the selected list followed by the number of items in the list within parentheses. The elements of the selected list are displayed in the List Content and Viewer panes. Use this drop-down to select a different list.

4.1.4 Structure Viewer: List Content Pane

In the List Content pane of the Structure Viewer, you can view the identifiers of the molecular structures from the ID list currently selected in the Lists drop-down. This can represent:

- The marked rows in the active data table.
- A previously created or imported ID list.
- The results of a structure search.

The List Content pane displays the identifiers of the rows in the list. The identifiers are taken from the column you selected as the ID column when the Structure Viewer was first opened. If the result of a structure query is shown, the metadata supplied by the information link are used.

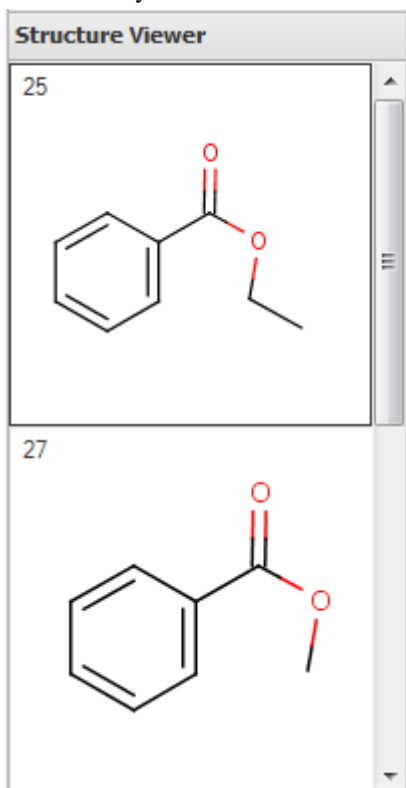
List Content	
ID	
	25
	27
	28
	29

The right-click pop-up menu of the List Content pane contains a number of options shown in the table below.

Right-click Menu Option	Description
Mark Selection in Active Visualization	Marks the rows with the selected IDs in the active visualization.
Create New List from Selection...	Creates a new ID list from the IDs selected in the List Content pane.
Export Selection to SDFFile...	Opens the Export to SDFFile dialog where you can export the selected IDs to an SDFFile.
Copy IDs	Copies the selected IDs to the clipboard.
Select All	Selects all IDs in the List Content pane.
Invert Selection	Inverts the selection in the List Content pane.
Remove IDs from List	Removes the selected IDs from the list in the List Content pane.
Manage Lists...	Opens the Manage Lists dialog where you can change the names and descriptions of all previously added lists. You can also remove unwanted lists from Structure Viewer.

4.1.5 Structure Viewer: Structure Viewer Pane

In the Structure Viewer pane, you can see the structures of either the marked rows of the data table, or of the currently active ID list. This pane also displays the structures of the search results after you run a Structure Search.




The right-click context menu of the Structure Viewer pane contains a number of options shown in the table below:

Right-click Menu Option	Description
Structure Search...	Displays the Structure Search dialog.
Copy	Copies information from the Structure Viewer to the Windows clipboard: Structure - copies the selected structure as a structure which can be edited in the structure renderer. Image - copies the selected structure as an image. Image with All Visible Structures - copies the visible contents of the Structure Viewer pane as an image.
Renderer	Use this option to select the default renderer used in the Structure Viewer pane (see Supported Renderers for more information). You can also change the renderer settings in the Renderer Settings dialog.
Print	All - when selected, specifies that all the structures from the current list will be printed. Visible Structures - when selected, specifies that only those structures from the current list that are visible in the Structure Viewer pane will be printed. Print - prints the structures according to the print settings (All or Visible Structures). Print Preview - displays the Print Preview window.
Show IDs	Shows or hides the molecule IDs for the structures displayed in the Structure Viewer pane.
Layout	Specifies the number of columns to be shown in the Structure Viewer pane.

