



GLYSADE

Lead Discovery ChemCharts

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Release Notes

Version 4.3.0.0

New Features

Bug Fixes

Version 4.2.0.0

New Features

Bug Fixes

Version 4.0.1.0

Bug Fixes

Version 4.0.0.0

New Features

Bug Fixes

Version 3.0.1.10

New Features

Bug Fixes

Version 3.0.1.9

Bug Fixes

Version 3.0.1.8

Bug Fixes

Version 3.0.1.7

Bug Fixes

Version 3.0.1.6

Bug Fixes

Version 3.0.1.5

Bug Fixes

Version 3.0.1

Bug Fixes

Version 3.0.0

New Features

Bug Fixes

Version 2.1.0

New Features

Bug Fixes

Version 2.0.0

New Features

Version 1.4.4.0

Bug Fixes

Version 1.4.2.0

Bug Fixes

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Front Matter

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Introduction

Lead Discovery ChemCharts extends TIBCO Spotfire® with a set of visualizations designed for use in the life science industry. The visualizations add functionality useful to scientists, such as 2D and 3D molecule depiction, R-Group analysis and advanced coloring rules. The visualizations work in both the Spotfire Professional client and Spotfire WebPlayer. There are currently 15 visualizations combined in Lead Discovery ChemCharts:

Biomolecule Viewer	3D interactive display of biomolecules linked to a sequence viewer
Dendrogram	View phylogenetic trees from multiple sequence alignments.
Details	Used in conjunction with any other Spotfire visualization to

	display data in the active row or marked rows. This visualization may be used as an alternative to the details-on-demand panel. The layout of the Details visualization is fully configurable.
Distributions	Display grouped numeric data and sample statistics.
Gallery	Presents data as a gallery of cards, where each card can be configured to display data as the user sees fit. Includes molecule depictions, molecule tooltips and single click limit by marking
MMP Filter	This visual is specific to filtering results from the MMP Database Search web service. It allows the user to filter putative transformations by selecting substructures of an MMP query.
Molecule Viewer	Typically used in conjunction with the Table visualization, this displays a 3D view of small molecules and macromolecules. This can be used to view the results of 3D superpositions, pharmacophore elucidation and the results of docking
MPO	Visualize and filter data using a distribution chart. The MPO visual includes the ability to create and update multi-parameter optimization (MPO) score columns.
Multiple Sequence Alignment	Explore structure activity relationships within a set of biopolymers. The Sequence Viewer includes an annotation viewer, LOGO plot, and a distribution chart.
Neighbor Properties	A network display of near neighbors based on chemical similarity, with the ability to visualize disparate properties associated with the structures. Neighbors are pre-computed by the Nearest Neighbors web service.
Radar	Used to display data from 3 or more numeric columns in a data table. Each axis starts from the same point at the center of the chart. The axes are distributed at equal angle increments around the center point. Each item plotted on the chart is represented as a polygon formed by joining the points for the item on each axis.
SAR Map	Displays the results of an R-Group decomposition as a grid by plotting the R-Groups along the x and y axes. Properties for the molecules contained in each cell of the grid can be displayed as color coded bars.
Structure Network	A hierarchical display of structural cores derived from the

	Core Analysis web service. This visual is used to identify and explore common cores within sets of chemical structures.
Table	Presents data as a table of rows and columns. Includes molecule depictions, tooltips, transpose mode and single click limit by marking.
Web Services	This visual provides a list of available Lead Discovery Web Services. Using this visual, users may submit data to Lead Discovery Web Services, view status of submitted tasks, retrieve completed results and configure visuals for viewing results from web services.

System Requirements

Lead Discovery ChemCharts may be used with any current Spotfire Long Term Support (LTS) version. Use of ChemCharts in the Web Player/Business Author requires installation of [.NET Framework 4.7.2](#) or greater on the Spotfire Node Manager server.

Installation

Lead Discovery ChemCharts is installed by adding the LeadDiscoveryChemCharts.sdn file to a Distribution Area on the Spotfire Server. This is the same process that is used for a standard Spotfire package installation. See the "Deploying Spotfire Packages" in the Spotfire Deployment and Administration Manual for more details on deploying distributions. The Lead Discovery ChemCharts distribution contains the following packages:

- GlysadePython
- Lead Discovery Biologics
- Lead Discovery ChemCharts
- Lead Discovery ChemCharts Forms
- RDKitChemistry
- RDKitRenderer
- ChemDraw Chemistry
- Rename Columns from CSV
- ScriptSync

The RDKitChemistry and RDKitRenderer packages are optional, but provide supplemental functionality. The RDKitChemistry package supports conversion of chemical structures loaded in MOL format to SMILES strings when copying structures to the clipboard or export CSV files from a ChemCharts Table plot. The RDKit renderer is able to highlight substructures in results

returned by the MMP Database Search web service. The highlights indicate modified portions of query and product structures.

The following packages installed from prior versions of Lead Discovery ChemCharts must be removed for normal operation: CDRenderer, ChemAxonRenderer, BioviaRenderer, RDKRenderer. Failure to remove these packages will result in errors when attempting to use current and future versions of Lead Discovery ChemCharts.

WAR File Installation

Beginning with the 4.0 release, installations of ChemCharts in the Business Author or Web Player instances require installation of static resources. While the installation of static resources adds an additional administrative burden, the performance benefit gained through the use of static resources is dramatic.

Static resources are contained in a WAR file included in ChemCharts distributions. The file will be named ChemChartsVERSION.war where "VERSION" matches the ChemCharts distribution version. There are a couple of different ways of installing the contents of WAR files on the Spotfire server. The following method is recommended to reduce the possibility of omitting installation steps.

Locate the Spotfire server installation directory. A typical path to the Spotfire server installation would be something like C:\tibco\tss\SPOTFIRE_VERSION where "SPOTFIRE_VERSION" is the version of Spotfire e.g. 11.4.0 or 12.0.0. The Spotfire server installation path will be referred to as SPOTFIRE_SERVER_DIR.

Open the SPOTFIRE_SERVER_DIR\tomcat\conf\server.xml file in a text editor. The default server.xml configuration will appear similar to the following:

```
<Host name="localhost"
      appBase="webapps"
      deployOnStartup="true"
      autoDeploy="false"
      unpackWARs="false">
```

Change the autoDeploy and unpackWARs fields to "true":

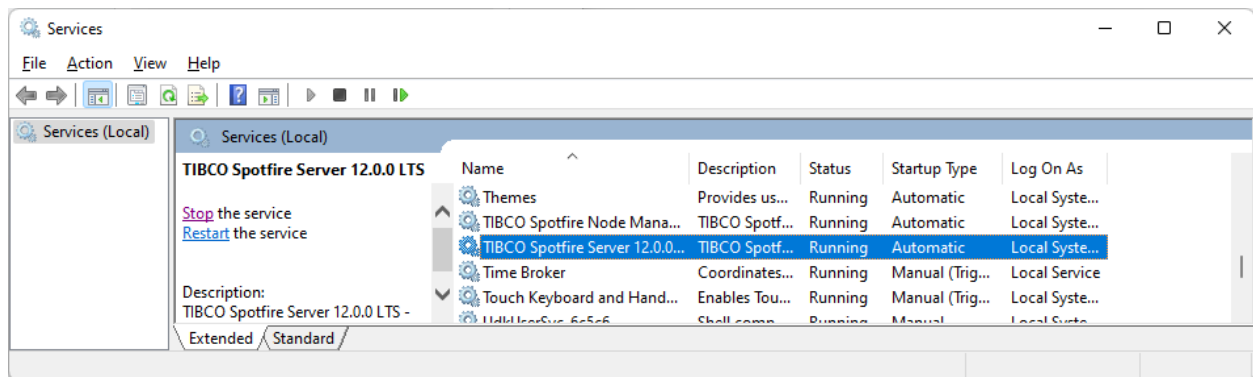
```
<Host name="localhost"
      appBase="webapps"
      deployOnStartup="true"
      autoDeploy="true">
```

```
unpackWARs="true">
```

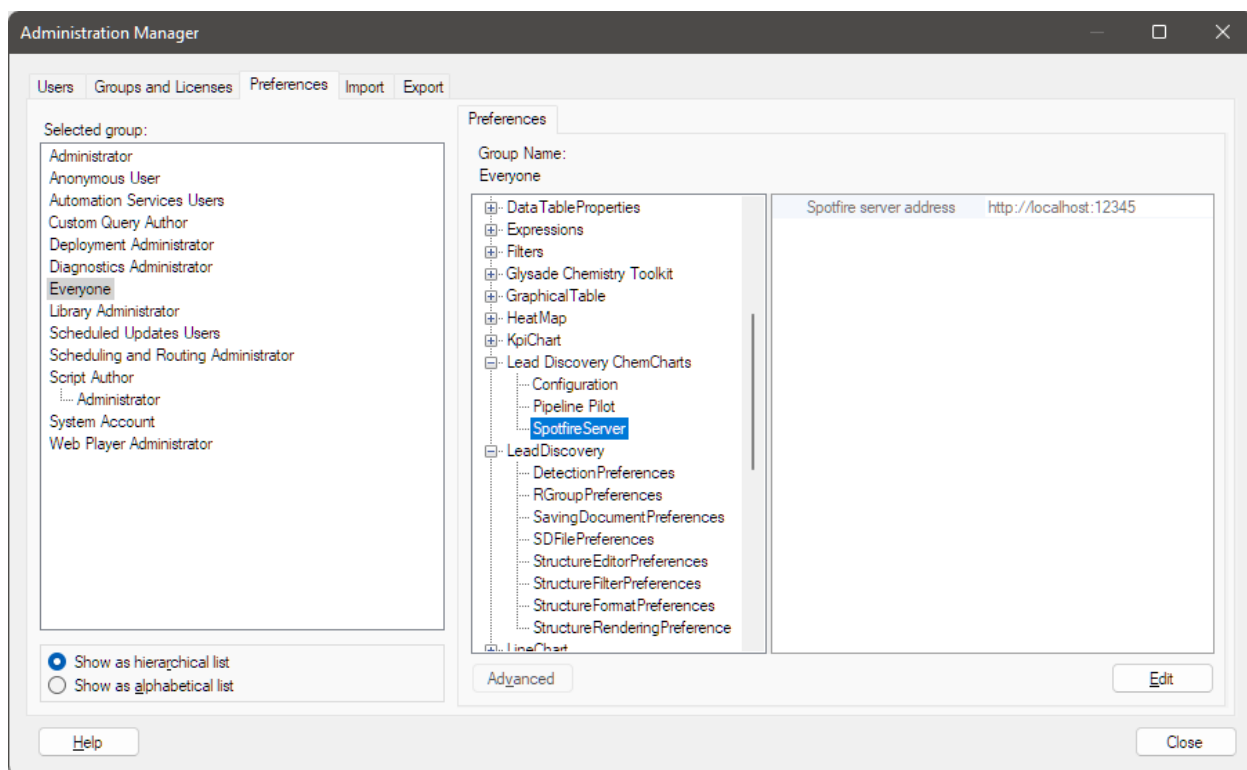
Save the settings and exit the text editor.

Copy the ChemChartsVERSION.war file into the folder indicated by the “appBase” setting in the server.xml file. “appBase” is set to the default folder “webapps” in the above example. Therefore, In this case, the ChemChartsVERSION.war file should be copied to the SPOTFIRE_SERVER_DIR\tomcat\webapps folder.

Restart the Spotfire server. If a windows service has been installed for the Spotfire server, it can be restarted using the windows “Services” dialog by selecting TIBCO Spotfire Server and clicking the ‘Restart the service’ link.



In certain network scenarios the network address for the Spotfire server provided by the Spotfire Node Manager may not be valid in the Web Player browser. If this is the case an additional ‘Spotfire server address’ must be configured via the Administration Manager > Preferences tab in Spotfire Analyst. This is shown in the figure below. Note that http/https must be included in the URL as well as the port number, if a non-standard port number is being used.



Configuration

Lead Discovery ChemCharts preferences may be configured through the Tools>Administration Manager menu option in the Spotfire Professional client. An example configuration is provided below.

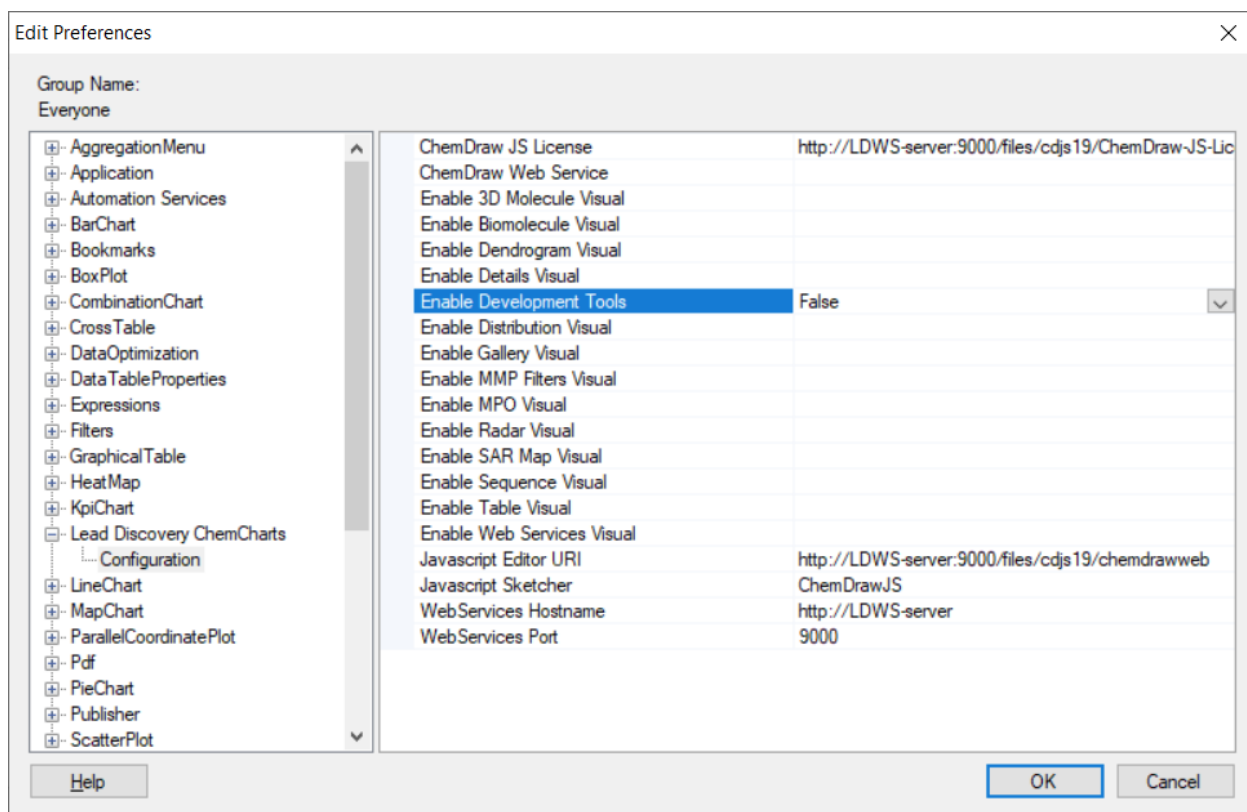


Figure: Lead Discovery ChemCharts preference settings.

Configuring Visualizations

When opening a new Lead Discovery ChemCharts visualization, a main page appears that contains a dropdown menu listing all available visualizations types. The contents of the main page may be altered by disabling visualizations through the preferences. If the "Enable" option corresponding to a visualization is set to "False" in the preferences, the visualization will be excluded from the menu on the main page.

Configuring a Structure Editor

Various visualizations make use of structure editors. Both ChemDrawJS and MarvinJS are supported in Lead Discovery ChemCharts.

ChemDrawJS is the default structure editor. This is bundled with Lead Discovery ChemCharts and requires no further configuration.

MarvinJS is not bundled with Lead Discovery ChemCharts and must be made available via a web server. To configure MarvinJS, first select MarvinJS from the list of options associated with the Javascript Sketcher preference field. Next, the Uniform Resource Identifier (URI) must be provided for Lead Discovery ChemCharts to retrieve the Javascript files for the editor. For MarvinJS, the value should be the server path to the directory that contains the "editor.html" file.

Web Services

*** Web services are now deprecated in favor of data functions and may be removed in a future version of Lead Discovery ChemCharts. Please see the Data Function User Guide for more details.**

Lead Discovery ChemCharts may be configured to access Lead Discovery Web Services. Lead Discovery Web Services is an open architecture, extensible, centralized web services framework for providing functionality to Spotfire that may be difficult or impossible to access locally from within Spotfire. Large centralized data and compute resources lend themselves well to access via web services. Please contact your Revvity representative for inquiries regarding web services support contracts.

Demonstration Web Services

Revvity hosts a demonstration version of Lead Discovery Web Services that may be made available for trial periods. Please contact your Revvity representative to obtain access and configuration details for the demonstration instance. Care should be exercised when submitting test data to the demo web services instance as it is not guaranteed to be secure. Proprietary corporate data and queries should not be used with the demonstration instance.

Installation

Lead Discovery Web Services are delivered as Docker containers or Amazon AWS Amazon Machine Instances (AMIs). Docker containers may be used for on-premises installations provided that the minimum operating system and hardware requirements are met for Docker (<https://docs.docker.com/install/linux/dockerce/binaries/>). An Amazon AWS account and familiarity with configuring AWS security groups are required for hosting Lead Discovery Web Services on AWS.

Configuration

To enable access to Lead Discovery Web Services from Spotfire, configure the Web Services Hostname and Web Services Port shown in the figure below. The Web Services Hostname should include the protocol prefix (<http://server-name> or <https://server-name>). The Web Services Port should be the integer port number on which the web services are hosted.

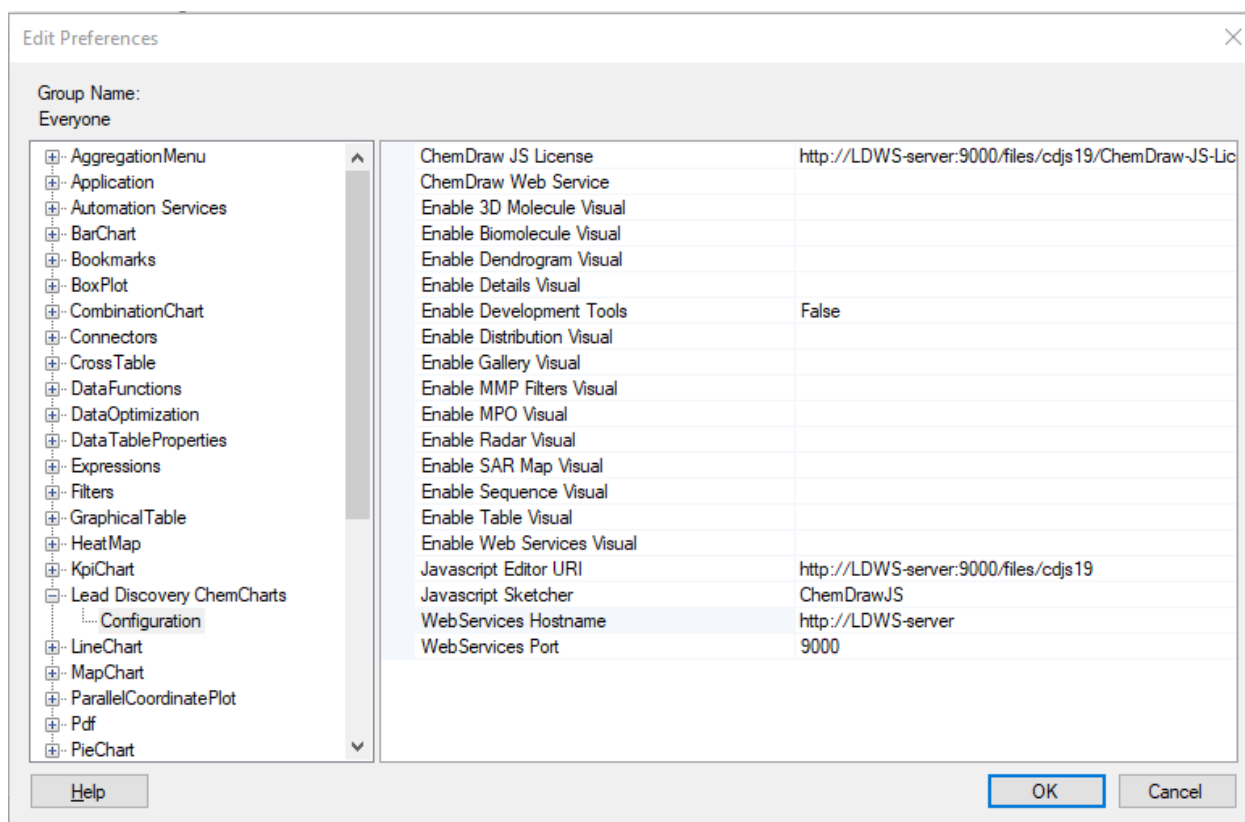



Figure: *Lead Discovery ChemCharts* example web service settings.