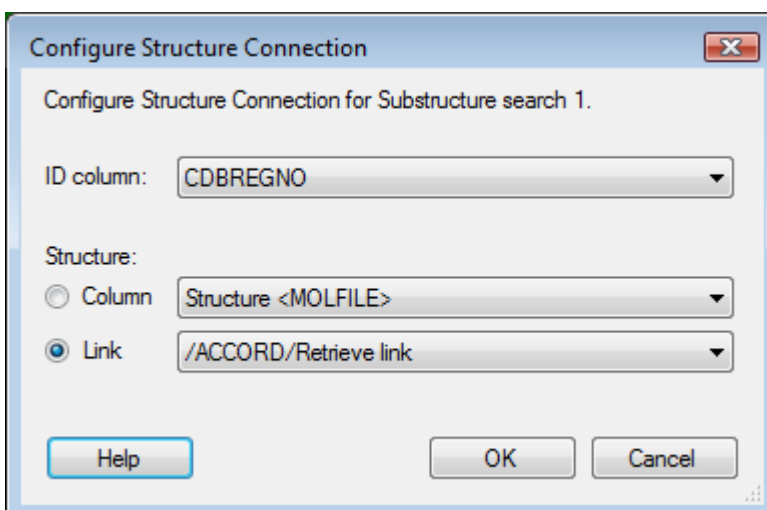
4.1.6 Details on Configure Structure Connection

In the Configure Structure Connection dialog, you specify the columns of the table which will be treated by the Structure Viewer as the columns containing structures and IDs. The structure connection can be different for different lists.

► To reach the Configure Structure Connection dialog:

- Click on the Structure Viewer button on the toolbar, .
 Comment: You can also select **View > Structure Viewer** from the menu.
 Response: The Configure Structure Connection dialog is displayed.

In Structure Viewer, you can also click on the Configure Structure Connection button, , to show the dialog again.



Option	Description
ID column	Select the column from the data table which you want to use as the identifier of the structure. The values from this column will be displayed in the List Contents pane of the Structure Viewer panel. Also, the Structure Viewer will use the IDs from this column for creating, exporting, and importing the ID lists.
Structure	
Column	Select a column that contains structures from those available in the active table visualization. The contents of this column will be rendered in the Structure Viewer pane.
Link	Select an information link that contains structures from those available in the drop-down list. The structures from this link is what will be displayed in the Structure Viewer pane. The information links that are available here are configured using Information Designer. See the TIBCO Spotfire Lead Discovery - Installation Manual for more information.


4.2 Working with ID Lists

4.2.1 Working with ID lists

The ID lists in the Structure Viewer let you keep track of groups of compounds. Each time you conduct a structure search, the result is added as a new list in the List Content pane of the Structure Viewer. All the lists that you create are stored locally and appear in the Lists drop-down of the Structure Viewer.

The Structure Viewer also maintains a dynamic list called "Marked Rows", which contains the current set of marked rows. To save the results of a structure query or the set of marked rows more permanently, create a new list and convert the list to a data table, or export a list file or an SDF file.

► **To display the Structure Viewer:**

1. Select **Tools > Structure Viewer**, or, click on the Structure Viewer button on the toolbar, .

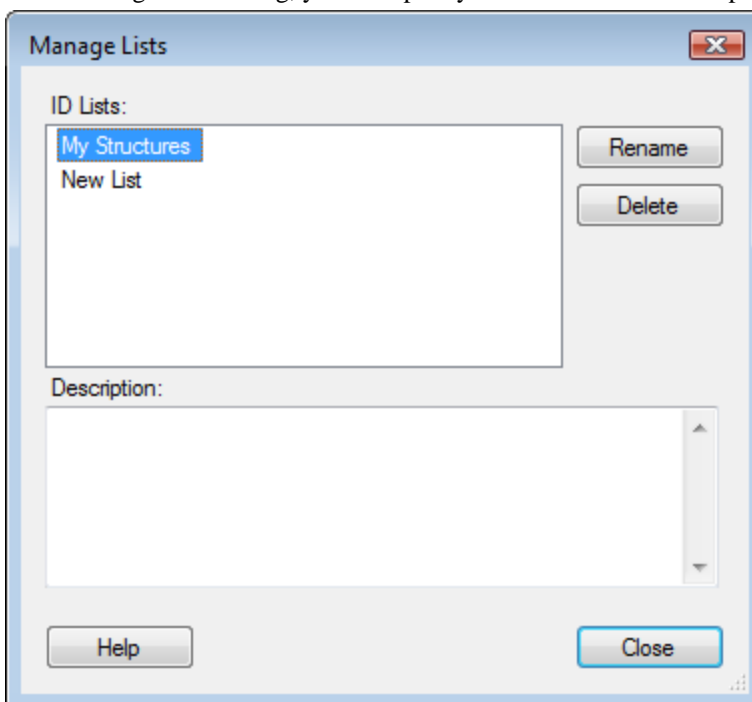
Comment: Another way to launch the Structure Viewer is to perform a structure search by right-clicking on a table column containing structures and selecting **Structure Search...** The Structure Viewer appears and the search results are displayed in the List Content and Structure Viewer panes.

Action	Instruction
Create a list	Do either one of: Perform a search using the Structure Search tool. Select the IDs in the current list, right-click and select Create New List from Selection...
Change list settings	Click the Manage Lists button,  , on the Structure Viewer toolbar. You can also right-click and select Manage Lists... from the pop-up menu. In the Manage Lists dialog, you can change the list name and description. In the Structure Connection dialog, reached from the Configure Structure Connection button,  , you can re-map the ID and structure columns, if necessary.
Rename a list	Click the Manage Lists button,  , on the Structure Viewer toolbar. You can also right-click and select Manage Lists... from the pop-up menu. In the Manage Lists dialog, click to select the list you want to rename, then click Rename.
Export the list as an LST file	Select the list in the Lists drop-down and click the Export button,  , on the Structure Viewer toolbar.
Import a list	Click the Import button,  , on the Structure Viewer toolbar and select the list file to import in the Open File dialog.
Export selected IDs to an SDF file	Right-click on any of the selected IDs and select Export Selection to SDF... from the pop-up menu to open the Export to SDF dialog.
Display structure for a compound ID	Click on one or more identifiers in the List Content pane. The Structure Viewer pane will display the structures corresponding to the selected identifiers.
Create a new data table with the compounds from the current list	Select the list in the Lists drop-down and click the Create Table button,  , on the Structure Viewer toolbar. A new data table will be created with the ID, structure, and any related data for the compounds in the list.
Mark compounds from the list	In the list, select the desired identifiers. Right-click and select Mark Selection in Active Visualization .


Copy a list	In the list, select the desired identifiers. Right-click and select Copy IDs .
Select all identifiers in a list	Right-click in the List Content pane and select Select All .
Invert the selection in the list	In the list, select the desired identifiers. Right-click and select Invert Selection .
Remove identifiers from the list	In the list, select the desired identifiers. Right-click and select Remove IDs from List .

4.2.2 Details on Manage Lists

In the Manage Lists dialog, you can specify the list name and description of all available lists.



► To reach the Manage Lists dialog:

1. Click the Manage Lists button, , on the Structure Viewer toolbar or right-click in the List Content pane and select **Manage Lists...**

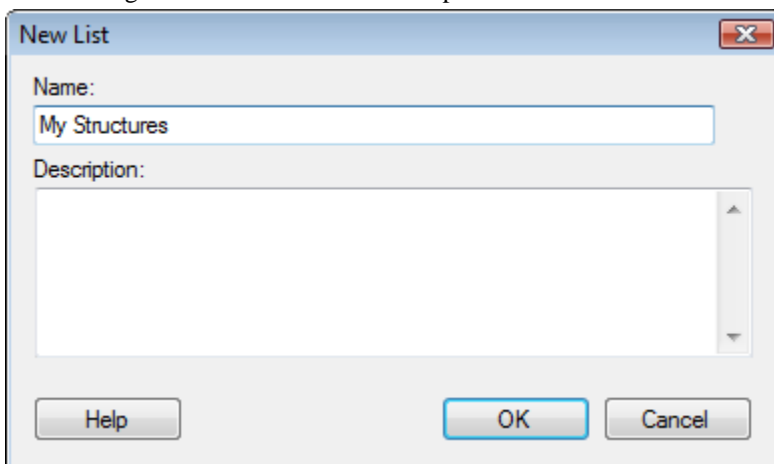
Option	Description
ID Lists	Lists all currently available ID Lists in Structure Viewer.
Rename	Click on a list in the ID Lists pane and then click Rename to change the name of the selected list.
Delete	Click on a list in the ID Lists pane and then click Delete to remove the selected list from the Structure Viewer.
Description	Optional. Type a description of the contents of the selected list.

4.2.3 New List Dialog

New lists are automatically created when you perform a structure search. To create a new list from a selection in another list, use this dialog.