Visualizations

Adding a New Visualization

A new Lead Discovery ChemCharts visual may be added to a page by clicking the New Lead Discovery ChemCharts visualization button. In Spotfire versions 7.11 through 7.14, the button appears as  on the top toolbar in Spotfire. In Spotfire versions 10.0 and later, navigate to the list of visualization types and click the Lead Discovery ChemCharts button that appears as:



A new Lead Discovery ChemCharts visualization will be added to the page. The visualization initially displays menus to select a data table and chart type (shown below). Once menu selections have been made, click the GO button.

LD ChemCharts

Data table:

Chart:

Figure: *The Lead Discovery ChemCharts 'home' page.*

Biomolecule Viewer Visualization

The Biomolecule Viewer visualization enables the 3D interactive display of biopolymers and links the structural data to a sequence viewer, which is used to display aligned sequences for the biomolecules. This visualization is used in conjunction with a second visualization to control the data displayed in the Biomolecule Viewer (such as a [Table](#) visualization). Biomolecules and sequences from the rows marked in a different chart are displayed in the Biomolecule Viewer visualization. For biomolecules and sequences to be displayed correctly, some configuration of the columns that contain these data may be required. See the [Configuration](#) section for details.

The Biomolecule Viewer has much of the same functionality as the [Molecule Viewer](#), and as such, reviewing the documentation for the Molecule Viewer may be useful. The Biomolecule Viewer adds the following features:

- Sequences are displayed in a panel at the bottom of the visual.
- Highlight and mark residues in both the sequence viewer and the biomolecule viewer.
- Regions of the biomolecule can be colored or hidden.

A screen capture of the Biomolecule Viewer visualization is shown in the figure below. The Table visualization on the right hand side is being used to mark rows and control the display of the Biomolecule Viewer. In this case, 1 row is marked and the Biomolecule Viewer is displaying the biomolecule and aligned sequence for the marked row. The molecule controls panel displayed on the left hand side works in the same way as the 3D Molecule Viewer visualization. See the Molecule Controls section of the [Molecule Viewer](#) documentation for more details. Use the context (right-click) menu to toggle display of the molecule controls panel.

The glycine residue that is highlighted in green was marked by clicking on the residue in the sequence viewer at the bottom of the visual.

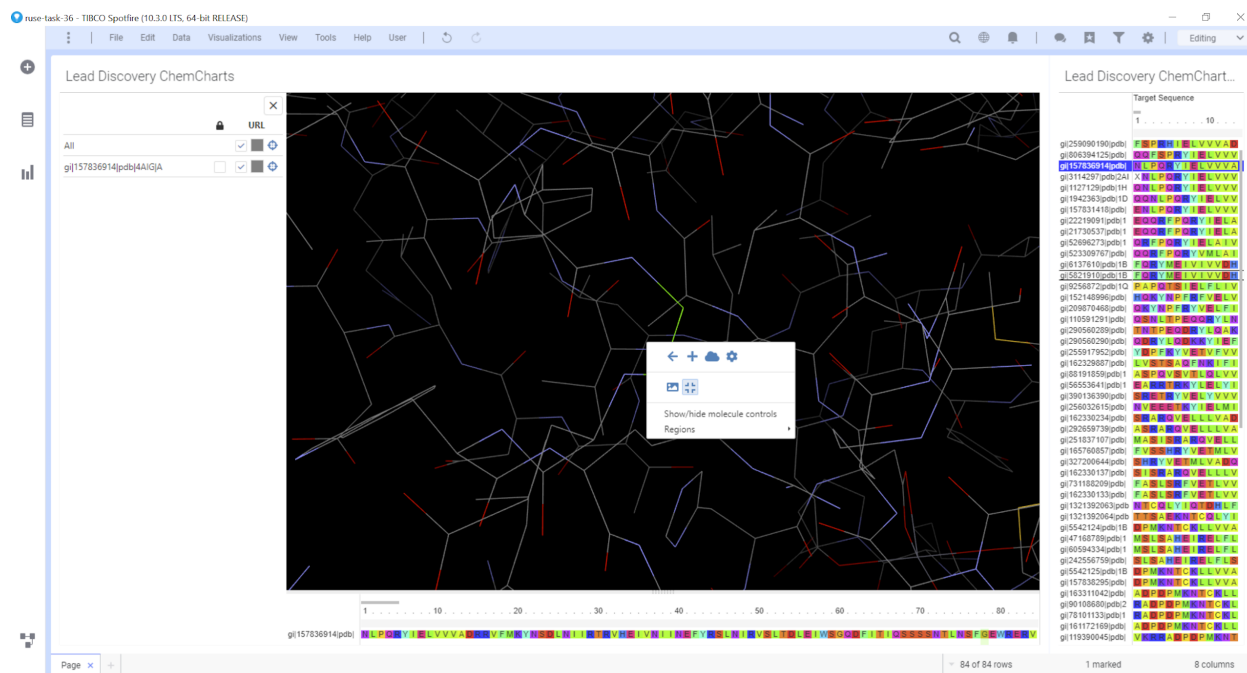


Figure: A protein structure and aligned sequence displayed in the Biomolecule Viewer.

Like the [Molecule Viewer](#), the Biomolecule Viewer is able to display multiple 3D structures from appropriately configured columns simultaneously.







Context menu

As with all the visualizations in Lead Discovery ChemCharts, much of the functionality of the Biomolecule Viewer visualization is accessed through the context menu, which is opened by right clicking anywhere in the visual. The context menu for the Biomolecule Viewer visualization is shown in the following Figure.




Figure: A screenshot of the Biomolecule Viewer visualization context menu.

The list below describes the function of each item in the context menu:

	Back: returns the user to the visualization 'home' page where the user can select a different visualization or data table to display in the current ChemCharts visualization.
	Add visualization: adds a new ChemCharts visualization to the current page. Used primarily in the web player.
	Web services: opens the web services dialog.
	Properties: opens the Properties dialog.
	Tooltips: opens the tooltips control for the visualization.
	Active residue: toggles active residue highlighting from the sequence panel.
Show/hide molecule controls	Toggles display of the molecule controls panel.
Regions	Opens the <i>Regions</i> submenu.

Create a Biomolecule Viewer visualization

Click the New Lead Discovery ChemCharts button  in the list of visualizations in Spotfire. A new Lead Discovery ChemCharts visualization will be added to the page. Select Biomolecule Viewer in the dropdown menu of available visualizations on the ChemCharts home page.

Display/hide biomolecules and sequence

The Biomolecule Viewer visualization is used in conjunction with a second visualization to control what is displayed in the Biomolecule Viewer. The [Table](#) visualization is a good visualization to use in this case. Biomolecules and sequences contained in each row of the table will be displayed if the rows are marked. Unmarking a row will hide the biomolecules and sequences in that row. For biomolecules and sequences to be displayed correctly some configuration of the columns that contain these data may be required. See the [Configuration](#) section for details

Rotate, translate and zoom

The list below describes the various mouse controls:

Rotate	Left mouse button + mouse move
Zoom	Mouse wheel or Shift + Left mouse button + mouse move
Translate	Middle mouse + mouse move button or Ctrl + left mouse button + mouse move

Measuring distances, angles and torsions

Distances, angles and dihedral angles (torsions) can be displayed. To start a measurement, right-click (or Ctrl + left-click) to select 1, 2, 3 or 4 atoms. The measurement is completed by clicking on the final atom twice. The atoms will be deselected on completion of the measurement. All atoms can be deselected by either a right-click (or Ctrl + left-click) in empty space. Measurements are removed by repeating the process used to add a measurement.

Highlight a residue (active residue)

In order to highlight a residue, (i.e. make a residue the active residue) open the context menu and click the active residue button. As the mouse is moved along the sequence shown in the sequence panel, the visualization will update to display the new active residue. The Figure below shows an example of highlighting an active row. In this case the mouse is being moved over the sequence panel at the bottom of the visualization. The residue position is highlighted in the sequence panel (with the residue index) and the active residue is rendered as cylinders in the 3D viewer. The way in which active residues are displayed in the 3D viewer is configurable (see [Configure active residue style](#)).

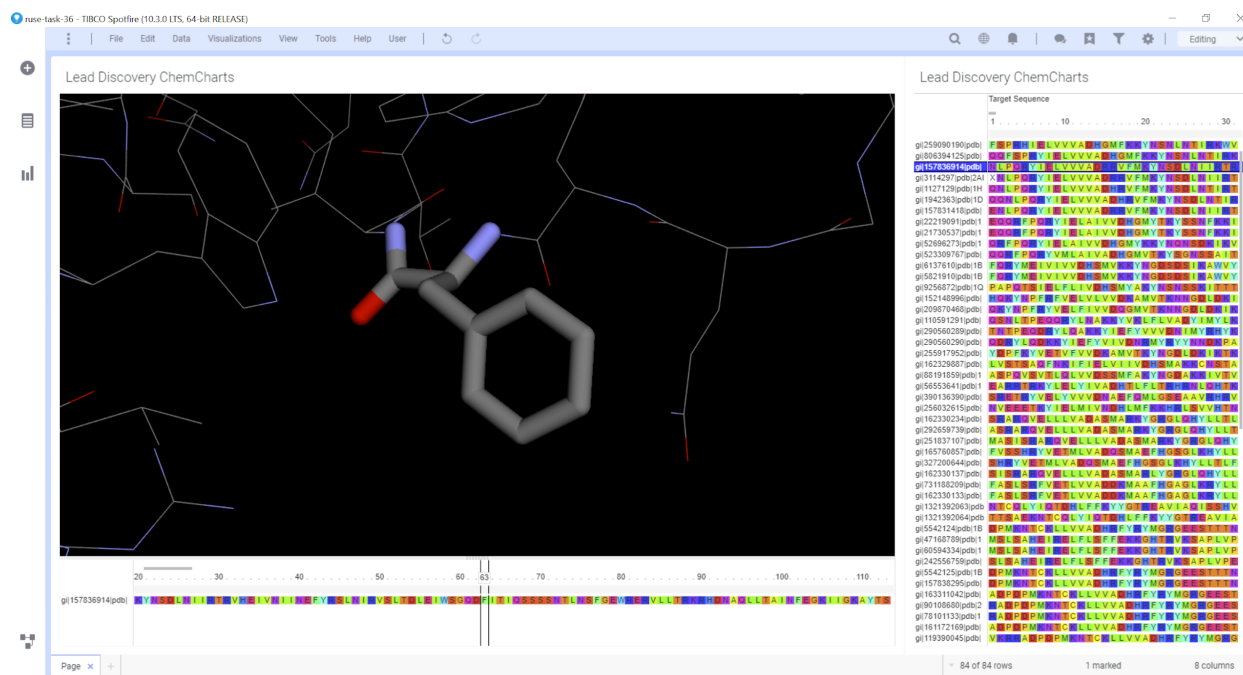


Figure: Active residue display.

Mark a residue

Residues can be marked by clicking on a residue in the sequence panel. Ctrl + mouse click can be used to toggle the marked state of a residue. Figure 4 shows an example of a set of marked residues. The carbon atoms of the marked residues are colored green in the 3D viewer and are highlighted with a green background in the sequence viewer panel. The way in which marked residues are displayed in the 3D viewer is configurable (see [Configure marked residue style](#)).

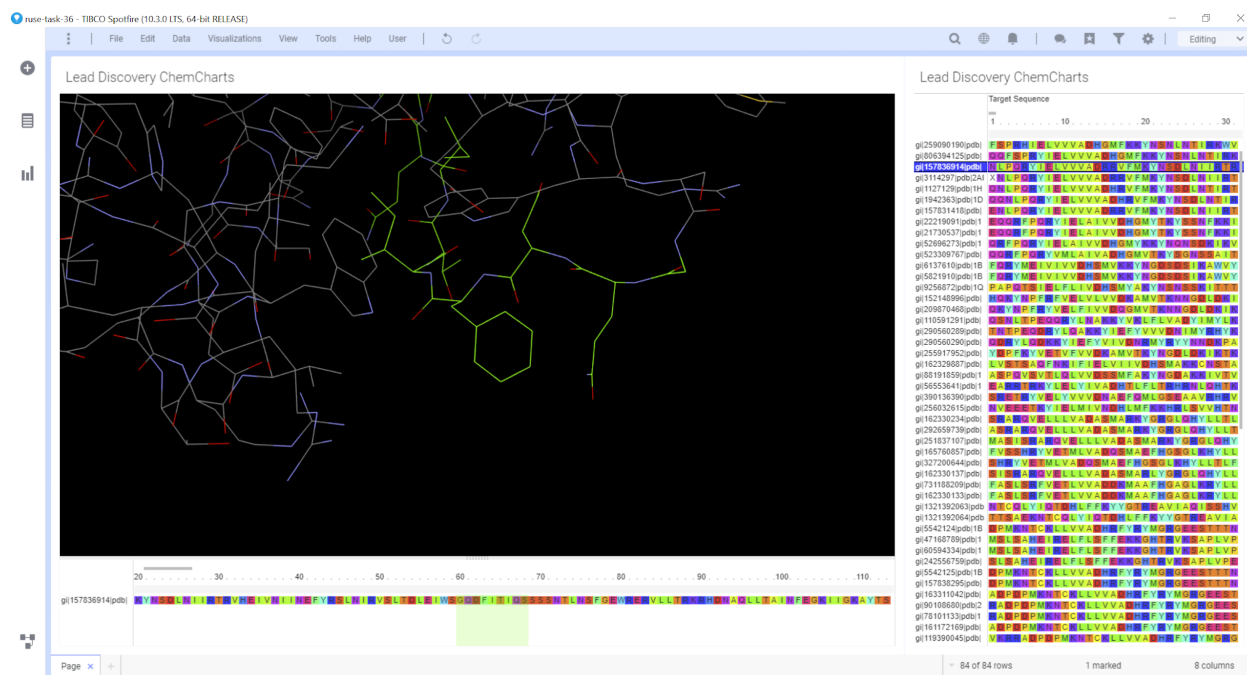


Figure: Marked residues.

Add a region

To add a region, right-click in the sequence panel to open the context menu and select *Regions > Add region*. This will add a single residue width region to the sequence panel. A region is denoted by the '[' and ']' characters on the number bar in the sequence panel. An example is shown in the following figure.

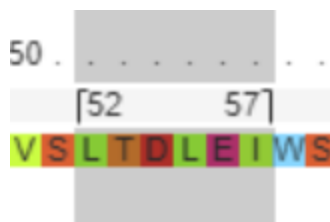


Figure: A region defined in the sequence panel.

Resize/move a region

Regions can be resized in two ways:

- If the region is expanded, use the mouse to drag-resize the region.
- Right click over the region (below the residue numbers in the gray bar) and select *Regions > Properties*. This will open the region configuration dialog. The region can be resized using the Range sliders.

A region can be moved by depressing the left mouse button when the cursor is positioned within a region just below the residue numbers in the gray bar, then dragging the mouse to a new position.

Expand or collapse a region

Regions can be expanded or collapsed by double clicking when the mouse is over the region in the sequence panel (below the residue numbers in the gray bar). Regions may also be expanded and collapsed using the *Regions > Expand all regions* and *Regions > Collapse all regions* context menu options. When a region is collapsed the residues within the region are hidden in both the sequence panel and the 3D viewer. An example of this is shown in the next two figures:

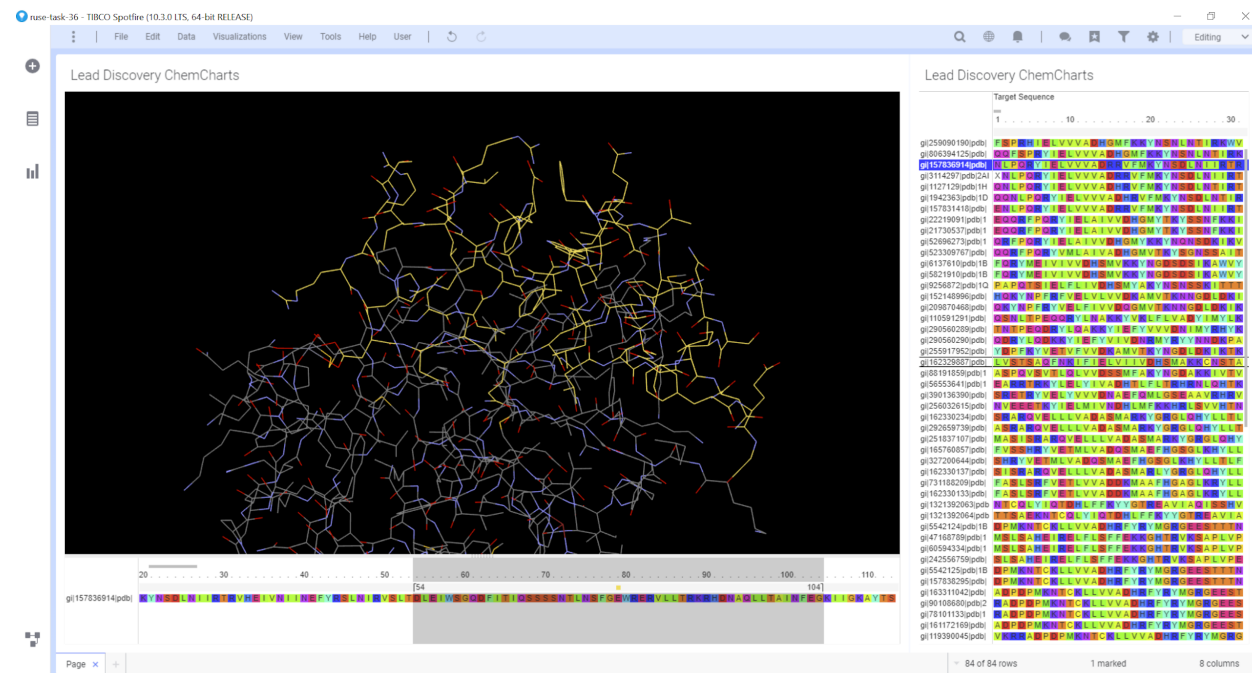


Figure: A region defined with a custom color.

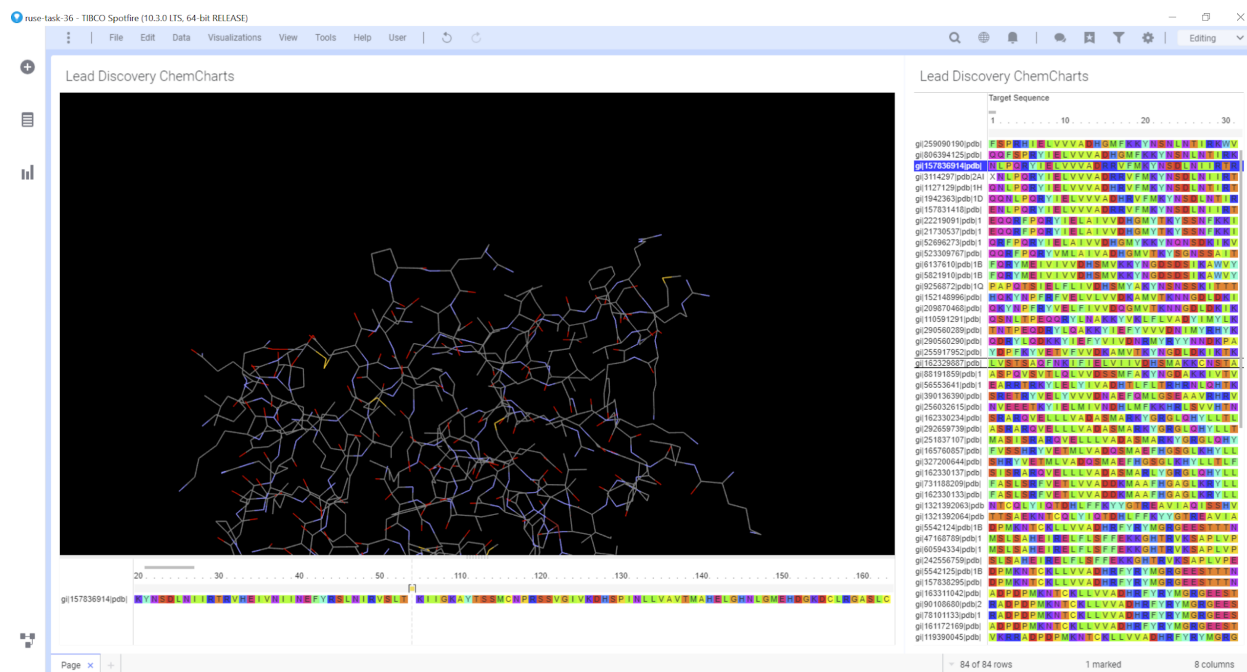


Figure: The region displayed in the prior figure has been hidden by collapsing the region.


Region Properties

Regions can be colored and named using the region properties dialog. In the case of the biomolecule viewer, the carbon atoms in the 3D viewer that are contained within the region will be similarly colored. See the [Region Properties](#) section of the Multiple Sequence Alignment visual for more information.

Remove a region


A single region can be removed by hovering over the region, right clicking and selecting *Regions > Remove* from the context menu. Alternatively, all regions can be removed by right clicking and selecting *Regions > Remove all*.

Show/hide the molecule controls panel

To display the molecule controls panel, open the context menu (right click) and select *Show/hide molecule controls*. To hide the molecule controls panel, either toggle the *Show/hide molecule controls* option from the context menu, or click the Close molecule controls button  at the top right of the molecule control panel.

Lock/unlock biomolecules/sequences

[Open the molecule control panel](#) and check/uncheck the checkboxes in the Locked column

(denoted by the column header symbol ). This will cause biomolecules/sequences to persist in the display regardless of the marked row state.


Set the visible state of biomolecules/sequence

[Open the molecule control panel](#) and check/uncheck the checkboxes in the under columns containing biomolecules/sequences that are to be displayed/hidden. By unchecking the box, even if a row is marked, the biomolecules/sequences contained in the column will no longer be visible. To enable visibility, click the checkbox again.

Change the biomolecule color

[Open the molecule control panel](#) and click the color control to the right of the visibility checkboxes under the column for the desired structure. The new color for the biomolecule can be selected from the color drop down that will appear. This new color is now used to color the carbon atoms for the structure. Note that this will not alter the color scheme for ribbons when displaying proteins or nucleotides.

Center on a biomolecule

[Open the molecule control panel](#) and click center button  for the biomolecule that is to be centered. The display is shifted such that the geometric center of the structure will be placed at the center of the Biomolecule Viewer.

Change the column used to name rows in the molecule controls panel and sequence panel

The column containing names used to identify each row displayed in the *Biomolecule Viewer* molecule controls panel and next to the sequences in the sequence panel is configurable. The name column may be changed in the [Properties dialog](#) by selecting the desired column from the Name column drop down.

Change the background color

The background color can be configured in the [Properties dialog](#) by clicking on the colored square next to Background color and selecting a different color from the color swatch.

Protein cartoon settings

Cartoons (ribbon diagrams) that highlight the secondary structure can be displayed for proteins. The appearance of protein cartoons may be configured in the [Properties dialog](#). The display of protein cartoons can be toggled using the *Display cartoons/ribbons* check box. The cartoon style can be chosen using the *Cartoon/ribbon style* drop down and the opacity of the cartoon can be set via the *Cartoon/ribbon opacity* number box (1 is opaque, 0 is completely transparent). Note that setting the cartoon opacity to anything other than 1 may impact performance.

Select biomolecule and sequence columns

The data table columns configured for the 3D structure and sequence displays can be configured in the [Properties dialog](#). Select the desired columns from the Sequence column or Biomolecule columns drop downs.

Configure active residue style

The style of active residues displayed in the 3D viewer can be configured in the [Properties dialog](#). Use the *Active residue style* dropdown to select the style used to display active residues. The *Active residue color* control may be used to set the active residue color to None, or a user-defined color by selecting a color from the color palette.

Configure marked residue style

The style of marked residues displayed in the sequence panel and 3D viewer can be configured in the Biomolecule Viewer [Properties dialog](#). Use the *Marked residue style* dropdown to select the style used to display marked residues. The *Marked residue color* control may be used to select the color for marked residues in the 3D display.

Configuration

In order to display biomolecules and sequences in the Biomolecule Viewer the data table must contain the following columns:

- A column containing sequences. The sequences here should relate to the biomolecules from the structure column (see below). The sequences contained in this column should be aligned, but this is not a requirement. The column should have one of the following ContentTypes: chemical/x-sequence or chemical/x-genbank. The ContentType typically depends on whether the sequences were imported from FASTA or Genbank files.
- A column containing the URIs of the biomolecules in PDB or gzipped PDB format. The biomolecules are not contained within the Spotfire data table, but are referenced by URI (Uniform Resource Identifier) in order to minimize the data table size. The web server must obviously be visible to the client running Spotfire or Spotfire WebPlayer. The ContentType of the column should be set to "chemical/x-uri" and the Dimension property should be set to "3".

Columns imported from results of Lead Discovery Web Services will likely have the appropriate properties set to make them displayable by the 3D Molecule Viewer. Columns originating from other data sources, such as SDF or CSV import may need to have their properties set manually. To set column properties manually, open the Column Properties through the Spotfire *Data > Column Properties* menu. Select the column from the list in the top half of the Column Properties dialog, then select the *Properties* tab in the middle of the dialog. Select the ContentType property and click the Edit button on the right hand side, and enter the appropriate value for the ContentType. The Dimension property may be added by clicking the New button to the right of the properties listing. Enter "Dimension" as the property name, leave the Data type as "String" and enter the value "3" into the Default value field. An example is shown in the following figure:

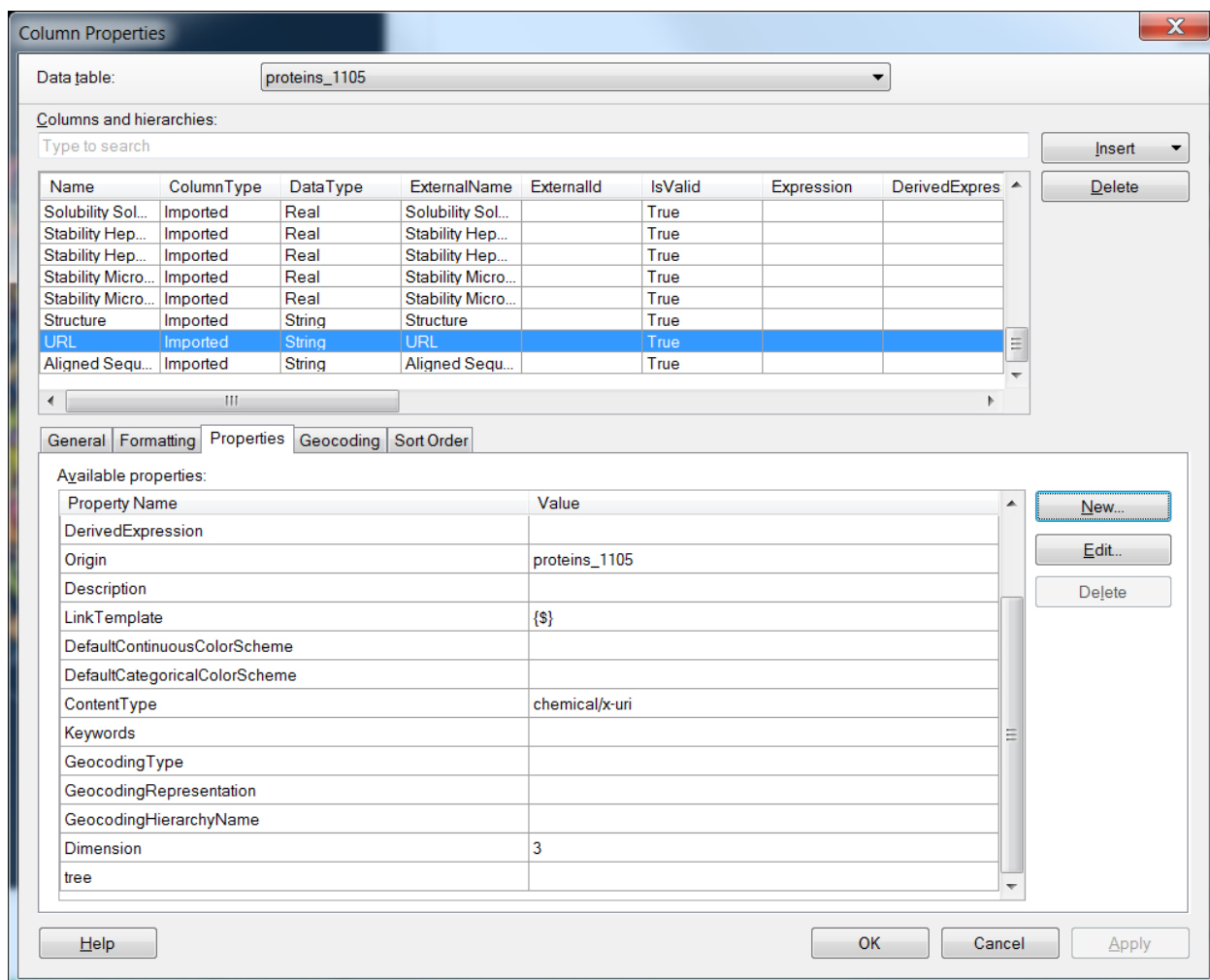



Figure: Editing properties using the Column Properties Dialog.

Once the properties are set correctly, the Biomolecule viewer will display molecules for marked rows in the data table.

Biomolecule Viewer Properties

Many chart specific settings are configured in the Properties dialog. To access the Properties dialog, open the content menu by pressing the right mouse button and click the *Properties*  button. After the dialog opens, click the *Biomolecule viewer* page on the left panel to configure Biomolecule viewer specific options.

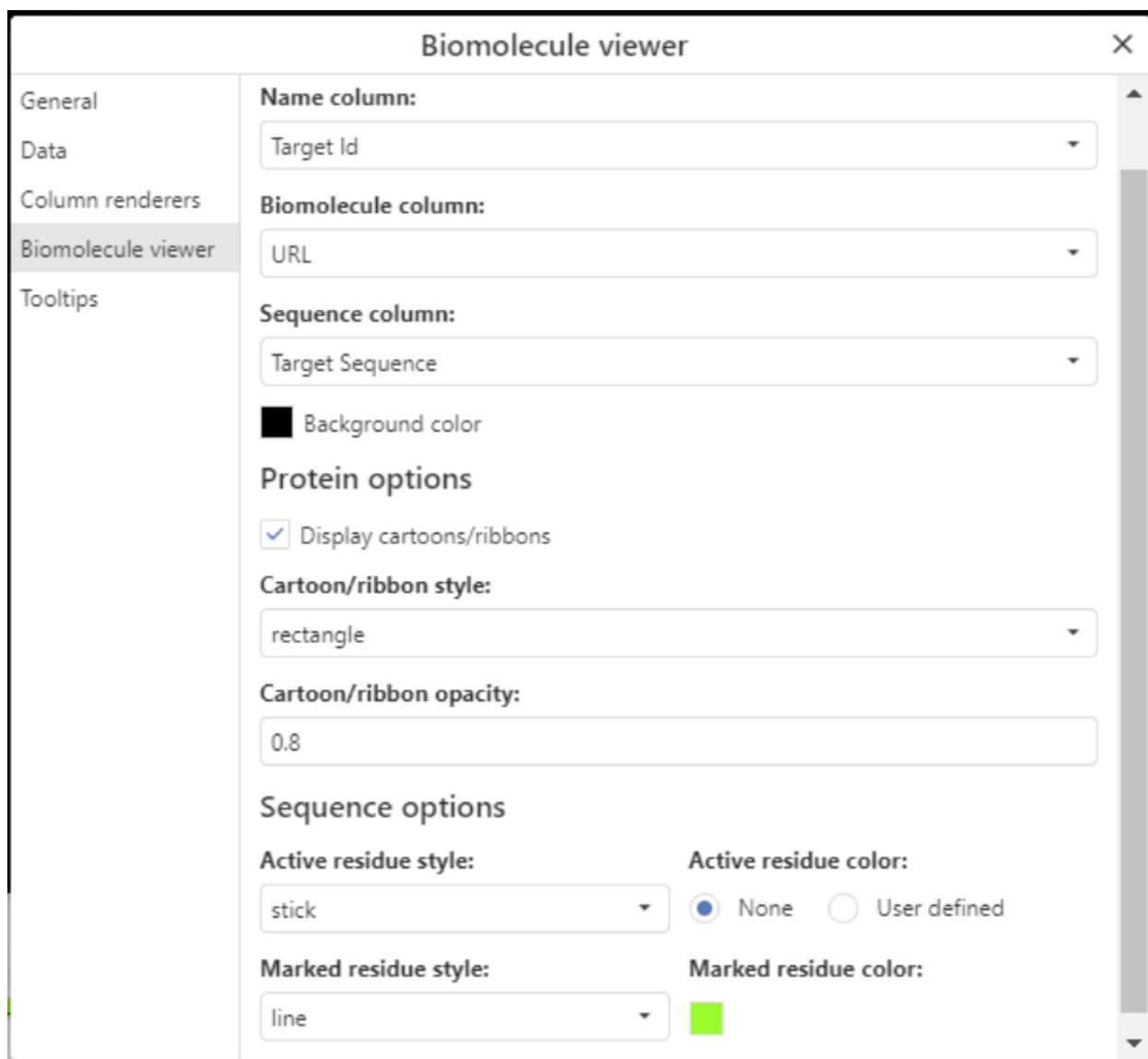


Figure: The Properties dialog.

Chemistry Visualization

The Lead Discovery ChemCharts Chemistry Visualization is used to perform chemical structure searches, structural similarity searches, property calculations, R-group decompositions, core identification, and other cheminformatics related tasks. Much of the functionality available in the Chemistry Visualization adds columns to existing tables using Spotfire DataFunctions. The Chemistry Visualization differs from other ChemCharts visualizations in that it allows users to view and manage calculations, rather than viewing the data itself.

Multiple DataFunction implementations are supported by the visualization. Although a default implementation of each function exists, alternate vendor toolkit implementations may be configured and used preferentially to the default. Users are able to customize their experience

and calculation results based on the relative merits of and personal preferences toward vendor cheminformatics toolkits.

A new Chemistry Visualization added to a document devoid of existing calculations will appear as:

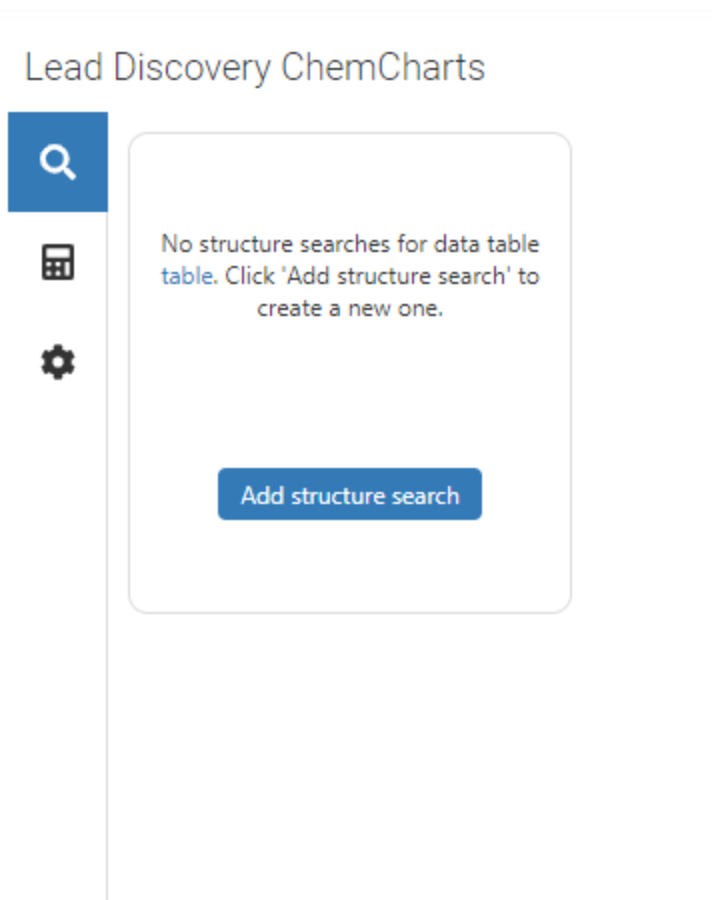


Figure: Initial appearance of the Chemistry Visualization.

If chemistry calculations are present in an existing document, they will automatically be displayed in the Chemistry Visualization. A navigation bar will appear either at the left hand side or the bottom of the visualization, depending on the size of the visualization.

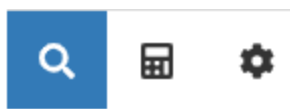




Figure: Chemistry Visualization navigation bar.


New Chemistry Visualizations display chemical structure searches  by default, if they exist. Cheminformatics functions other than structure searches are grouped in the calculations

tab . Preferences for the Chemistry Visualization may either be accessed through the

settings tab  of the navigation bar or the context menu.

Chemical Structure Search

Substructure, similarity, and exact match searches may be added to a document using the

Chemistry Visualization. Click on the chemical structure search button  in the navigation bar if it is not already selected. To add a new structure search, click the button in the *Add Structure search* control.

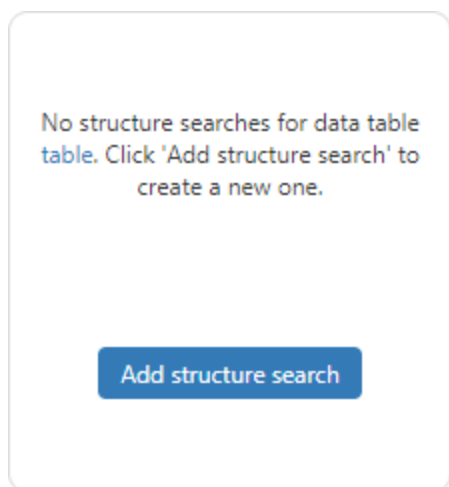


Figure: The Add structure search control.

The visualization will temporarily maximize to display a *New Search* dialog.

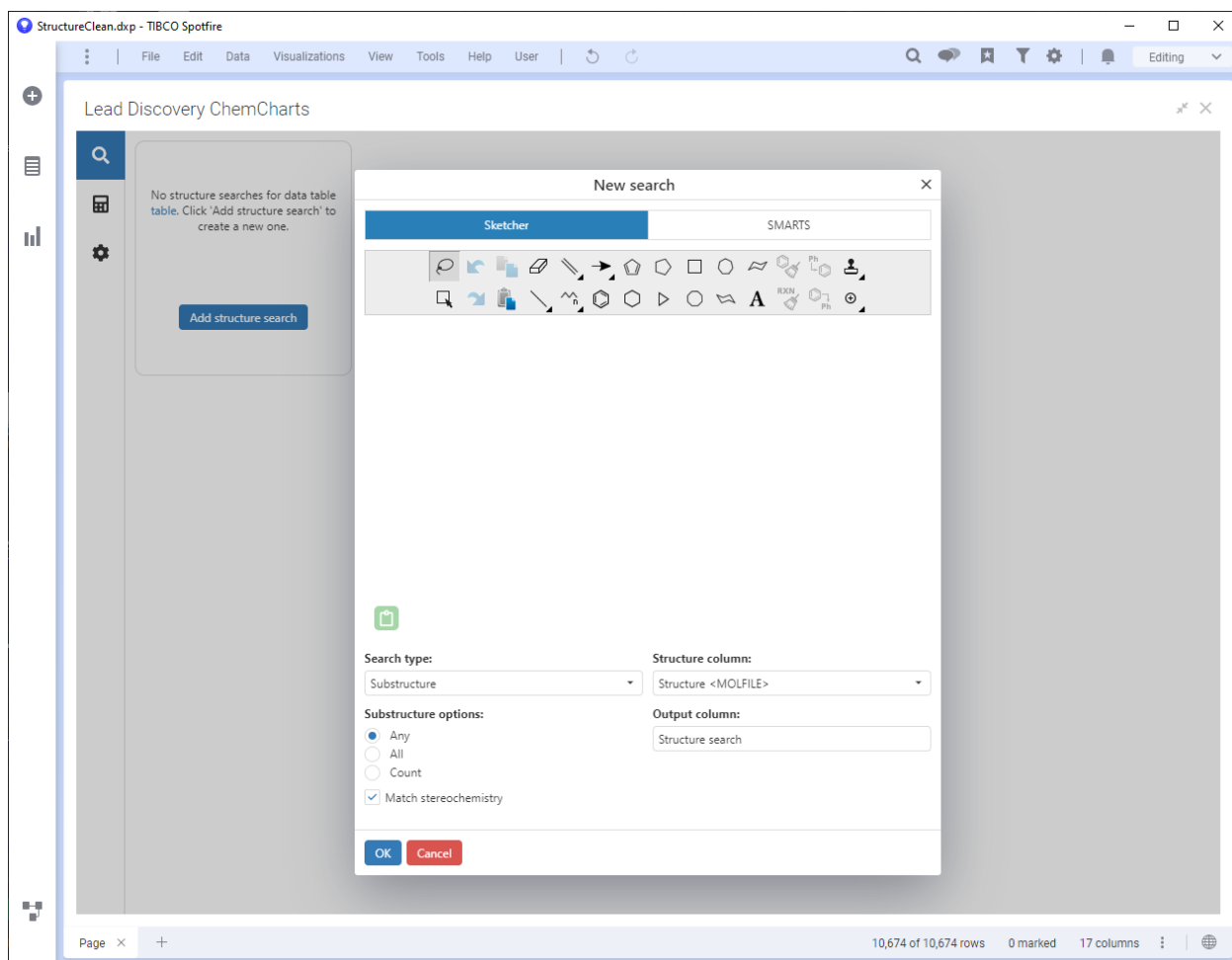


Figure: The New Search dialog.