► **To reach the New List dialog:**

1. Make sure that the interesting IDs are selected in the List Contents pane of the Structure Viewer. See *Working with ID Lists* for more information.
2. Right-click in the List Contents pane and select **Create New List from Selection...**



Option	Description
Name	Type a suitable name for the new list.
Description	Optional. Type a description of the contents of the list.

4.3 Searching Structures

4.3.1 Searching for Compounds Using Structure Search

The Structure Search tool allows you to perform substructure and similarity searches. See *Details on Structure Search* for more information regarding the individual search methods. The search returns a list of identifiers that is displayed in the Structure Viewer.

► **To search for compounds in a structure database:**

1. In the Structure Viewer or in a table visualization with structures, click to activate the compound on which you want to base the search.
2. Right-click on the structure and select **Structure Search...** from the pop-up menu.
Comment: You can also select **Tools > Structure Search...** from the main menu.
Response: The Structure Search dialog is displayed.
3. Select one of the alternatives under **Search for**.
Comment: You can search for Substructure or Similarity.
4. If the **Parameters...** button becomes available, click on it to edit the parameters available for the selected search method.
Comment: If you select Similarity search, you must enter a range of similarity values in the Similarity Search Parameters dialog. Similarity values range from 0 (least similar) to 100 (most similar).
5. If you want to import a structure from a file, click **Import Structure...**

Response: The Open File dialog appears. Select the file you want to import and click **Open**. The structure from the file will be displayed in the Structure Search dialog.

6. If required, click **Edit...**. If more than one structure editor is available, you can choose which editor to use from a drop-down list.

Response: Your selected structure editor is launched. Edit the structure and click the button that returns the structure to Spotfire (in ChemDraw: **OK**, in Symyx® Draw (MDL): **Transfer**). Please refer to the documentation of your current structure editor for more details.

7. Select an information link in the **Search in** drop-down.

Comment: See chapter 2.4 Configuring Information Links in the TIBCO Spotfire Lead Discovery - Installation Manual for more information about how information links should be configured to be shown here.


8. If required, limit the search to the current list of identifiers.

Comment: This option is only available when performing the search from the Structure Viewer and when any list except for the Marked Rows list is selected in the Lists drop-down of the Structure Viewer. When you start a structure search from a table visualization without activating the Structure Viewer, or, if the Marked Rows list is selected, the Data Source option will be the only one available.

9. Specify the name for the resulting list.

10. Click **OK**.

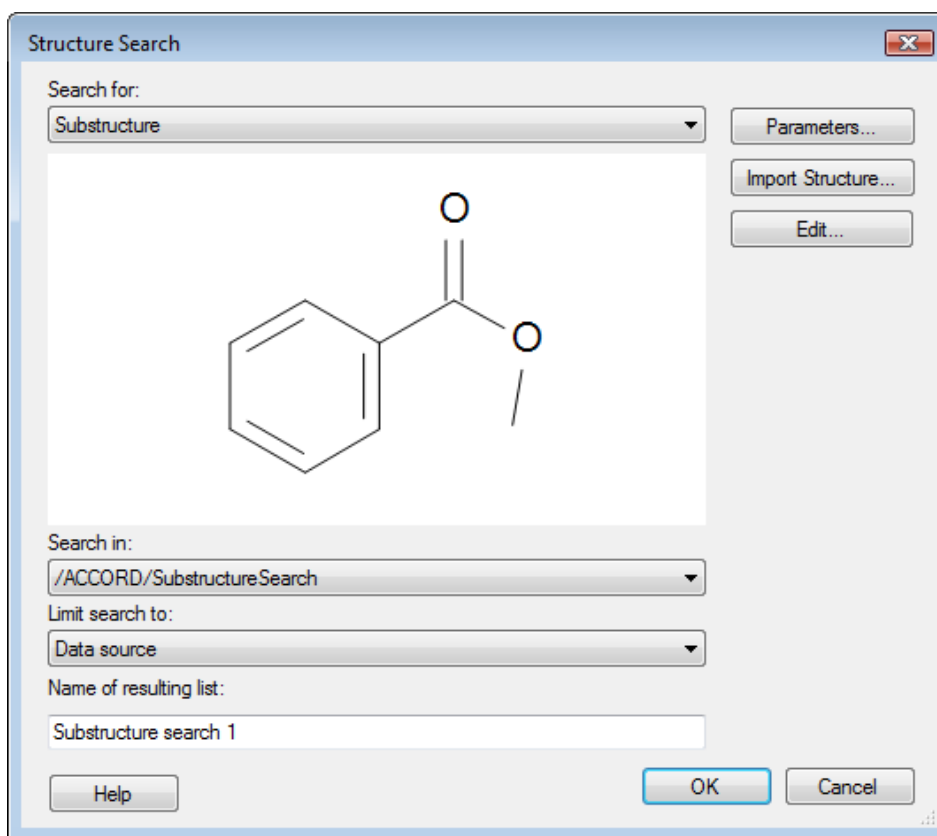
Response: Structures in the database that match the search criteria are displayed in the Structure Viewer (Viewer pane). A new ID list is added and displayed in the List Content pane. To show the search results as a separate data table, select the search