The structures or substructures to be used in a search may be pasted from a clipboard into the sketcher, drawn using the sketcher, or input as SMILES or SMARTS by switching from the Sketcher tab in the dialog to the SMARTS. Note that disconnected structures and substructures are supported in the default implementation based on RDKit. Please check the documentation for alternate chemistry toolkit implementations for information on whether disconnected structures and substructures searches are supported.

Figure: SMARTS structure input in the New Search dialog.

After entering a query structure, the type of search to be performed may be selected from the *Search type* dropdown menu.

Figure: Selecting the type of structure search.

The options presented for substructure, similarity and exact match searches differ depending on the selected search type. They are described in the following three sections.

The column of structures to be searched may be altered using the *Structure column* control. Note that structure columns are identified by the *ContentType* assigned for the data column. Not all chemistry toolkits are capable of handling all possible chemical formats, and if the toolkit configured for structure searching is not capable of reading and searching structures in a particular format, the structure column will not appear in the *Structure column* dropdown.

The name of the output column may be configured in the *Output column* text box. If the target data table for search results already contains a column name specified in the *Output column*

text box, column name collisions are resolved by appending a “(#)” suffix where the number in parentheses is incremented to the next highest number that will resolve the collision.

Substructure Search

Substructure search is the default search type selected upon opening a *New Search* dialog. Search options include *Any*, *All*, *Count*, and *Match stereochemistry*.

Search type:

Substructure

Substructure options:

Any

All

Count

Match stereochemistry

Figure: Substructure search options.

The *Any* and *All* options are superfluous when only a single contiguous substructure query is entered. When the options are applied to searches with disconnected query structures, the resulting hits identified will differ. A structure in a data table will be considered a match if *Any* one of multiple disconnected query substructures are identified in the structure. Alternatively, all disconnected substructures must be present in a structure when the *All* option is selected. Substructure searches produce a boolean column containing True or False values indicating the presence or absence of substructure(s), while taking into account the *Any* or *All* criterion for disconnected queries. The *Count* option differs in that a column of integers containing the number of occurrences of symmetry unique matches of substructure(s) is produced.

When performing substructure searches, queries that do not contain stereochemistry will match structures that have stereochemistry specified. Queries that contain stereochemistry will only match structures that have identical stereochemistry specified unless the *Match stereochemistry* checkbox is unchecked.

After substructure search configuration is complete, the search will be submitted and the Chemistry Visualization will display all searches in progress.

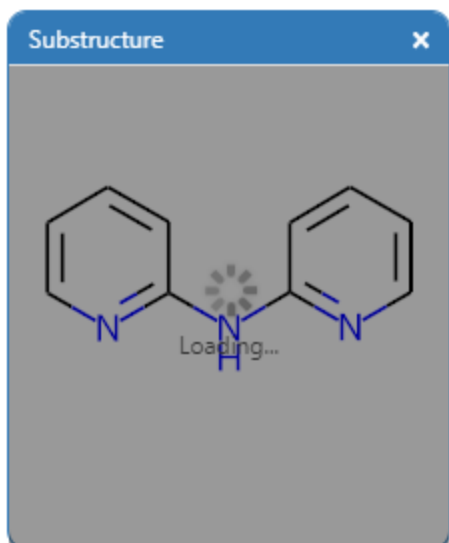


Figure: A substructure search in progress.

Substructure searches are run in the background so that Spotfire will remain responsive. Upon completion of the search, the *Substructure* control will alter its appearance and have *Include* and *Exclude* filter controls. Unchecking the *Include* filter checkbox will cause rows that match the substructure to be filtered out. Unchecking the *Exclude* checkbox will cause rows that do not match the substructure to be filtered out. Note that corresponding filters in the filter panel are updated, and altering corresponding filters in the filter panel will also cause the checkboxes in the *Substructure* control to be updated as well.

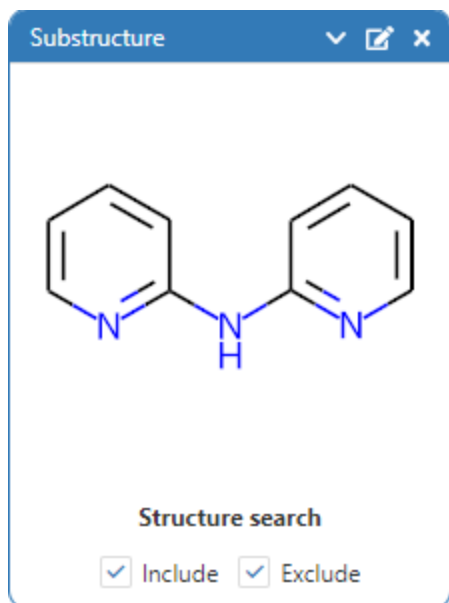



Figure: Substructure control.

The Substructure control can be used to configure highlighting of the matching substructures in the structure column that was searched and/or align structure depictions to the substructure. By default both of these are not enabled. To enable highlights, change the highlight color, or to align structure depictions to the substructure, expand the Substructure control using the *expand*  button to expose alignment and highlight controls.

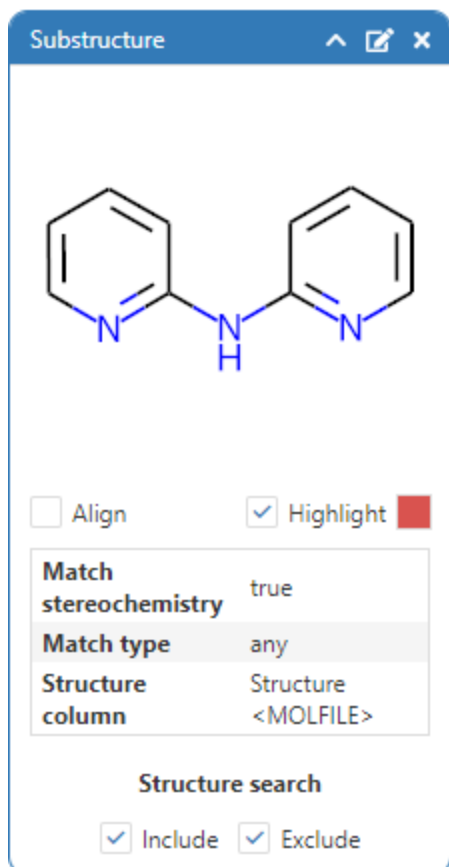


Figure: Expanding the substructure control to access alignment and highlight controls.

Similarity Search

Setting the *Search type* dropdown to *Similarity* will update the search options displayed in the New Search dialog. The type of *Fingerprint* to be used in the similarity search, and the *Metric* used to compute the similarity.

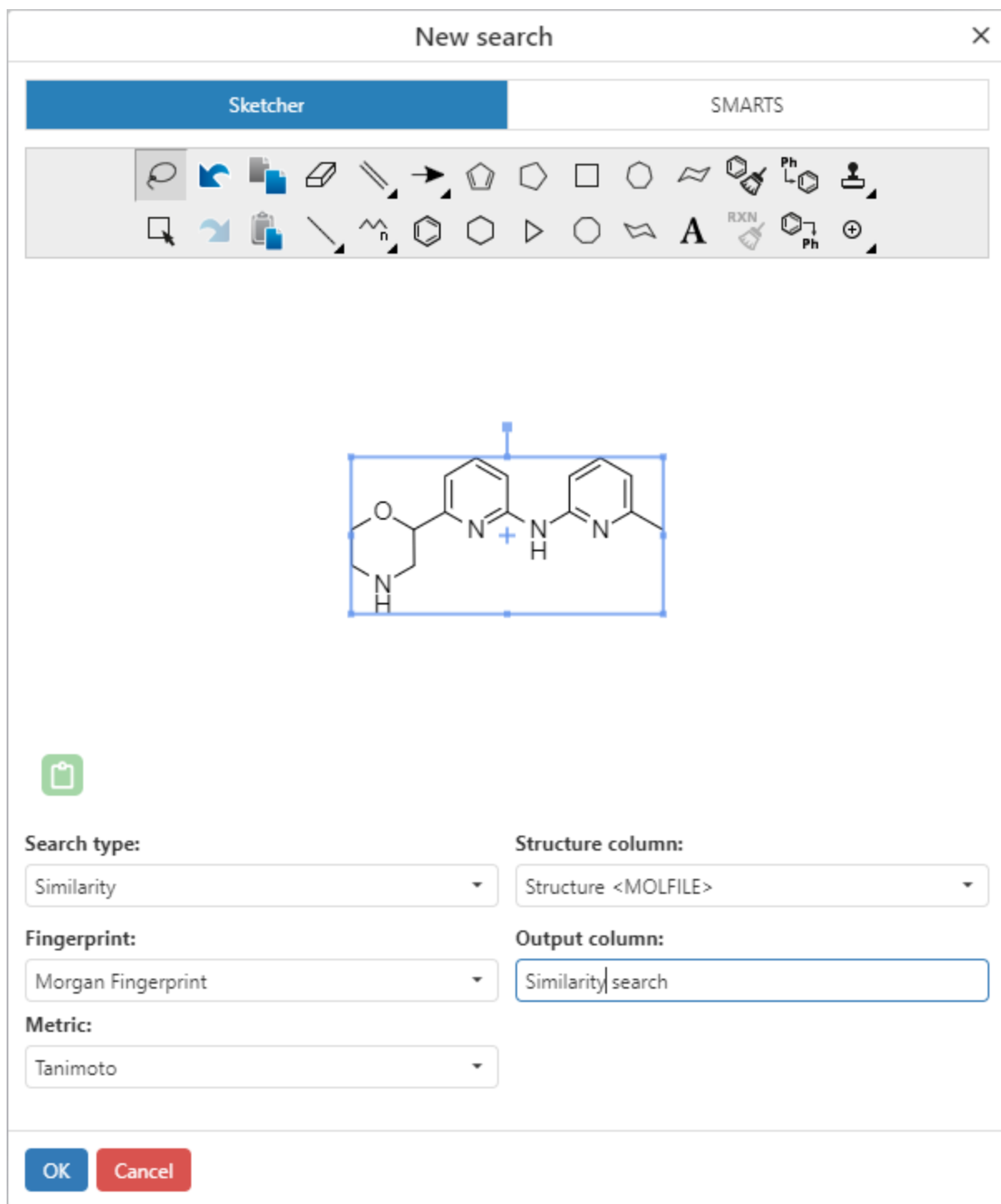


Figure: Similarity search options.

Fingerprint types differ in how the topological features of each structure are captured, and will produce different values for similarity metrics. Differences in rank ordering by similarity to a structure for different fingerprint types are expected. There are four different fingerprint types available in the default toolkit based on RDKit: MACCS, AtomPair, Morgan, and Topological

(Torsions). The MACCS fingerprint is based on the 166 public substructures of the original MACCS fingerprint screens used for substructure searches. MACCS fingerprints are poor at comparing overall topology of structures, but are appropriate when comparing structures by presence or absence of functional groups and ring systems. Topological torsions and Morgan (aka circular) fingerprints are able to relate elemental composition and local connectivity, but capture less of the overall connectivity. AtomPair fingerprints are good at capturing long range connectivity. The fingerprint type used for comparison should be selected to match the intended use. Please consult the documentation for descriptions of fingerprint types implemented in alternate vendor chemistry toolkits.

Exact Match Search

Structures that have the identical composition and connectivity as a query structure may be identified using exact match search. Matching stereochemistry is required by default, but may be disabled in the search options.

Structure Search Tag Columns

It is sometimes useful to create a column that contains text entries that denote whether a molecule in each row contains one (or more) named substructures. For example, project teams may want to label each row according to a named core that each molecule contains. Alternatively users may want to denote the presence of a set of reactive functional groups. In order to facilitate this, ChemCharts allows the creation of 'structure search tag columns' from one or more structure searches that have been defined in the Chemistry visualization.

The figure below shows the chemistry visualization where 2 substructure searches have been performed for 2 notional cores. The output columns from the substructure search have been carefully named 'Core 1' and 'Core 2' using the 'Output column' text box in the substructure search dialog (see [above](#) for more details).

table-1000 - TIBCO Spotfire

Lead Discovery ChemCharts

	Code	Structure	Core 1	Core 2
1	MBX000043		False	False
2	MBX000205		False	True
3	MBX000230		False	True
4	MBX000273		False	True
5	MBX000274		False	True
6	MBX000277		False	True
7	MBX000278		False	True
8	MBX000279		False	True

Lead Discovery ChemCh...

Substructure

Core 1

Include Exclude

Substructure

Core 2

Include Exclude

Displaying structure searches for data table table-1000.

Add structure search

Reorder structure searches

Structure search tag columns

999 of 999 rows 1 marked 21 columns

Figure: Two substructure searches in the Chemistry visualization denoting the presence or absence of 'Core 1' or 'Core 2'.

To create a structure search tag column, click the 'Structure search tag columns' button shown in the figure above. This will open the 'Edit structure search tag columns' dialog. To create a new structure search tag column, click the 'Add' button in the dialog, enter a name for the new column and either hit enter or click the tick button on the right (shown in the figure below).

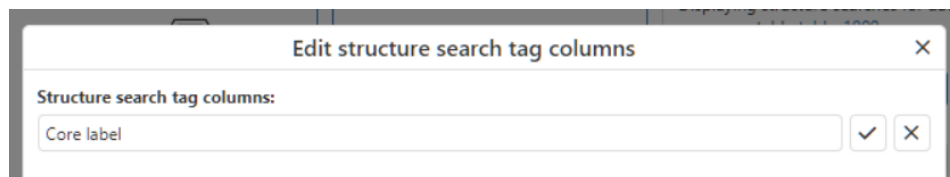


Figure: Adding a new structure search tag column.

Once a structure search tag column has been added the user can select which of the Chemistry visualization structure search result columns they want to include as potential tags for the structure search tag column. In the figure below both the substructure searches have been added as potential tags for the new structure search tag column. Note the options section at the bottom of the dialog that determines whether all matching tags appear in the structure search tag column or just the first matching tag. If 'All matches' is selected, and there is more than one matching tag, the tag names will be separated by a '[' character. If 'First match' is selected, only the first matching substructure will be displayed in the structure search tag column. The user can reorder the chosen structure search columns which can be important if the 'First match' option is selected.

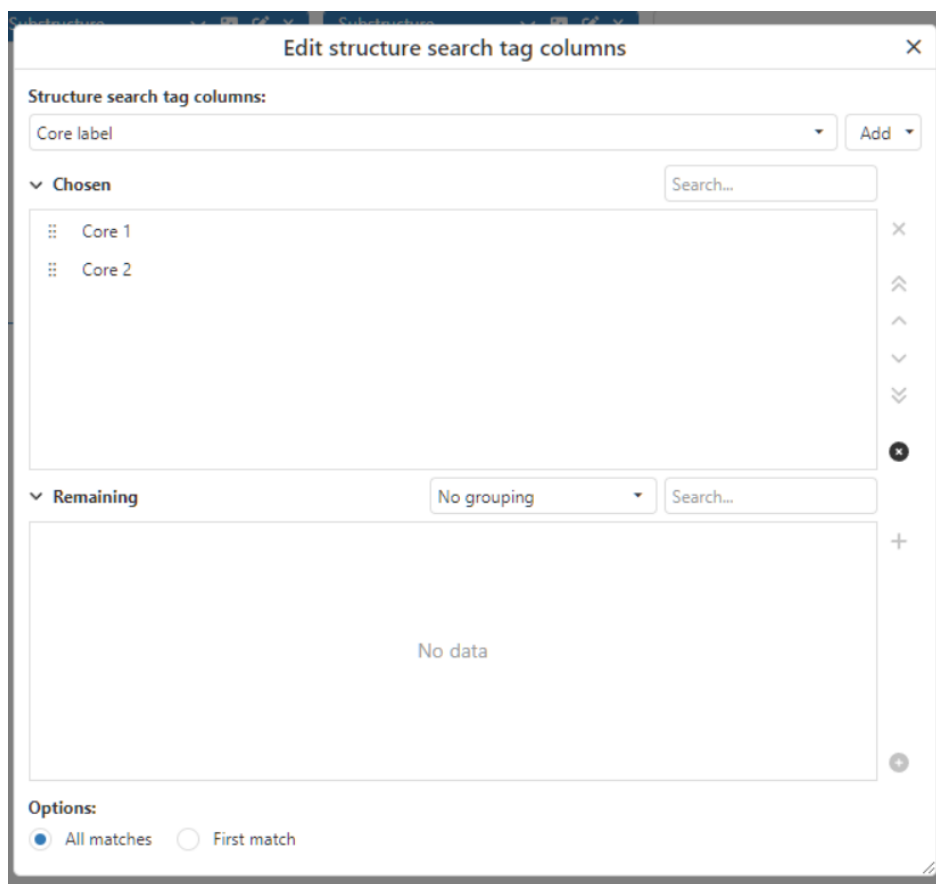


Figure: Configuring which substructure search results columns are used as potential tags for the new structure search tag column.

The results of the configuration of the structure search column are displayed in the figure below. As can be seen, the table visualization now contains the new structure search tag column and the labels for the various cores have been added as values in each of the cells.

The screenshot displays a TIBCO Spotfire interface with a table titled 'Lead Discovery ChemCharts'. The table has the following columns: Code, Structure, Core 1, Core 2, and Core label. The data rows are as follows:

	Code	Structure	Core 1	Core 2	Core label
74	MBX021674		False	True	Core 2
75	MBX021675		False	True	Core 2
76	MBX026870		True	False	Core 1
77	MBX026871		True	False	Core 1
78	MBX026920		True	False	Core 1

On the right side of the interface, two 'Substructure' configuration panels are visible. The top panel is for 'Core 1' and shows a chemical structure of a pyridine ring attached to a pyrrolidine ring. The bottom panel is for 'Core 2' and shows a chemical structure of a pyridine ring attached to a six-membered ring containing five 'A' atoms. Both panels have 'Include' and 'Exclude' checkboxes checked.

Figure: Results of structure search tag column configuration. The 'Core label' column is added and each row is now labeled with the name of the core that each molecule contains.

Existing structure search tag columns can be edited by clicking on the 'Structure search tag columns' button in the Chemistry visualization, selecting the column you want to edit and configuring as described above.

Cheminformatics Calculations

Cheminformatics features other than structure searches are grouped in the *Calculations* tab



of the Chemistry Visualization. New calculations can be added to a document in the *Add Calculation* control that appears on the Calculations page.

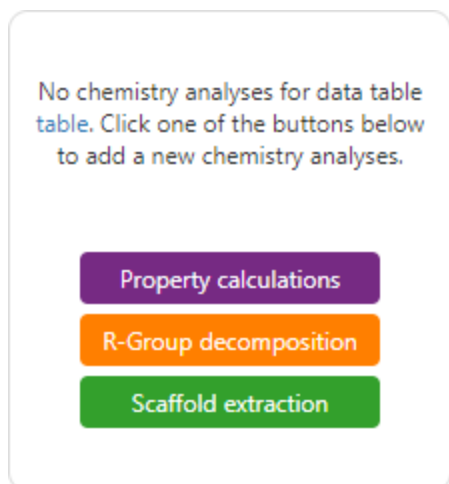


Figure: The Add Calculations control.

Property calculations

Topological and predicted physical property calculations based on chemical structures may be added to a data table using the Property calculations DataFunction. One column per calculated property is added to the same table that contains the chemical structures. Click the Property calculations button in the *Add Calculation* control to open the *Property Calculation* dialog.

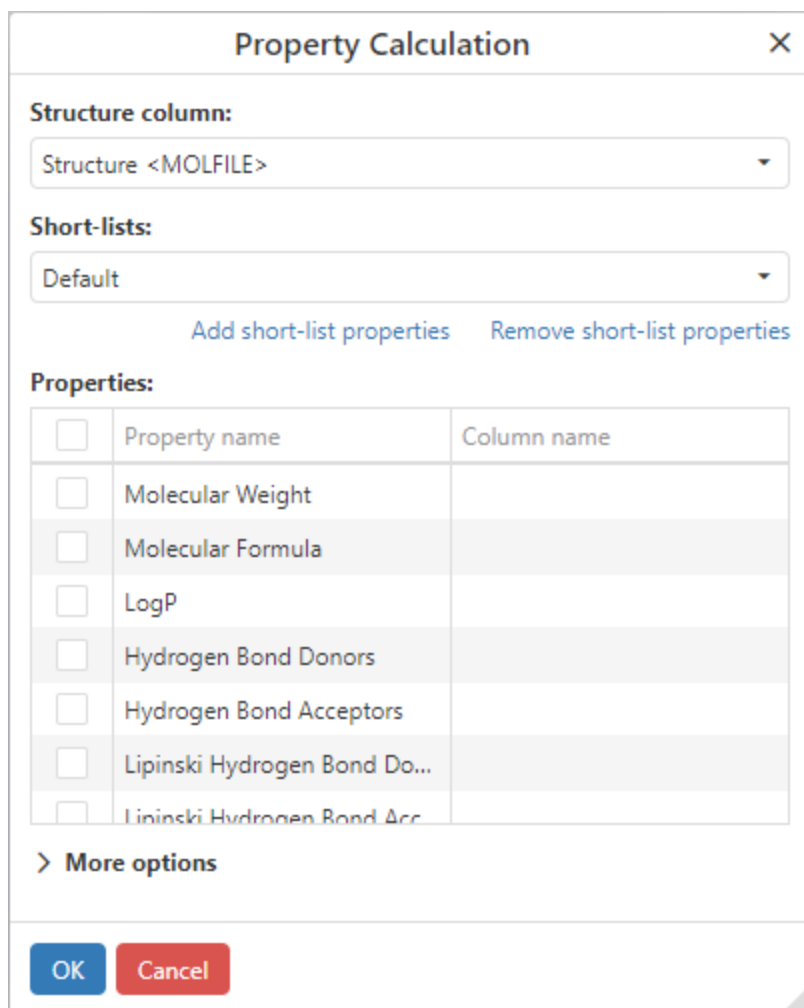


Figure: The Property Calculation dialog.