results list in the Lists drop-down and click the  button on the Structure Viewer toolbar.

4.3.2 Details on Structure Search

► To reach the Structure Search dialog:

1. Select **Tools > Structure Search...** or right-click on a structure in a table or the Structure Viewer and select **Structure Search...** from the pop-up menu.



Option	Description
Search for	
Substructure	Performs a search for structures containing the specified substructure.
Similarity	Performs a search for structures similar to the specified master structure. Open the Similarity Search Parameters dialog and specify a range of values between 0 (least similar) and 100 (most similar).
Parameters...	Launches the Parameters dialog where you can provide search parameters for similarity search.
Import Structure...	Launches the Open dialog where you can select a structure file to use in the search.
Edit...	Launches your current structure editor where you can edit the structure before performing the search. The same thing is achieved by double-clicking the structure. If more than one structure editor is available, you can choose which editor to use from a drop-down list. After editing the structure and sending it back to TIBCO Spotfire, the Structure Search dialog is updated with the edited structure.
Search in	Specifies the information link (predefined query) to the data source in which the search will be performed. See chapter 2.4 of the TIBCO Spotfire Lead Discovery - Installation Manual for more information about Configuring Information Links. See Information Links topics in the TIBCO Spotfire online help for general information about information links.

Limit search to	Allows you to limit the search to a set of identifiers from the list currently selected in the Lists drop-down. This option is only available when any (not empty) list except for the Marked Rows list is selected.
Name of resulting list	Allows you to give the resulting structure search list a name of your choice.

4.4 Viewing Structures in Virtual Columns

In the table visualization, you can view structures from remote data sources using virtual columns. You can connect to a virtual column and collect structure data from the remote data source both when showing structures in a table visualization and when structures are shown in the Structure Viewer.

► To add a virtual column:

1. Right-click on a table visualization and select **Properties**.
2. Select **Virtual Columns** and click **Add > Structure Column**.
3. In the **Structure Column Settings** dialog, select the key column - for example, the column that contains the IDs of the structures in your visualization.
4. Click on **Browse...**
Response: The Open from Library dialog is displayed.
5. Select the information link that contains the data you want to retrieve in your virtual columns and click **Open**.
Note: Make sure that columns containing the key column data (in our example - structure IDs) and the data you would like to view in the virtual column (for example, molecular structures) are included in the information link.
6. Click **OK**.
Response: The virtual Structure column is displayed in the active table visualization.

4.5 Viewing Structures in Labels or Tooltips

In TIBCO Spotfire 3.3 and forward, it is possible to display structures and other images in the labels or tooltips of many visualizations.

► To show structures from the loaded data in labels:

1. Open the **Properties** dialog for the visualization.
Comment: This is done by right-clicking on the visualization and selecting Properties from the pop-up menu.
2. Click on the **Labels** page in the list on the left.
Response: The Labels page is displayed. Note that not all visualizations support labels.
3. Select the structure column under **Label By**.
Comment: This is possible if the loaded data contains the structure information directly (e.g., if the loaded data is an SDF file). For example, select "Structure <MOLFILE>". If you want to retrieve the structures from an information link instead, see below.
4. Specify whether to **Show labels for: All** or **Marked rows**.
5. Make sure that **Get content from** is set to **(Selected column)**.
6. Make sure that **Show as** is set to your current structure renderer. For example, Symyx® Draw (MDL).
7. If desired, change the **Size** of the structures using the slider.
8. Click **Close**.

► **To show structures from an information link in labels:**

1. Open the **Properties** dialog for the visualization.
Comment: This is done by right-clicking on the visualization and selecting Properties from the pop-up menu.
2. Click on the **Labels** page in the list on the left.
Response: The Labels page is displayed. Note that not all visualizations support labels.
3. Select an identifier column under **Label By**.
Comment: Here you select the identifier column in your data table that will be used to match the identifier in the information link from which structures are to be retrieved.
4. Specify whether to **Show labels for: All** or **Marked rows**.
5. Select **Get content from: Structure Column**.
Comment: This specifies that rather than displaying the information from the selected Label by column directly, the selected column will be used as an identifier when retrieving data from an information link.
6. Click on the **Settings...** button next to Get content from.
Response: The Structure Column Settings dialog is displayed.
7. Make sure that the correct Key column is selected, then click **Browse...**
Response: The Open from Library dialog is displayed.
8. Click to select the information link containing your structures and then click **Open**.
Note: Make sure that columns containing the key column data (in our example - structure IDs) and the data you would like to view in the virtual column (for example, molecular structures) are included in the information link.
9. Click **OK**.
10. Make sure that **Show as** is set to your current structure renderer. For example, Symyx® Draw (MDL).
11. Click **Close**.

► **To show structures from the loaded data in tooltips:**

Most visualizations can display images from a binary image column, a shape file, or chemical structures in tooltips.

1. Open the **Properties** dialog for the visualization.
Comment: This is done by right-clicking on the visualization and selecting Properties from the pop-up menu.
2. Click on the **Tooltip** page in the list on the left.
Response: The Tooltip page is displayed.
3. Click on the **Add...** button.
Response: The Add Tooltip Value dialog is displayed.
4. Select the structure **Column** of interest.
5. Type a **Name** to display.
Comment: This is the text that will be shown together with the expression value in the tooltip, and also what will be shown in the list of available tooltip values.
6. Make sure that **Get content from** is set to **(Selected column)**.
Comment:
Make sure that **Show as** is set to your current structure renderer. For example, Symyx® Draw (MDL).
7. If desired, change the **Size** of the tooltip image by moving the slider,
8. Clear the **Include value name in tooltip** check box if you only want to display the image in the tooltip and not the name.
9. Click **OK**.

Response: The Add Tooltip Value dialog is closed and the newly added value is shown in the Tooltip property page.

10. Click **Close**.

► To show structures from an information link in tooltips:

Most visualizations can display images from a binary image column, a shape file, or chemical structures in tooltips.

1. Open the **Properties** dialog for the visualization.
Comment: This is done by right-clicking on the visualization and selecting Properties from the pop-up menu.
2. Click on the **Tooltip** page in the list on the left.
Response: The Tooltip page is displayed.
3. Click on the **Add...** button.
Response: The Add Tooltip Value dialog is displayed.
4. Select an identifier **Column**.
Comment: Here you select the identifier column in your data table that will be used to match the identifier in the information link from which structures are to be retrieved.
5. Type a **Name** to display.
Comment: This is the text that will be shown together with the expression value in the tooltip, and also what will be shown in the list of available tooltip values.
6. Select **Get content from: Structure Column**.
Comment: This specifies that rather than displaying the information from the selected Label by column directly, the selected column will be used as an identifier when retrieving data from an information link.
Click on the **Settings...** button next to Get content from.
Response: The Structure Column Settings dialog is displayed.
7. Make sure that the correct Key column is selected, then click **Browse...**.
Response: The Open from Library dialog is displayed.
8. Click to select the information link containing your structures and then click **Open**.
Note: Make sure that columns containing the key column data (in our example - structure IDs) and the data you would like to view in the virtual column (for example, molecular structures) are included in the information link.
9. Click **OK**.
10. Make sure that **Show as** is set to your current structure renderer. For example, Symyx® Draw (MDL).
11. If desired, change the **Size** of the tooltip image by moving the slider,
12. Clear the **Include value name in tooltip** check box if you only want to display the image in the tooltip and not the name.
13. Click **OK**.
Response: The Add Tooltip Value dialog is closed and the newly added value is shown in the Tooltip property page.
14. Click **Close**.