Checking boxes next to each property name will cause that property to be computed and added to the result data table. Predefined lists of properties may be created in the [Property calculation preferences](#) as short-lists. Short-lists will appear in the *Short-lists dropdown menu*, and either be applied or used to remove selections from the *Properties* control of the *Property Calculations dialog*. Expanding *More options* reveals *Output columns prefix* and *Output columns suffix* text boxes that are used to prepend or append text to the output column names created by a property calculation. Text added to output columns may help the user identify the source of the calculated column.

R-Group decomposition

R-Group decompositions may be performed by selecting *R-Group decomposition* from the *Add new chemistry analysis* drop down control. The default chemistry toolkit R-Group decomposition supports multi-core decomposition, and attempts to correctly group R-group results by similarity in cases where the core(s) are perfectly symmetric. Matching cores and

R-Groups are written to the same data table that contains the input structures. The matching core will be written to a column titled "Core". R-Groups are written to columns titled "R#" where # begins at "1" and is incremented to the total number of R-Groups. The input structure column is selected in the *Structure column* dropdown menu. Cores and R-Groups may be output in either Molfile or SMILES format. The original orientation taken from each input structure will be preserved in Molfile output records.

Cores may be entered with undefined or user defined R-Group positions. Undefined R-Group positions are automatically identified based on the set of input structures. Users may define R-Group positions on cores to exert control over the ordering of R-Group output columns. Incomplete specification of user defined R-Group positions is acceptable, and the default chemistry toolkit will automatically identify unspecified R-Group positions unless the *Only match R-Group atoms defined in core* checkbox is checked. If the *Only match...* control is checked, the user must define at least one R-Group position on the cores, otherwise the decomposition will fail. R-Groups will only be output for each user defined position defined in the core(s). Structures with R-Groups at other positions will be excluded from the decomposition.

Disconnected structures in the sketcher will normally be treated as separate cores and the first core to match an input structure will be selected as the core in the decomposition of the input structure. Alternatively, by selecting the *Allow fragmented single core* checkbox a decomposition can be performed on a disconnected core and structures will need to match all sketched fragments.

Expanding *More options* reveals *Output columns prefix* and *Output columns suffix* text boxes that are used to prepend or append text to the output column names created by an R-group decomposition.

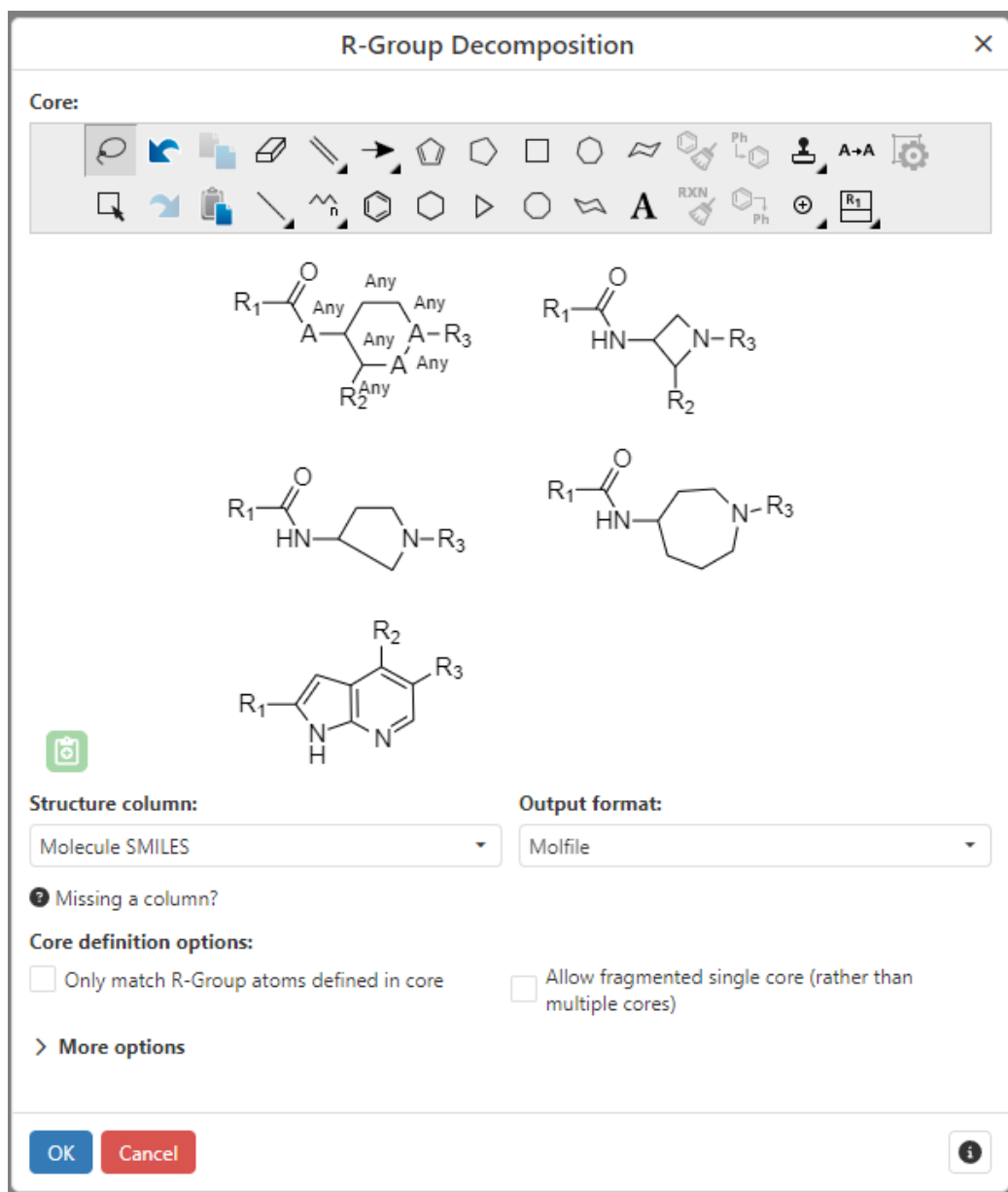


Figure: The R-Group decomposition dialog

Following completion of the R-Group decomposition, a card for the data function is added to the calculations view and the decomposition is visible in the input data table.

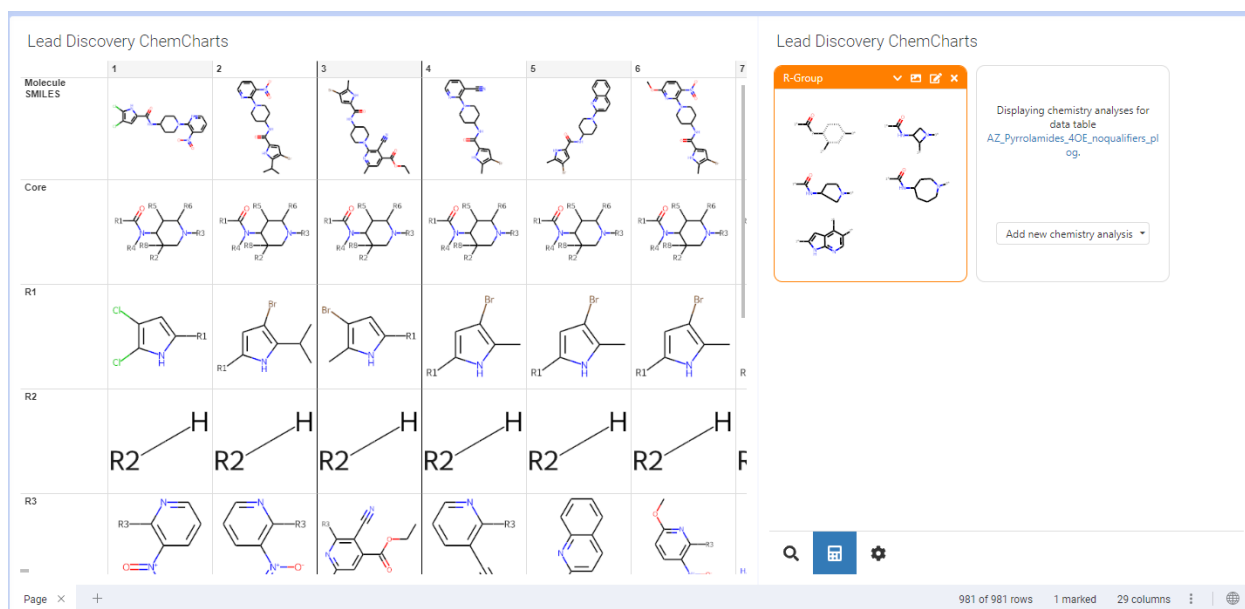


Figure: Completed R-Group decomposition

Scaffold extraction

Reduced and simplified representations of molecules may be created automatically by scaffold extraction calculations. Click the *Scaffold extraction* button in the *New Calculation* control to open the *Scaffold extraction* dialog.

Scaffold extraction ✕

Structure column:

Structure <MOLFILE>
▾

Output column:

Scaffold
▾

Output format:

SMILES
▾

Options:

Remove atom and bond types from scaffolds

OK

Cancel

Figure: The Scaffold extraction dialog.

The default chemistry toolkit performs Bemis-Murcko scaffold extraction. Input structures from which scaffolds will be extracted are taken from the column selected in the *Structure column dropdown* menu. The output column name and output format (SMILES or Molfile) may be set in the *Output column* and *Output format* controls, respectively. An interesting feature of scaffold output in SMILES format is that structures can be grouped together simply by sorting the scaffold column. Canonical SMILES strings may be used as unique structural identifiers, so sorting scaffolds represented as SMILES has the effect of grouping identical scaffolds.

Free-Wilson analysis

Free-Wilson analysis performed machine learning on a data set containing an R group decomposition and compound activities. Every R group in the decomposition is assigned a contribution to compound activity. The predicted activity for every compound is then the sum of the activity contributions for each of the compound's R groups and a constant bias term. Following the Free-Wilson analysis, the R group contributions may be used to predict the activity of new, virtual, compounds.

The Free Wilson analysis creates three new data tables: a *Free Wilson* data table containing input compounds and their activity predictions together with the virtual compounds that have the highest predicted activity; a *Free Wilson R-groups* table that contains all R groups and cores and their contributions to activity; and a *Free-Wilson Properties* table that contains model training and cross-validation statistics.

Free-Wilson analysis may be performed by selecting *Free-Wilson* from the *Add new chemistry analysis* drop down control.

Free-Wilson [X]

Core column:
Core

? Missing a column?

R-Group columns:
R1 X R2 X R3 X

? Missing a column?

Property columns:
SAU Gyr Ki X

Predicted values for 'SAU Gyr Ki' are used to rank enumerated compounds. The top 10000 will be output (see more options).

Extra columns:
External_ID X

∨ **More options**

Max enumerated compounds:
10000

Number of folds for cross-validation:
5

Enumerate ascending (lower property values are better)

Automatically detect log distributions

Exclude compounds with untrained R-Groups from cross validation

Output tables prefix: [] **Output tables suffix:** []

OK Cancel

Figure: The Free Wilson analysis dialog

The Free Wilson dialog is used to select the columns containing the R group decomposition and the activity. The R group analysis may be created using the R group decomposition cheminformatics calculation described above, or any other analysis may be used, assuming that R group core and attachment points are correctly labelled in the input columns. The *Property columns* column selector is used to choose one or more property columns to perform Free-Wilson analysis on. If more than one column is selected predictive models will be constructed for multiple properties, but the property in the first column will be used to rank the enumerated compounds. The *Extra columns* column selector is used to pick other columns in the input table whose values will be copied to the *Free Wilson* output data table for structure rows used in training the models. It is recommended that, if possible, a column containing a

structure identifier is chosen (so that input compounds can be easily identified in the Free-Wilson visuals). On expanding *More options*, the *Max enumerated compounds* field contains an integer specifying the maximum number of enumerated compounds added to the *Free Wilson* output table. If the number of enumerated compounds is larger than the maximum number chosen here, those virtual compounds with the highest predicted property will be retained. For each property for which a Free Wilson model is created N-fold cross validation is performed to gauge the effectiveness of the model for that property. The number of folds is specified in the *Number of folds for cross validation* field. By default the analysis enumerates compounds predicted to have high property values. If it is desired to enumerate compounds with low predicted property values the *Enumerate ascending* checkbox should be selected. Free-Wilson will perform poorly if trained on arithmetic values that are distributed on a log scale, for example if raw Ic_{50} concentrations are used instead of $\log Ic_{50}$ (or pIc_{50}). When *Automatically detect log distributions* is selected a Shapiro–Wilk test will be used to determine if a log transform should be applied to a property prior to performing the analysis. During cross-validation, if a particular R group occurs infrequently in the input table then it may be present in a validation fold but absent from the corresponding training fold. In this case the group will not contribute to predicted activity and a poor cross validation R squared will be seen. To exclude such compounds from the cross validation R squared calculation check *Exclude compounds with untrained R-Groups from cross validation*. Finally, a prefix and or suffix may be added to the name of each of the three output tables via the *Output tables prefix* and *Output tables suffix* fields.

Once the Free Wilson analysis is complete the data function card contains a synopsis of the analysis. Clicking on the *Configure visuals* button will open customized visuals to view the output tables.

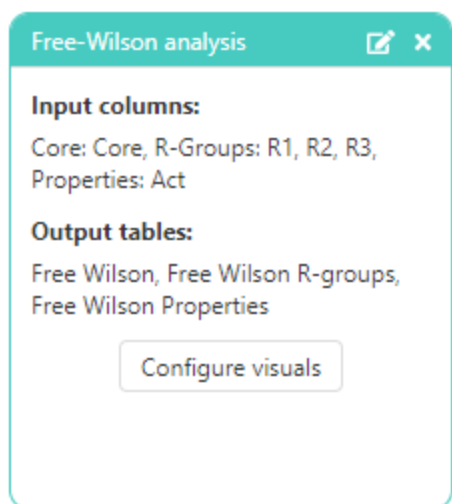


Figure: The Free-Wilson data function card

Preferences

Chemistry Visualization preferences determine the behavior of searches and calculations performed from the visual, in addition to the chemistry handling behavior in other visuals. There are tabs in the Chemistry preferences: *Toolkit preferences*, *Property calculation preferences*, and *Depiction templates*.

Toolkit preferences

Chemistry Visualizations are compatible with multiple cheminformatics toolkits. The default chemistry toolkit, based on RDKit, implements all available search and calculation features. Alternate vendor toolkit implementations exist, and may be selected to override the default chemistry toolkit functionality. Toolkit preferences can be configured on the Toolkit preferences tab in the Chemistry Preferences page.

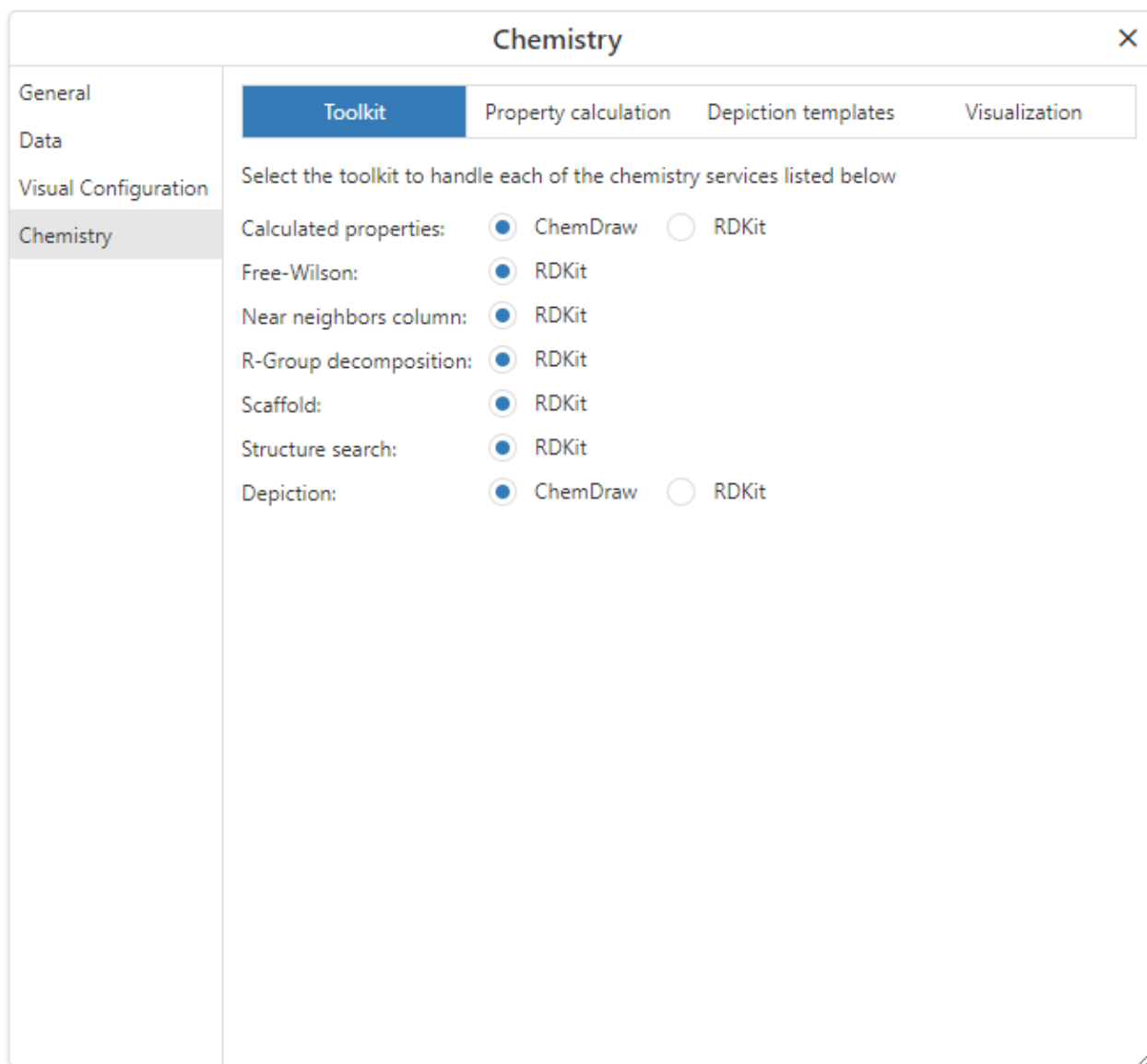


Figure: Toolkit preferences in the Preferences dialog.

Chemistry toolkits available in Spotfire will appear for each feature category if the toolkit implements that feature. It is not a requirement that toolkits implement all features. In the above example, depiction of query structures on the search page of the Chemistry visualization may be performed by any one of three available toolkits. Note that the *Near neighbors* calculation is used by the Neighbor Properties visualization, not directly by the Chemistry visualization.

Chemistry toolkit implementations may differ in the physical property predictions available, and the accuracy of physical property predictions. Chemistry toolkit implementation may also differ in their handling of aromaticity perception and Molfile query features, thereby producing different results for substructure searches. Alternate chemistry toolkits provide the flexibility and extensibility to meet specific demands of the cheminformatics calculations in Spotfire.

Please direct questions regarding availability and licensing of vendor chemistry toolkits to business@glysade.com.

Property calculation preferences

Short-lists containing user-defined lists of calculated properties as described [previously](#) may be created in the *Property calculation preferences* tab. To add a new short-list, click the *Add* button. To edit or delete a short-list, click the caret on the right side of the *Add* button, and select the desired operation. After adding a new short-list, or selecting an existing short-list and selecting *Edit*, checking or unchecking boxes next to each calculated property will immediately update the short-list.