5 Settings

5.1 Supported Renderers

TIBCO Spotfire Lead Discovery modules provide support for several different renderers to display molecular structures. See the system requirements for TIBCO Spotfire Lead Discovery on <http://support.spotfire.com/sr.asp> for more information. However, note that a few of the supported renderers can only be used to render structures in the table visualization and the Structure Viewer; they cannot be used to edit structures in the Structure Search tool. You can add one or more of these renderers to the list of default renderers, select any of them as default for a content type, and change the renderer settings.

► **To add a renderer to the list of default renderers:**

1. Select **Tools > Options**.
2. Select the **Application** tab.
3. Click the **Renderer Settings...** button.
4. Click **Add...**

Response: The Add Default Renderer dialog is displayed.

5. Specify the Content type and select the default renderer from the drop-down list in the dialog.

Comment: You can only specify one default renderer per content type. See the table below for a description of content types.

► **To change the default renderer for a certain content type:**

1. Select **Tools > Options**.
2. Select the **Application** tab.
3. Click the **Renderer Settings...** button.
4. Click to select the content type of interest and then click **Edit...**

Response: The Edit Default Renderer dialog is displayed.

5. Select a new default renderer from the drop-down list.

Note: The content type you enter can be an arbitrary string, but it is recommended that you use the MIME types defined for molfiles, CHIME strings, and SMILES strings as shown in the table below.

Structure Format	Content Type
MDL molfile	chemical/x-mdl-molfile
MDL Chime string	chemical/x-mdl-chime
Daylight SMILES string	chemical/x-daylight-smiles

► **To change the renderer and/or renderer settings for the structures displayed in the table visualization:**

1. Right-click on a row in the table visualization and select **Properties > Columns**.
2. Select the column that contains chemical structures.
3. In the **Renderer** drop-down list, select the renderer to use.
4. Click the **Settings...** button to change the renderer settings.

Response: The Renderer Settings dialog for the currently used renderer is displayed.

5. Change the renderer settings and click **OK**.

► **To change the renderer used in Structure Viewer:**

1. In the Structure Viewer pane of the Structure Viewer, right-click on the structure.
2. Select **Renderer**.
3. Select the renderer to use.

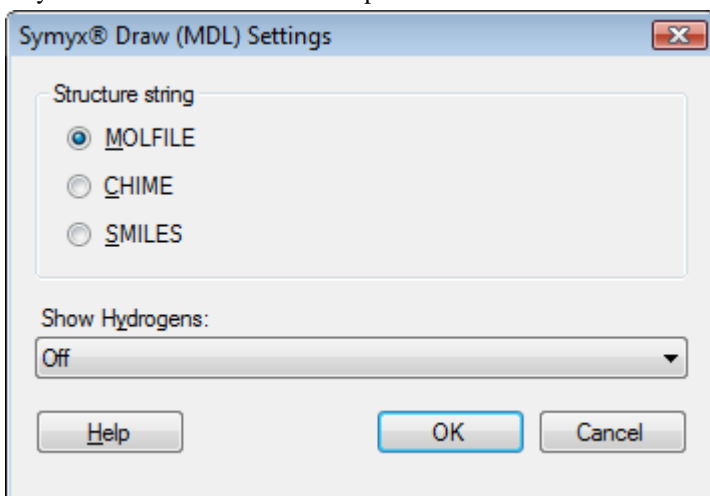
► **To edit the renderer settings in Structure Viewer:**

1. In the Structure Viewer pane of the Structure Viewer, right-click on the structure.
2. Select **Renderer > Settings...**
Response: The Renderer Settings dialog for the currently used renderer is displayed.
3. Change the renderer settings and click **OK**.

5.2 Renderer Settings

The renderer is the program that is responsible for the display of structures in Structure Viewer, Structure Search and when structures are shown in a visualization.

Note: Other structure renderers may display different type of settings, hence, the dialog you see may look different from the example shown here.



► **To reach the Structure Renderer Settings dialog from a table visualization with structures:**

1. Right-click on a row in the table visualization and select **Properties > Columns**.
2. Select the column that contains chemical structures.
3. Click on the **Settings...** button.

► **To reach the Structure Renderer Settings dialog from Structure Viewer:**

1. In the Structure Viewer pane of the Structure Viewer, right-click on the structure.
2. Select **Renderer > Settings...**
3. Response: The Renderer Settings dialog for the currently used renderer is displayed.
4. Change the renderer settings and click **OK**.