The screenshot shows a window titled "Chemistry" with a close button (X) in the top right corner. On the left is a sidebar with three items: "General", "Data", and "Chemistry". The "Chemistry" item is selected and highlighted. The main area of the window has three tabs: "Toolkit preferences", "Property calculation preferences" (which is active and highlighted in blue), and "Depiction templates". Below the tabs, the text reads "Configure short-lists of calculated properties for the selected toolkit". Under the heading "Short-list:", there is a dropdown menu showing "Default" and an "Add" button with a small downward arrow. Below that, under the heading "Properties:", there is a list of properties, each with a checkbox. The properties and their checkbox states are: "Property name" (unchecked), "Molecular Weight" (checked), "Molecular Formula" (checked), "LogP" (checked), "Hydrogen Bond Donors" (checked), "Hydrogen Bond Acceptors" (checked), "Lipinski Hydrogen Bond Donors" (unchecked), "Lipinski Hydrogen Bond Acceptors" (unchecked), "Rotable Bonds" (checked), "Topological Polar Surface Area" (checked), "Labute Accessible Surface Area" (unchecked), "Amide Bonds" (checked), "Rings" (checked), "Heteroatoms" (checked), and "Heterocycles" (checked).

Depiction templates

Depiction templates are used to standardize the display of chemical structures rendered in Spotfire visuals using coordinates from user-defined substructures. This functionality was formerly only available in the *Align To This Substructure* control in the *Lead Discovery Structure Filter* panel. In contrast, depiction templates in the chemistry visualization allow users to define numerous depiction templates that are applied to all chemical structure columns in a document. To add depiction templates, navigate to the *Depiction templates* tab of the *Chemistry* page in the Chemistry visualization preferences.

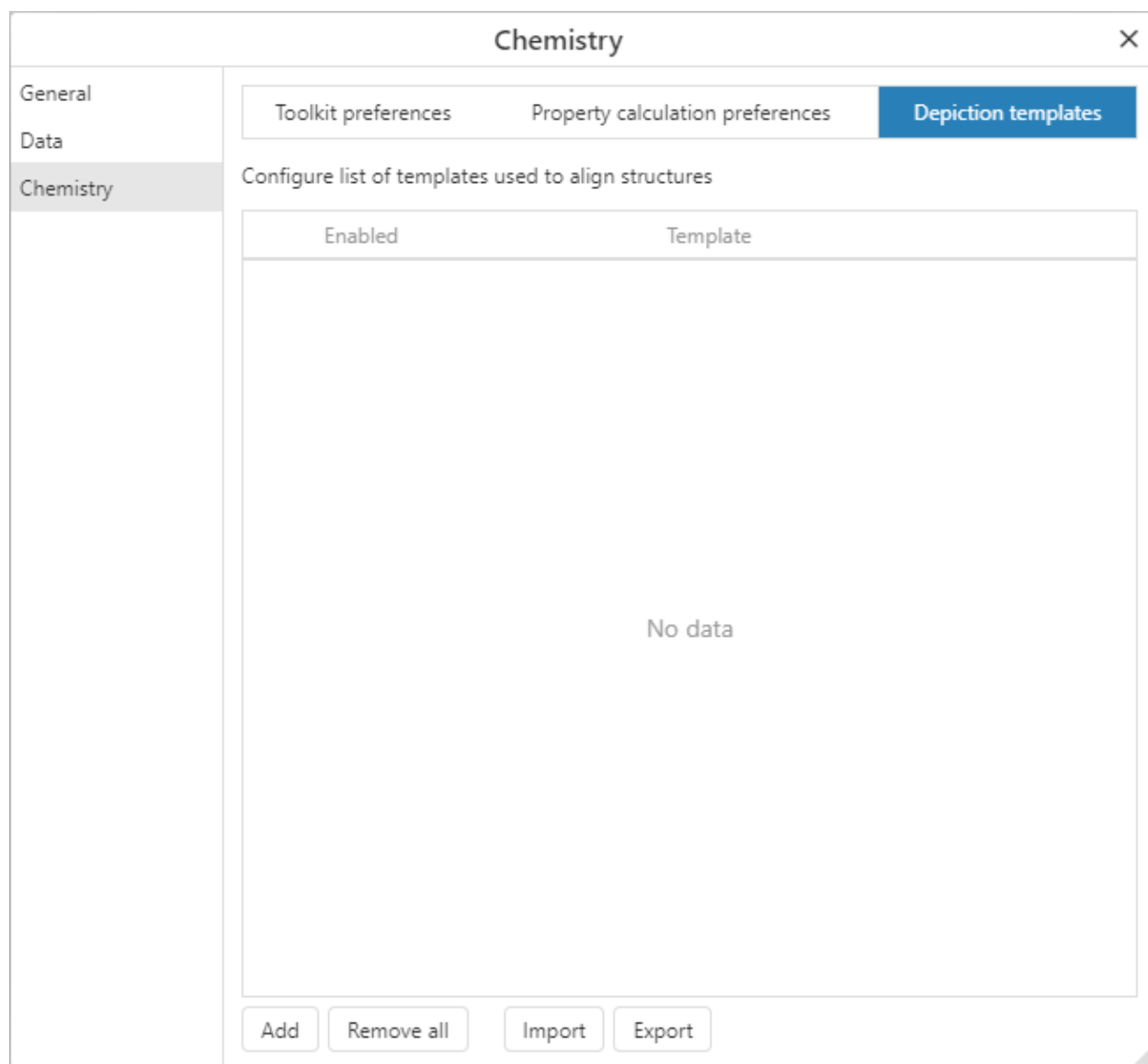


Figure: The Depiction template preferences page.

Use the *Add* button to open a chemical sketcher that can be used to sketch or paste a new depiction template from the clipboard.

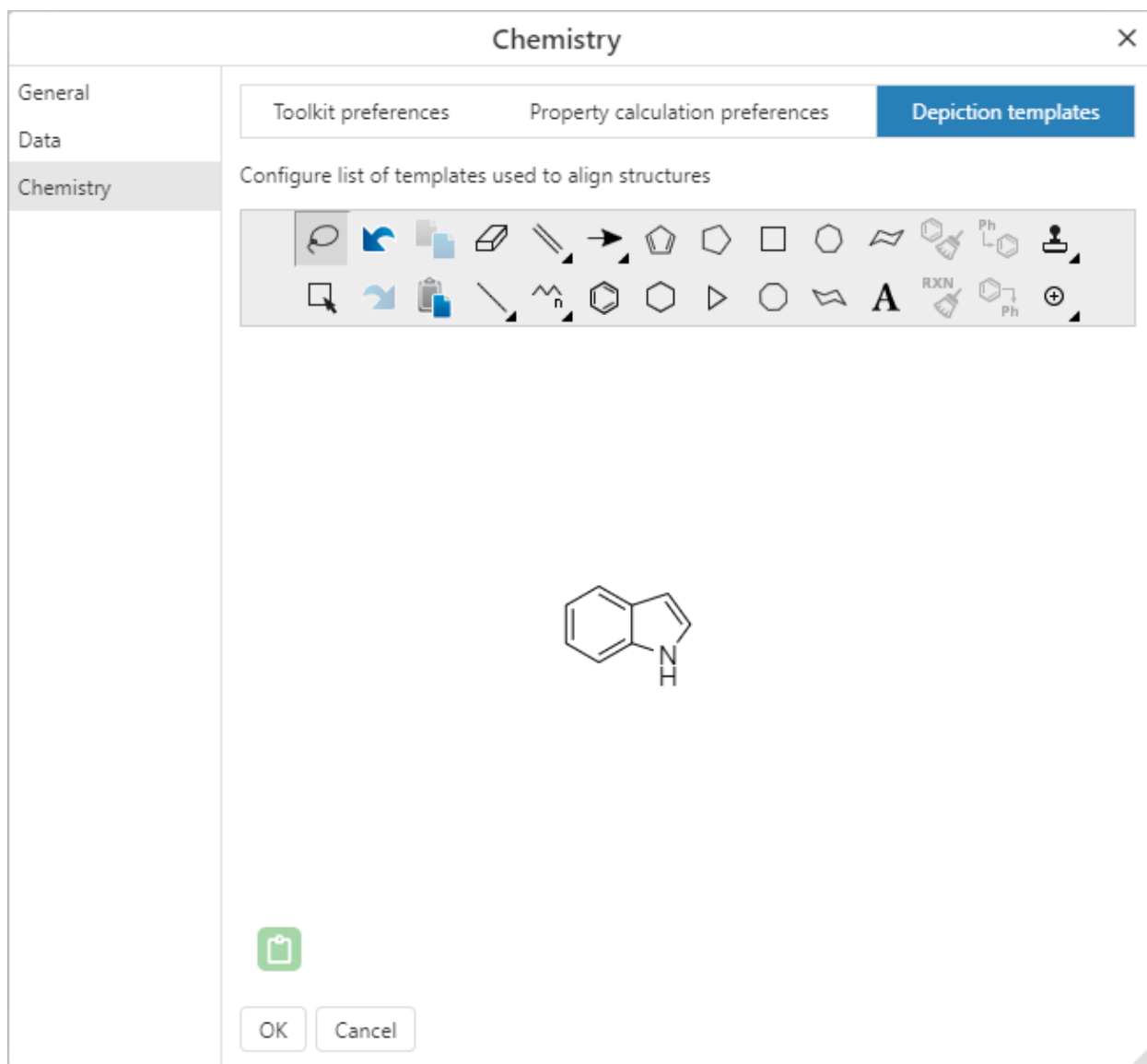


Figure: Adding a new depiction template.

After clicking OK, the new depiction template will appear in the list of saved templates.

Chemistry ✕

General
Data
Chemistry

Toolkit preferences Property calculation preferences **Depiction templates**

Configure list of templates used to align structures

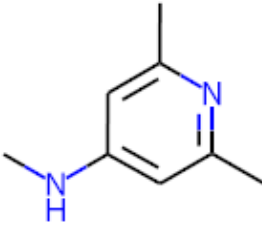
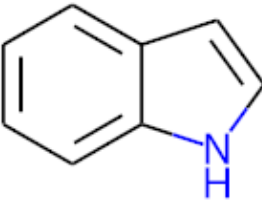
	Enabled	Template	
⋮	<input checked="" type="checkbox"/>		✎ 🗑
⋮	<input checked="" type="checkbox"/>		✎ 🗑
<input type="button" value="Add"/> <input type="button" value="Remove all"/> <input type="button" value="Import"/> <input type="button" value="Export"/>			

Figure: Saved depiction templates.

When structures are depicted, the first depiction template that matches the structure is used. Depiction template list order is therefore important. Specific templates should be added higher in the list, and generalized templates should be added lower in the list. Depiction templates may be reordered by using the *drag-handle* ⋮ on the template and dragging the item higher or lower in the list. Lists of depiction templates may also be imported or exported using the corresponding buttons at the bottom of the page. Substructure alignment based on structure searches in the Chemistry visualization will override depiction template alignment.

Data Functions Visualization

The Lead Discovery ChemCharts Data Functions visualization is used to add, edit, interact with, and remove data functions in a document.

The Data Functions visualization requires a set of data function definitions to be downloaded locally from a data function definition Git repository using ScriptSync. Please refer to the Data Functions section of the ScriptSync User Guide for ScriptSync configuration instructions.

Once ScriptSync has been configured with a data function definition repository, the Data Function visualization will display available data functions:

Lead Discovery ChemCharts

Search... Search tags...

- ▼ Biopolymer
 - Ab Component Analysis
 - Antibody Numbering
 - Blast Local Column Search
 - Blast Local Text Search
 - Blast Table Search
 - Blast Web Search
 - Extract Genbank Regions
 - Identify Enzyme Restriction Sites
 - IG Blastn Local Text Search
 - IG Blastp Local Text Search
 - Multiple Sequence Alignment
 - Pairwise Sequence Alignment
 - Sequence Pattern Match
 - Sequence Regular Expression Match
 - Translate DNA to Protein
 - Translate Sequences (bidirectional)
 - Translate Sequences From All Open Reading Frames
- ▼ Chemistry
 - ADMET Properties
 - Core Decomposition Analysis
 - Deprotect Structures
 - Exact Mass (.NET)
 - Exact Mass (Python)
 - MMPDB Database Search
 - MMPDB Project Search
 - R Group Analysis
 - R Group Decomposition
 - Reaction Matched Pairs
 - Substructure Search Asinex

Visualization tags for Biopolymer functions:

- MAB, sequence, analyze, new
- MAB, sequence, tform, modified
- sequence, search, modified
- sequence, search, modified
- sequence, search, modified
- sequence, search, modified
- sequence, tform, new
- sequence, nucleotide, search, modified
- sequence, nucleotide, search, modified
- sequence, search, modified
- sequence, tform, modified
- sequence, search, modified
- sequence, filter, modified
- sequence, filter, modified
- sequence, nucleotide, tform, modified
- sequence, nucleotide, tform, modified
- sequence, nucleotide, tform, modified

Visualization tags for Chemistry functions:

- PipelinePilot, chemistry, calprop, new
- chemistry, analyze, modified
- chemistry, tform, new
- chemistry, calprop, new
- chemistry, calprop, modified
- chemistry, search, modified
- chemistry, search, modified
- chemistry, analyze, modified
- chemistry, tform, modified
- chemistry, analyze, new
- PipelinePilot, chemistry, search, new

New Results Developer

Figure: The Data Function visualization displaying available data functions.

The list of data functions appears on the left hand side of the body of the visualization. Data functions are organized by category. In the previous Figure, data functions are categorized as either “Biopolymer” or “Chemistry”, depending on the type of data the data function depends on as input, or produces as output. Data function categories are configured in data function definitions, and may appear differently than the previous example if the categories have been

modified. The *Search* text box at the top left of the visualization allows users to search for data functions based on their name.

Data functions may also be searched based on associated tags. Clicking on the *Search tags* selector at the top right of the visualization will display a list of available tags that may be used to filter the data functions displayed.



Figure: Searching data functions by tag

Selecting the 'filter' tag will cause the visualization to only display data functions associated with the filter tag.

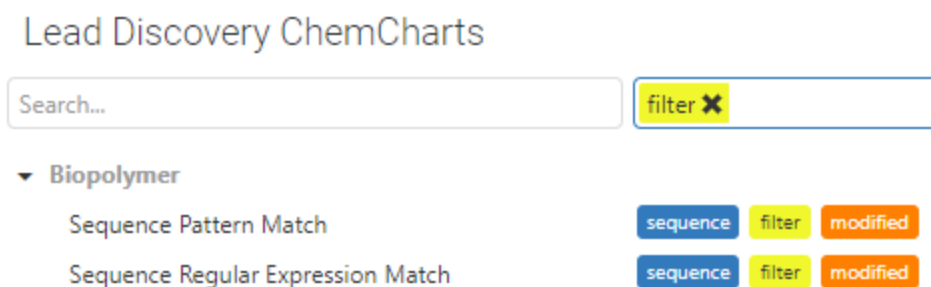


Figure: Searching data functions based on tags

Note that the *new* and *modified* tags are added automatically based on the timestamps of the data function definitions in the repository.

Clicking on the name of a data function will open the input dialog for that data function. For example, clicking on the Exact Mass (Python) data function will open the input dialog shown in the figure below:

Data Function [X]

Exact Mass (Python) chemistry calcpop

Calculates exact mass for structures using Python code in data function definition

Data table

Project Compounds

Select structure column

Structure <MOLFILE>

OK Cancel

Figure: The Exact Mass (Python) data function input dialog.

Data function table and column input selectors will be automatically populated with valid selections, if they exist. Once all required data function fields are configured in the input dialog, click the *OK* button to add a data function to a document. The Data Function visualization will automatically switch to the Results tab after a data function has been added.

Lead Discovery ChemCharts

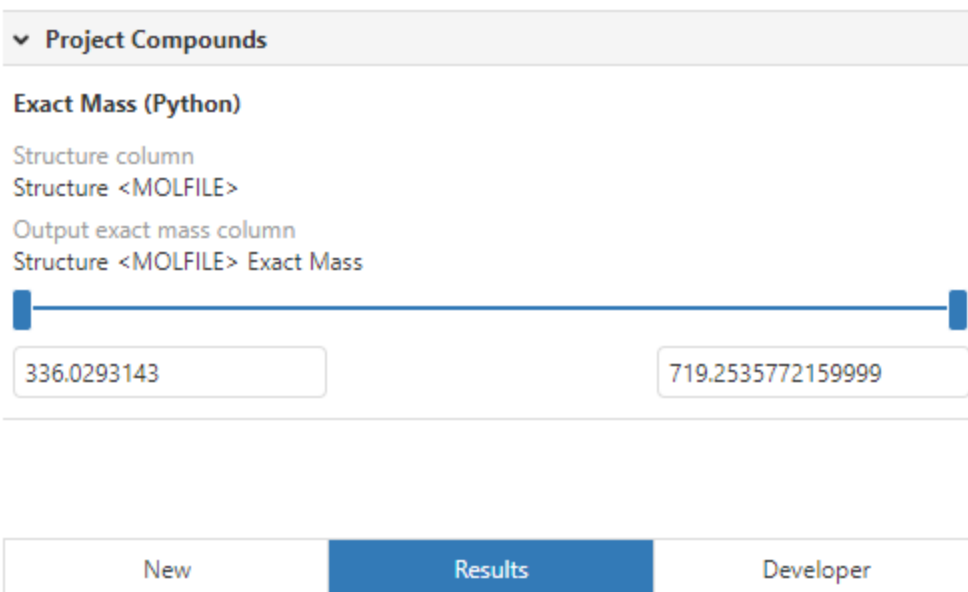


Figure: The Results tab of the Data Function visualization.

The results tab will display all data functions present in a document that have been added through the Data Functions visualization. Data functions are grouped by the data table from which input data is derived. In the above figure, one data function exists in the document, and the exact mass calculation was performed on the “Structure <MOLFILE>” column of the “Project Compounds” data table. Data functions that do not require an input data table will be categorized under the heading “No input data table”.

Expanding a data table heading displays a vertical list of data function output controls. Data function output controls provide information about input and output tables and columns. In the example above, the input “Structure <MOLFILE>” and output “Structure <MOLFILE> Exact Mass” columns are shown in the Exact Mass (Python) output control. Output controls may contain filter controls, as in the above example. The *range filter* in the output control is used to filter the data table on the “Structure <MOLFILE> Exact Mass” output column. Output controls may also include query molecule structures, query sequences, and additional input and output fields associated with a data function.

Additional buttons are displayed in data function output controls when the mouse cursor hovers over the control.

▼ Project Compounds

Exact Mass (Python)



Structure column

Structure <MOLFILE>





Output exact mass column

Structure <MOLFILE> Exact Mass



Figure: Data function output control buttons.

The function of each output control button is described in the following table.

	Run visual configuration script: If a data function has an associated script to configure visualizations specific to view the results, clicking this button will configure visualizations.
	Refresh/run data function: this button will run the data function again using the existing configuration.
	Edit: will open the data function input dialog and allow users to edit input selections and run the data function with the edited configuration.
	Delete: deletes the data function from the document.

Dendrogram Visualization

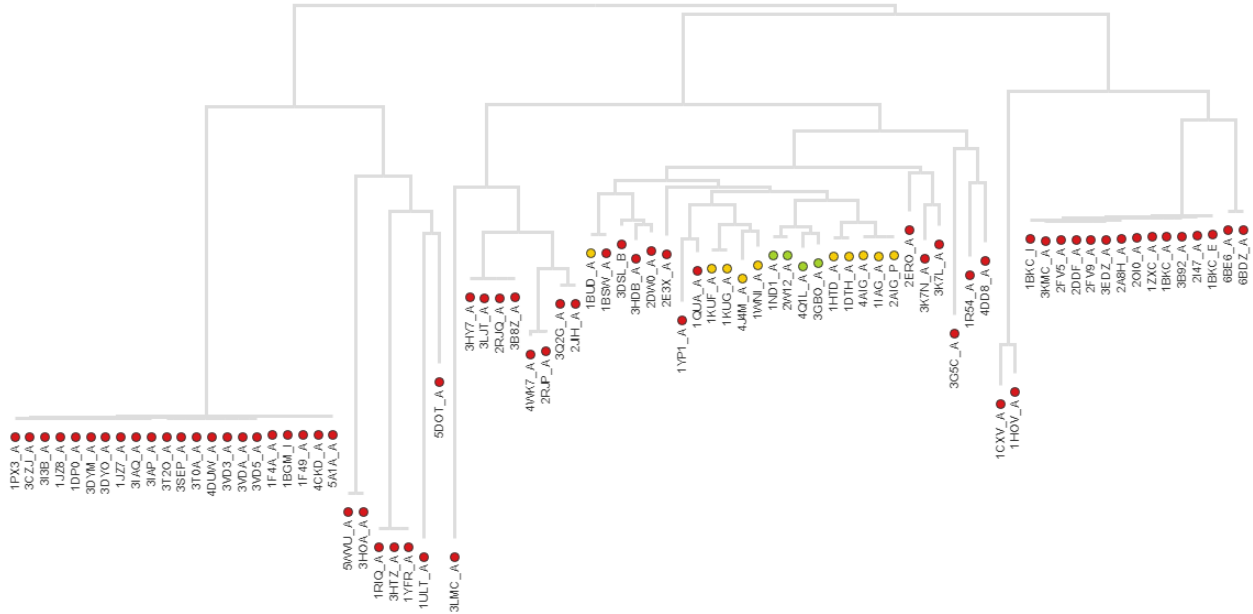
The Lead Discovery ChemCharts Dendrogram visualization is used to view the phylogeny tree produced by a multiple sequence alignment. The dendrogram is always returned as part of the results obtained from the Multiple Sequence Alignment web service defined in Lead Discovery Web Services. The tree is stored as a property of the aligned sequences column returned from the web service.

The Dendrogram visualization has the following features:

- The dendrogram can be displayed vertically, horizontally or radially.
- Color rules can be displayed on the leaf nodes of the dendrogram.

- Zoom and pan around the dendrogram.
- Active row/item highlighting is supported.
- Branch and leaf nodes can be marked.
- The dendrogram updates to display the current filtering state where paths and nodes in the dendrogram are grayed out if they do not pass through the filter.

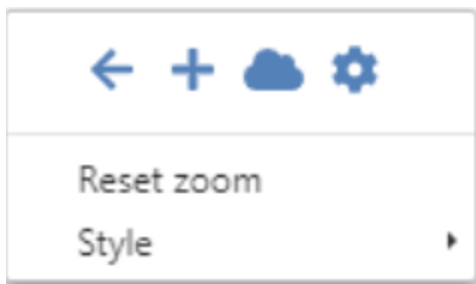
The following is an example of the Dendrogram visualization:



A screen shot of the Dendrogram visualization. In this case a vertical dendrogram is displayed.





Context menu

Much of the functionality of the Dendrogram visualization is accessed through the context menu. The context menu is opened by right clicking anywhere in the visual. An example of the context menu for the Dendrogram visualization is show below in the figure below:




Screenshot of the context menu for the Dendrogram visualization.

The list below describes each context menu item:

	Back: returns the user to the visualization 'home' page where the user can select a different visualization or data table to display in the current ChemCharts visualization.
	Add visualization: adds a new ChemCharts visualization to the current page. Used primarily in the web player.
	Web services: opens the web services dialog.
	Properties: opens the Properties dialog.
Reset zoom	Resets the display of the dendrogram to fit within the bounds of the visualization
Style	Opens the "Style" submenu. Used to select horizontal, vertical, or radial style dendrograms.

The following sections detail how to configure and interact with the Dendrogram visualization.

Create a Dendrogram visualization

Click the New Lead Discovery ChemCharts button  in the list of Spotfire visualizations. A new Lead Discovery ChemCharts visualization will be added to the page. Select Dendrogram in the dropdown menu of available visualizations on the ChemCharts home page. The column containing the dendrogram in the current data table will be automatically detected, if present.

Zoom and pan the dendrogram

Use the mouse wheel or shift + mouse drag to zoom in and out of the dendrogram. The dendrogram can be panned by moving the mouse while holding the left mouse button down.

Resize the space for leaf node labels

It is possible to resize the space available for leaf node labels for each style of dendrogram. This can be carried out by using the mouse wheel with the alt key or by opening the [Properties dialog](#) and entering the desired value in the Max leaf label size number box.

Change the style of the dendrogram

There are three possible styles for the dendrogram. To change the style, right-click to produce the context menu and choose the style from the Style sub menu. Alternatively, open the [Properties dialog](#) and select the style from the Style radio buttons.

Marking

The dendrogram can be marked by clicking on nodes. If a branch node is clicked then all the child nodes beneath the selected nodes will be marked. If a leaf node is marked the label for the node will be highlighted. Users can extend or toggle marking using the shift and ctrl key modifiers while left-clicking. An example of a dendrogram with marking applied is shown in the figure below.

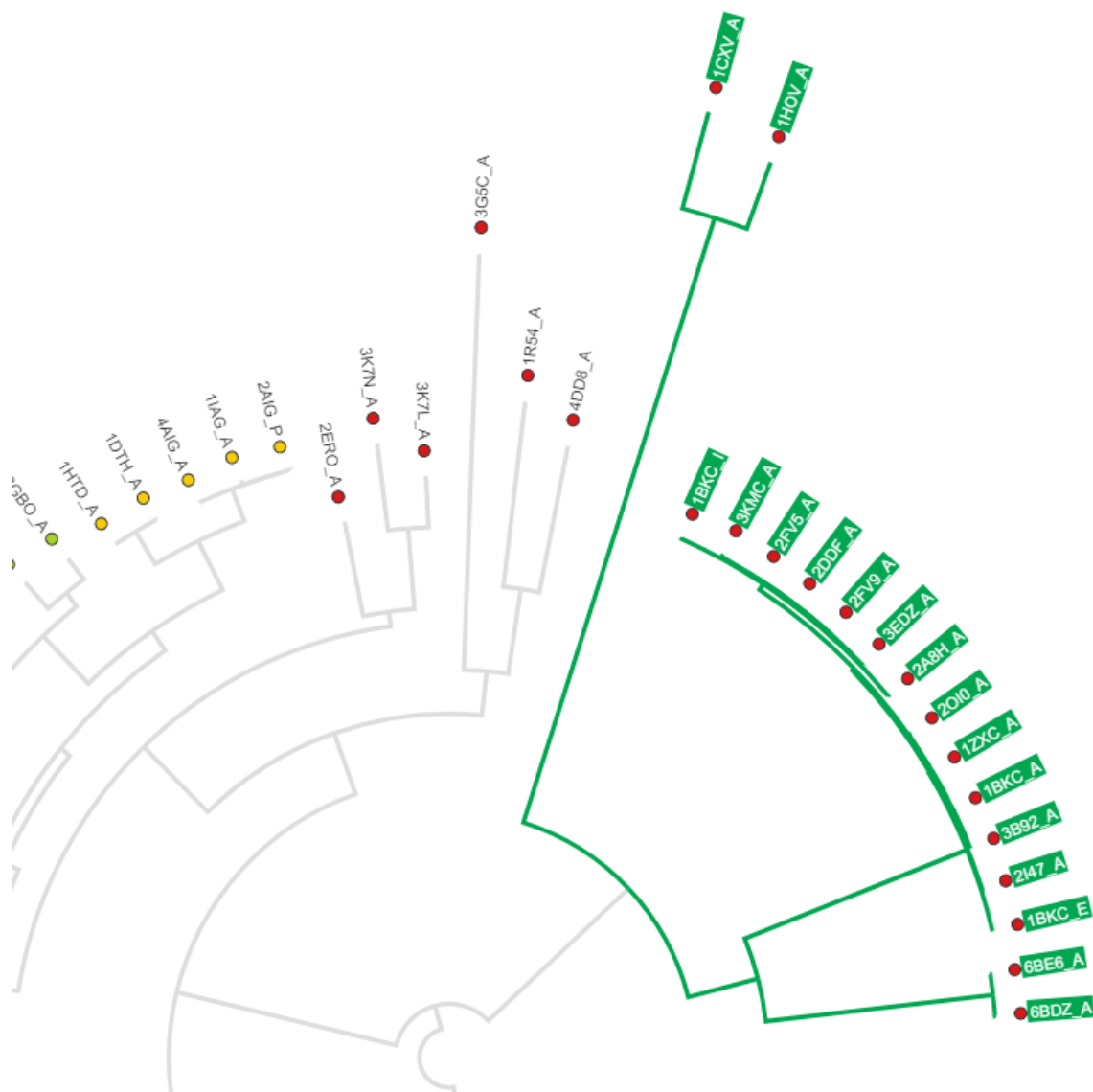



Figure: Dendrogram visualization with marked rows.

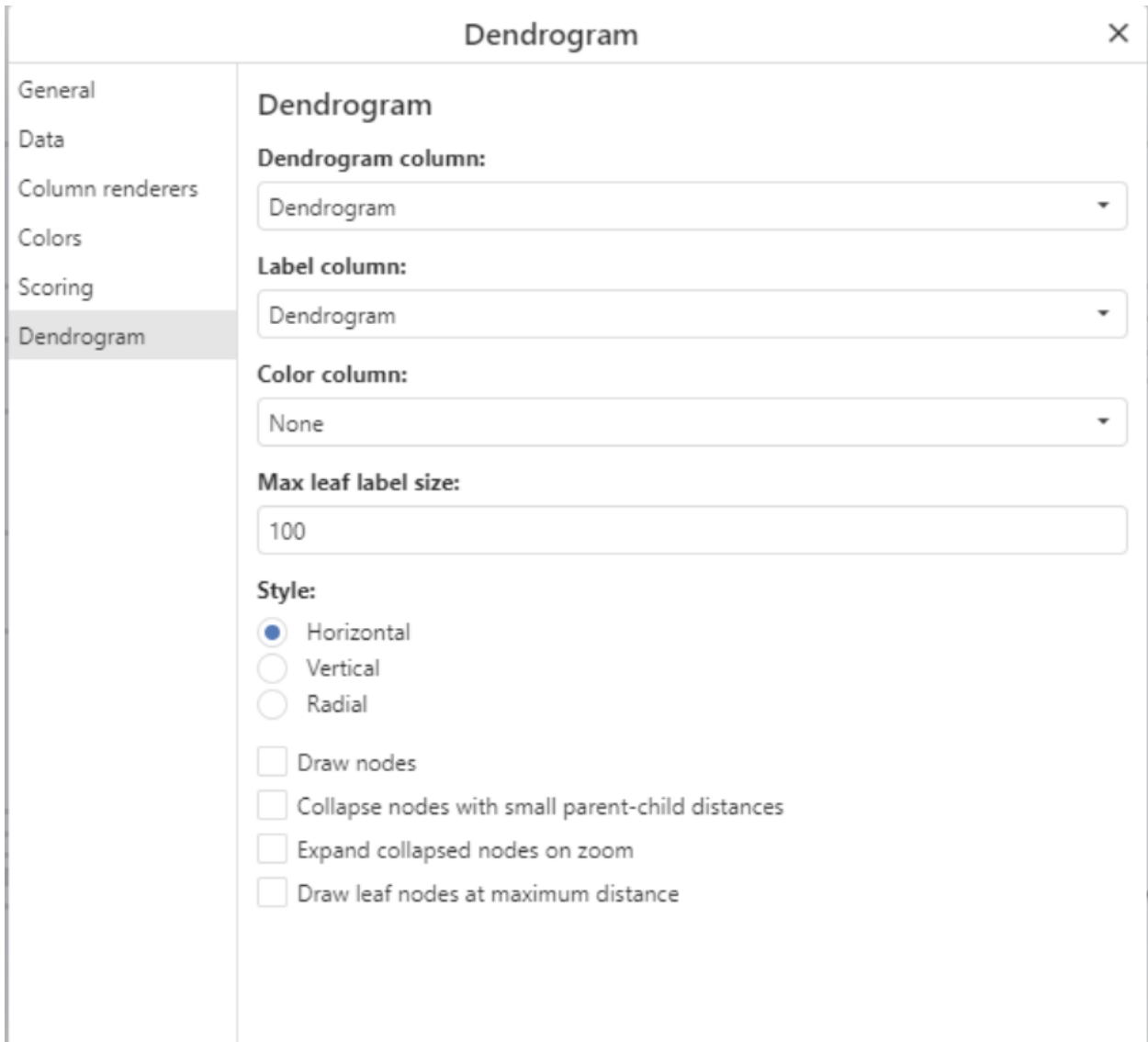
Applying color rules

Color rules defined for the dendrogram are used to determine the display color of leaf nodes. In order to apply color rules to the dendrogram, a color rule must be defined for a column in the

configured data table. Next, the column to which the color rule was applied must be selected in the Dendrogram visualization. To select the color column, open the [Properties dialog](#) from the context menu, and navigate to the Dendrogram tab. The *Color column* may be selected from the drop down in the dialog. See the [Coloring](#) section for additional information.

Dendrogram Properties

Many chart specific settings are configured in the Properties dialog. To access the Properties dialog, open the content menu by pressing the right mouse button and click the *Properties*  button. After the dialog opens, click the *Dendrogram* tab on the left panel to configure Dendrogram visualization specific options.



Dendrogram [X]

General
Data
Column renderers
Colors
Scoring
Dendrogram

Dendrogram

Dendrogram column:
Dendrogram

Label column:
Dendrogram

Color column:
None

Max leaf label size:
100

Style:

- Horizontal
- Vertical
- Radial
- Draw nodes
- Collapse nodes with small parent-child distances
- Expand collapsed nodes on zoom
- Draw leaf nodes at maximum distance

Figure: Dendrogram visualization properties.

Details Visualization

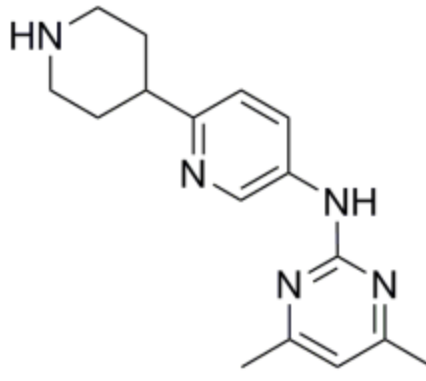
The Details visualization is designed to display a subset or all of the information for the active row/item or a set of marked rows/items from another visualization. An active item is typically a row, point or some graphical object in Spotfire that is under the mouse pointer. As the user moves the mouse around a visualization, the details visualization should update to display the information for the active item. If multiple rows/items are marked, *VCR* buttons will appear at the bottom of the details visualization that allow the user to page through the marked rows. This visualization makes use of the Form Editor that allows the user to arrange and customize various widgets used to display data.

The Details visualization has the following features:

- Create layouts made up of various widgets (text, tables, molecule images, charts) using the Form Editor.
- Multiple forms can be created for a single Details visualization. Users may select from a list of pre-defined forms to alter the data display layout of the Details visualization.
- Coloring rules are applied to the display when possible.
- Displays either the active item, or the data from a set of marked items with *VCR* buttons to page through the data.

A screen shot of the details visualization is shown in the following figure:

Lead Discovery ChemCharts



Code	MBX000280
Salt	-
Parent_MW	283.38
MW	283.38
Salt_MW	-
Name	4,6-dimethyl-N-[6-(piperidin-4-yl...
StereoComment	None
cLogP	1.45
HBA	5
HBD	2
Rot_Bonds	3
TPSA	62.73
Heavy_Atoms	21
N+O	5

Figure: A screenshot of the Details visualization.

Context menu

Much of the functionality of the Details visualization is accessed through the context menu, which is opened by right clicking anywhere in the visual. An example of the context menu for the Details visualization is shown in the figure below.

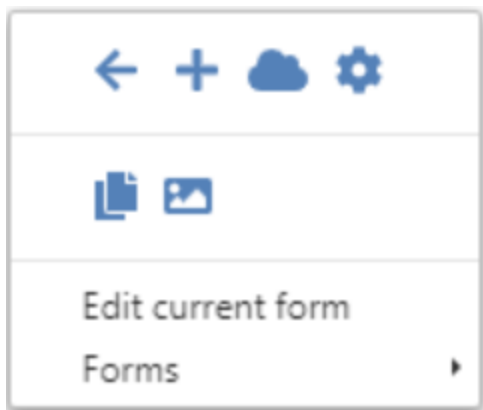









Figure: The Details visualization context menu.

The list below describes the function of each item in the context menu.

	Back: returns the user to the visualization 'home' page where the user can select a different visualization or data table to display in the current ChemCharts visualization.
	Add visualization: adds a new ChemCharts visualization to the current page. Used primarily in the web player.
	Web services: opens the web services dialog.
	Properties: opens the Properties dialog.
	Copy: The context menu Copy command will vary depending on the visualization in which it is contained. In most cases a tab delimited set of data will be copied on to the clipboard for the marked data in the visualization. In some cases the context menu Copy entry will be a sub menu, allowing the user to copy data to the clipboard in different formats.
	Tooltips: Enables or disables tooltips, including user-defined form tooltips. See Tooltips .
Edit current form	Switches the visualization to form editor mode.
Forms	If multiple forms (layouts) have been created for the current visualization, the user can switch between them by selecting a predefined form layout from this sub-menu.

Create a Details visualization

Click the New Lead Discovery ChemCharts button  in the list of Spotfire visualizations. A new Lead Discovery ChemCharts visualization will be added to the page. Select Details in the dropdown menu of available visualizations on the ChemCharts home page. A default layout will automatically be generated based on the columns configured for the Details visualization.

Form configuration

The current form used to display data can be edited by right-clicking on the visualization to open the context menu, then selecting *Edit current form*. The visualization will display the [Form Editor](#) where the user can add/remove and arrange the controls making up the form as they see fit. Once form editing is complete, click *Save and return* to exit the form editor and return to the standard Details visualization

Switching between forms

Multiple forms may be configured for a visualization that contain forms. See the [Form Editor](#) section for instructions on how to configure each form. To switch between forms, click the right mouse button to open the context menu and select the desired form from the Forms sub-menu.

Coloring

Open the visualization Properties dialog, select the *Coloring* tab and use the controls to configure the coloring. See the [Coloring](#) section for additional information.

Distributions Visualization

The Lead Discovery ChemCharts Distributions visualization is used to display individual value and grouped numeric data. For example, a user could create a Distributions visualization that shows the distribution of activity data when grouped by hydrogen bond acceptor count. The distributions may be depicted as box/bar plots, notched box/bar plots or violin plots. Below is a list of how statistical features of the distributions are drawn. Unless otherwise stated, these are displayed with each plot type.

- The median value is denoted by a dark horizontal line.
- The outliers are displayed as circles.
- The interquartile range (IQR) is depicted using a rectangle around the median.
- The whiskers in the bar and notched bar plots are drawn at the lower quartile minus 1.5 IQR, and the upper quartile plus 1.5 IQR.
- The notched bar plot displays the 95% confidence interval around the median using notches in the rectangles.
- The violin plot also displays the distribution of the data as both a histogram and a smooth distribution.

The Distribution visualization also displays statistical data about the distributions for each grouping in a table. Distributions can be marked by dragging the mouse and the visualization will react to marking from other visualizations in the expected way. Additionally, the Distributions visualization will update according to the current filtering state. A screen shot of the Distributions visualization is shown below in the following figure.

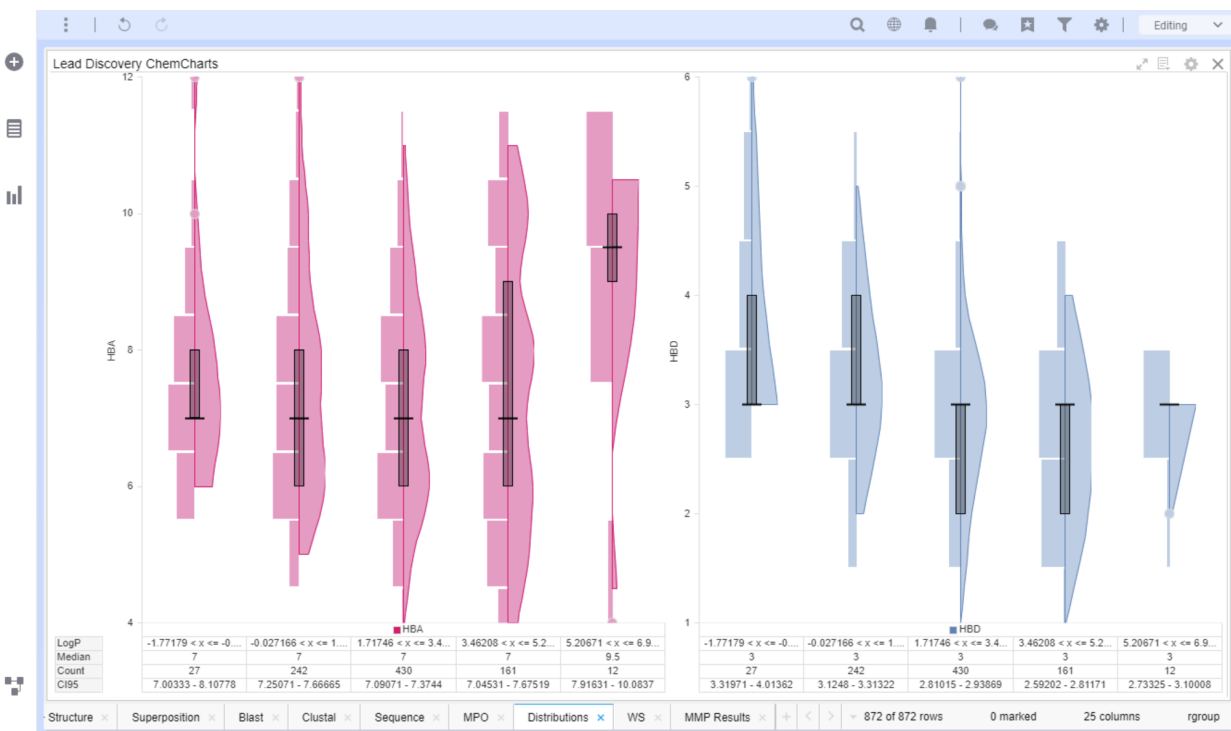


Figure: The Distributions visualization.