Option	Description
Structure string	Select the format of the structure string. The supported formats are MDL molfile, MDL Chime, and Daylight SMILES.
Show Hydrogens	Changes the hydrogen display settings. Possible options: For Symyx® Draw (MDL) - Off, Hetero, Terminal, HeteroOrTerminal, All For ChemDraw - True, False For Accord - True, False For Marvin - Off, Hetero, HeteroOrTerminal, All

6 Glossary

Column

A vertical list of values in a data table.

Column Name

The name of a column as displayed in the user interface. It is a normalized, trimmed, and unique text string. It is initially set to a tidied form of the external name, but it may be modified through a Rename Column operation.

Data Source

A handle to an external data source, such as a file or information link. A data source produces a single table of data.

Data Table

A data table in TIBCO Spotfire is defined as either data loaded from an external source, or new data created within the application. It has one or more columns and zero or more rows. A visualization is based on a single data table.

Data tables loaded from an external source can be linked or embedded. Linked data tables can be loaded completely into the application, but if the source is an information link they can also be configured to load data on demand only.

Data tables can be related to each other, using primary and/or foreign keys (key columns), but they can also be unrelated.

Details-on-Demand

The concept of expanding a small set of items to reveal more data behind it.

DXP File

The file type used for analysis files created with TIBCO Spotfire. Can be saved to disk and to the library. Defines what data to include and how to present it. Can include linked or embedded data based on user settings when saving the file. Includes one or more pages. There can only be one analysis file open at a time, but it is possible to run several instances of TIBCO Spotfire simultaneously, and one analysis file can also contain several data tables.

Filter

Used to reduce the amount of data to work on in TIBCO Spotfire. The same as Query Devices in TIBCO Spotfire DecisionSite. Filters can be either column filters, directly related to a column, or hierarchy filters (tree filters) which represent a hierarchy. Filters can be grouped into folders in the Filters panel.

ID column

A column in the table that contains structure identifiers.

ID list

A list of structure identifiers.

Information Link

Information links are predefined database queries, specifying the columns to be loaded, and any filters needed to reduce the size of the data table prior to visualization.

Library

The library is a space on the server where you can publish or open shared analysis files. Information links and the elements used to create information links are also stored in the library.

Marked Row

An item in a visualization becomes marked when you click on it, or, when it is captured using the rectangle method (left mouse button pressed while moving pointer). Marked rows are given a definable color to distinguish them from the rest of the data.

Marked Rows list

A dynamic list in the Structure Viewer called "Marked Rows" that contains the marked rows in the active visualization.

Marking

A marking identifies marked rows in the data tables of an analysis. If the data tables are related, the marked rows are propagated using the specified key relation between the data tables. Setting a marking in one data table does not affect the marking of unrelated data tables. Each analysis can hold multiple markings and each marking has its own marking color. One or more markings can be used to limit what data are displayed in a visualization.

Page

A page can be thought of as a "container" for visualizations, filters, a Details-on-Demand, etc. Pages make it possible to set up several sheets of visualizations that you can switch between in an analysis. Pages can contain visualizations and text areas that guide you through the analysis. Visualizations can only exist inside a page (they cannot be dragged outside even partly).

All visualizations in an analysis can be linked, both within and between pages, but they do not have to be. The visualizations on a page use one or more filtering schemes, and the filtering schemes determine whether visualizations are linked or not. The visualizations in a page can use one or several data tables.

Personalized Information Links

A personalized information link returns a subset of data depending on which user is logged in. See more details in the TIBCO Spotfire online help.

Row

A horizontal list of values in a data table.

Structure Viewer

The Structure Viewer can be used to display structures of the marked compounds in the visualizations. It can also be used to manage and view lists from various structure searches.

Structure Search

A tool used to search for compounds similar to or containing a specified master structure.

Table

A visualization with information arranged in rows and columns.

Table Column

A vertical list of values in a table.

Table Column Header

An area used to identify a table column.

Table Row

A horizontal list of values in a table.

Table Row Header

An area used to identify a table row.

URL

Uniform Resource Locator. (A world wide web address.)

Visualization

A representation of some data in TIBCO Spotfire. For example, a table, a bar chart, a pie chart, etc. A visualization displays data from one data table. The data displayed can be limited by one or more filtering schemes and by zero, one or several markings. A visualization shows and allows modification to one marking.

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