Context menu

As with all the visualizations in Lead Discovery ChemCharts, much of the functionality of the Distributions visualization is accessed through the context menu, which is opened by right clicking anywhere in the visual. An example of the context menu for the Distributions visualization is shown below in the next figure.




Figure: The Distribution visualization context menu.


The list below describes each context menu item:

	Back: returns the user to the visualization 'home' page where the user can select a different visualization or data table to display in the current ChemCharts visualization.
	Add visualization: adds a new ChemCharts visualization to the current page. Used primarily in the web player.
	Web services: opens the web services dialog.
	Properties: opens the Properties dialog.
	Limit by marking: toggles the limit by marking behavior of the visualization

Create a Distribution visualization

Click the New Lead Discovery ChemCharts button  in the list of visualizations in Spotfire. A new Lead Discovery ChemCharts visualization will be added to the page. Select Distributions in the dropdown menu of available visualizations on the ChemCharts home page.

Open the Distributions Visualization Properties dialog

Right click to open the context menu and click the *Properties*  button. Visualization specific settings will be found in the Distribution page of the Properties dialog.

Select the chart type

[Open the Distributions visualization Properties dialog](#), click the *Distribution* tab, then click the *General* tab in the *Distribution* property page. The chart type may be selected: *None*, *Bar*, *Notched*, *Violin* or *Violin and histogram*. Only selected statistics are displayed if chart type *None* is selected.

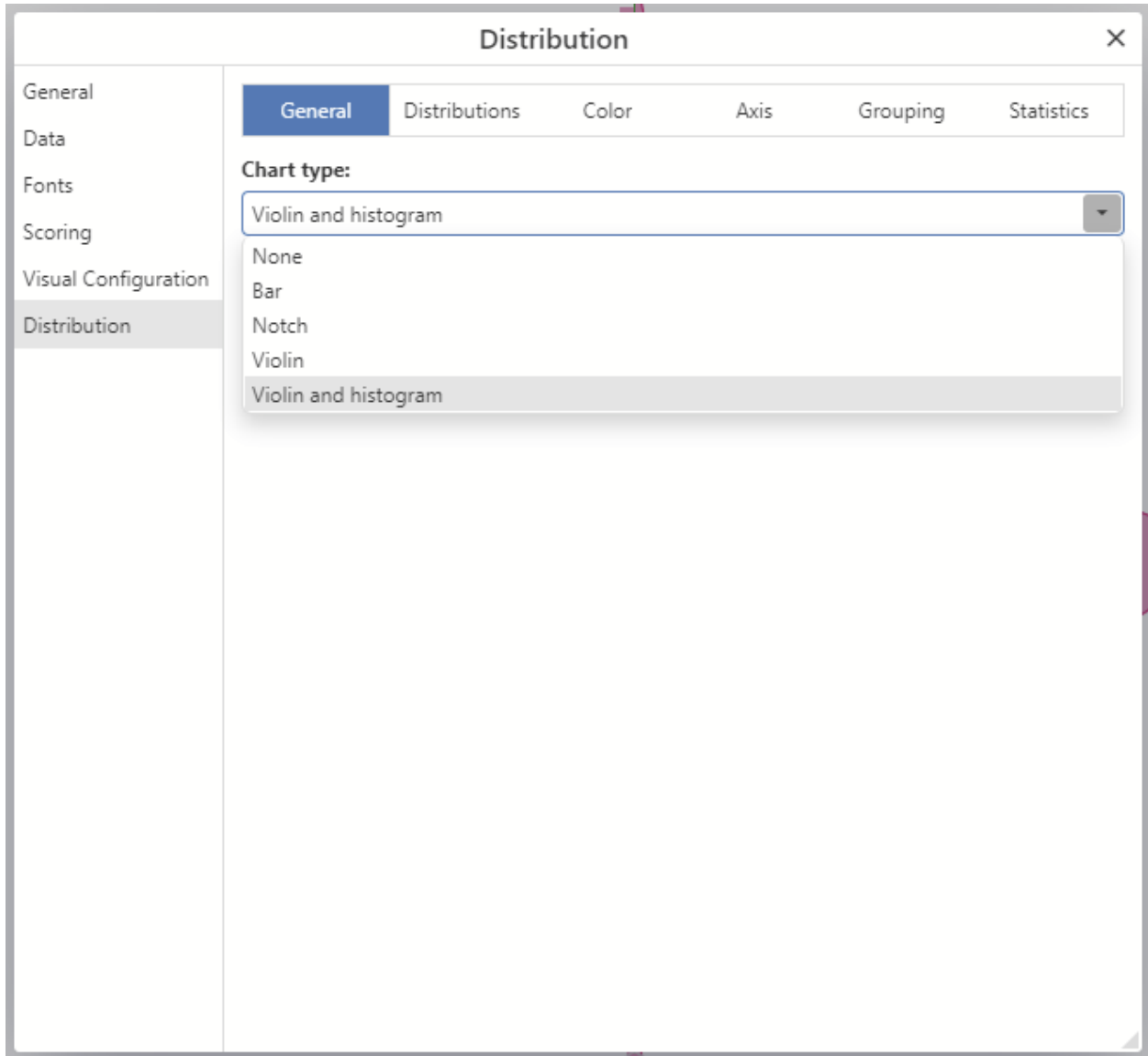


Figure: Selecting the chart type for a Distribution visualization.

Edit the distribution settings

Editing the distributions settings allows the user to select the columns from which distributions are created. [Open the Distributions Visualization Properties](#) dialog and click the *Distributions* tab in the *Distribution* property page. Here the user can select one or more of the numeric columns from the data table that are to be displayed as grouped distributions in the Distributions visualization from the *Display distributions for the following columns* column selector. Users can also order the distributions by dragging and dropping the corresponding columns.

Edit the color settings

The color for each of the distributions can be configured on the *Color* tab in the distribution property page. Here the columns that are currently displayed as distributions are listed along with a color picker that the user can use to configure the color of the eac distribution.

Edit the axis settings

Distributions may either be plotted using a single axis that encompasses all values for all selected columns, or with an axis per-column. Users can edit the settings for the axes in the *Axis* tab in the distribution property page.

The minimum and maximum values for axes may be altered using the min and max *Range* text boxes to the right of each column listed. If a single axis is selected, the minimum and maximum values for the single axis may be altered in the same fashion. Clicking the *Log* checkbox will create distributions by applying the base 10 Log function to column values. By default, the minimum and maximum axis values are displayed at the bottom and top of the chart respectively. Clicking the *Invert* checkbox inverts the axis such that the minimum value is at the top of the chart and the maximum value is at the bottom.

If the minimum and maximum are determined automatically, by default, these are set to the bounds defined by the contents of each column before filtering. As such, when filters are applied to the data set, the bounds of the axes for the distributions will not change. Clicking the checkbox to the left of the *Range* text boxes will alter this behavior such that the automatic bounds are determined after filtering. Note that if values are entered for the minimum and maximum values, this setting has no effect.

By default if an empty grouped distribution is created, it is omitted from the chart. This behavior can be altered by checking the Display empty check box which will result in distributions of empty values being displayed in the chart.

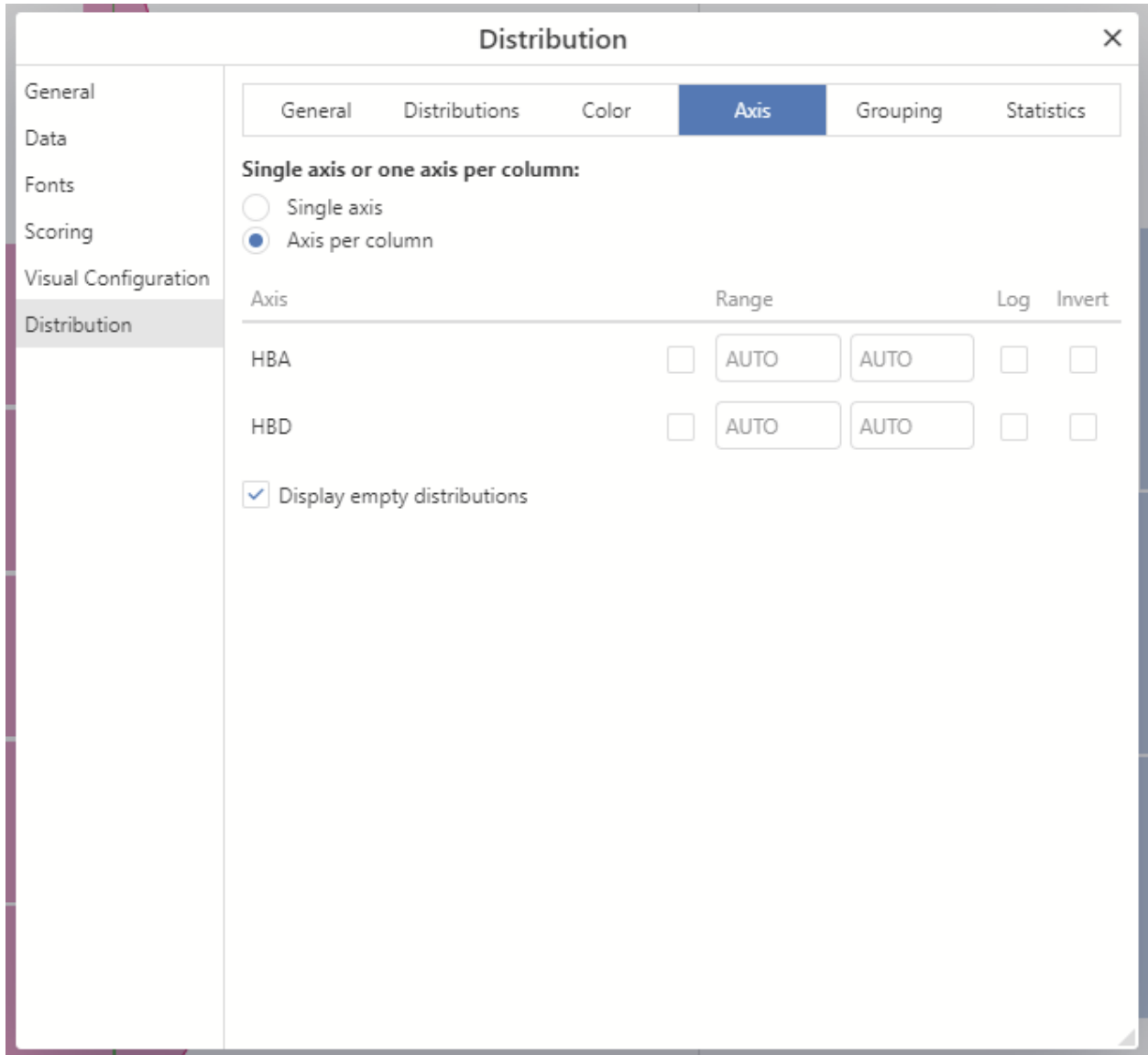


Figure: Configuring the axes for a Distribution visualization.

Edit the grouping settings

Editing the grouping settings allows the user to create per-group distributions for each column configured for distribution display. [Open the Distributions Visualization Properties](#) dialog and click the *Grouping* tab in the *Distribution* property page. Here the user can select a column from the data table that is used to group values, with a distribution displayed for each group. If the column is numeric, either *Automatic binning* or *Manual binning* may be selected. The user may enter *Min* and *Max* values for the selected *Group distributions by column* and the number of bins. All rows that fall within the range of binned values are considered a group, and a distribution is displayed in the Distribution visualization per-group.

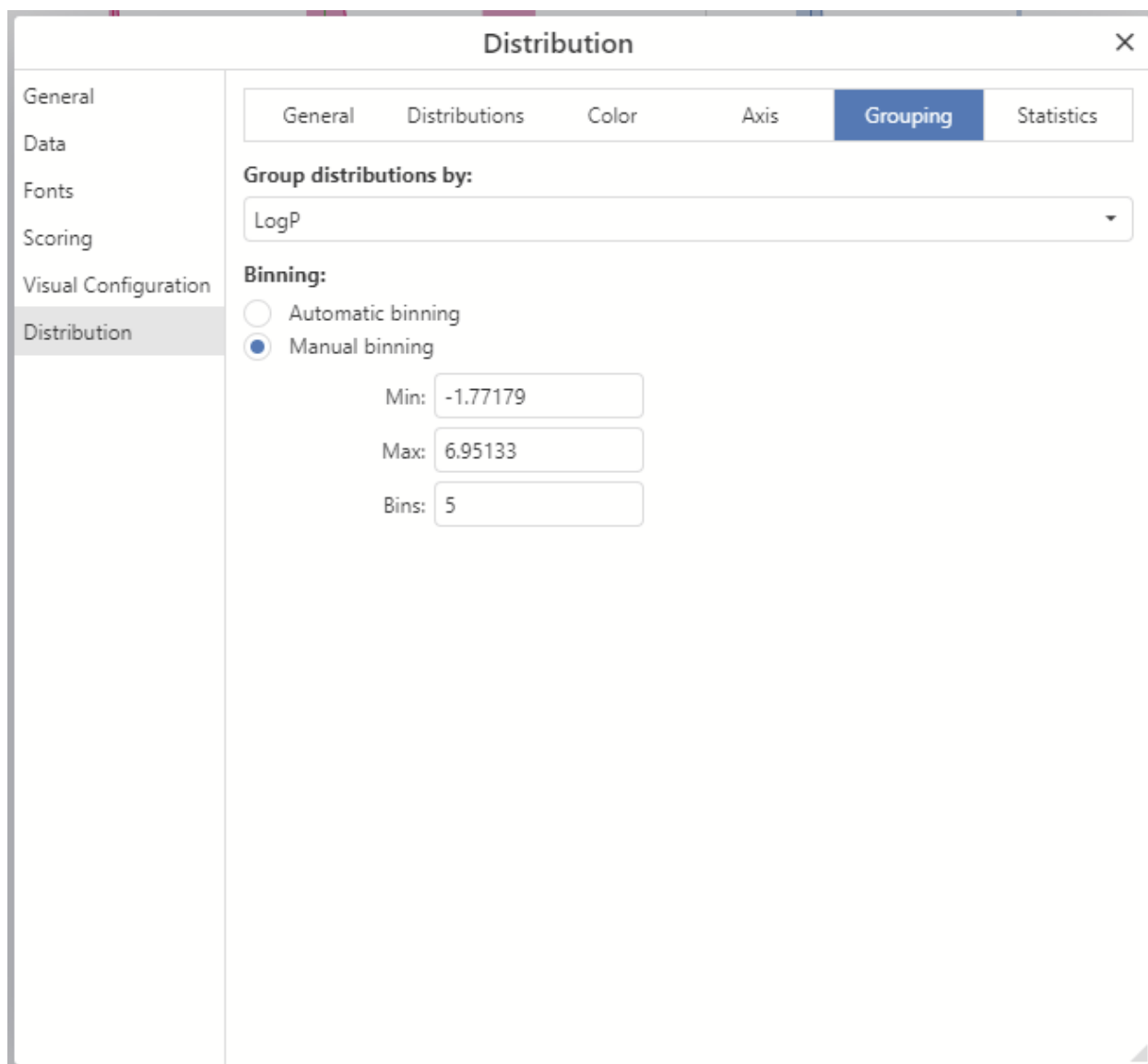


Figure: Configuring the grouping for a Distribution visualization.

Edit the displayed statistics

Editing the displayed statistics alters the statistics displayed under each distribution in the Distribution visualization. [Open the Distributions Visualization Properties](#) dialog and click the *Statistics* tab in the *Distribution* property page.

There is a large set of statistics that can be displayed in the table at the bottom of the Distributions visualization. By default these are: Count and Median. To include additional statistics in the Distribution visualization, click the checkbox next to the desired statistic. The set of available statistics are described in the table below.

Statistic	Description
Mean	Arithmetic mean of the dataset.
Median	The value separating the higher half of the dataset from the lower half.
Minimum	The minimum value in the dataset.
Maximum	The maximum value in the dataset.
Count	The number of values in the dataset.
Q1	The first quartile.
Q3	The third quartile.
IQR	The interquartile range.
Variance	The sample variance of the dataset.
StdDev	The sample standard deviation of the dataset.
StdErr	The sample standard error.
CI90	The 90% confidence interval of the dataset.
CI95	The 95% confidence interval of the dataset.

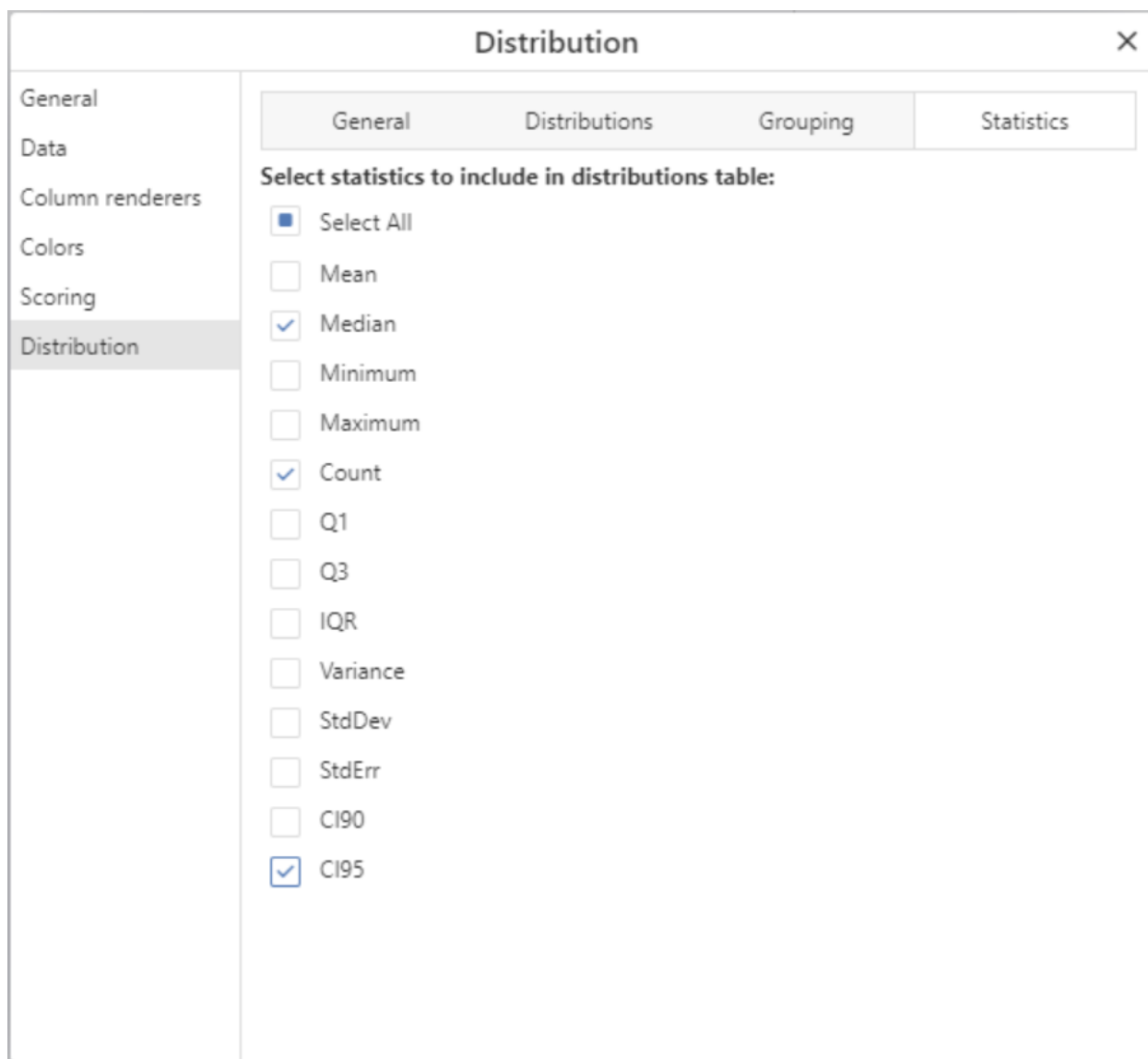


Figure: Configuring the statistics table for a Distribution visualization.

Gallery Visualization

The Lead Discovery ChemCharts Gallery visualization is used to display a set of items (or cards). Cards are composed of a set of controls, where each control displays data taken from a row in a Spotfire data table. The controls can be simple pieces of text, small graphical displays or molecule depictions. The layout of the controls in the gallery item is fully configurable and can be achieved using the [Form Editor](#). The gallery visualization interacts with Spotfire in the expected manner:

- Clicking a gallery item will mark it.
- Hovering over a gallery item will set the active item. The active item will be highlighted in other open visualizations in Spotfire.

- The gallery items can be sorted by the values in up to 3 columns from the underlying data table.
- The data displayed in the gallery can be limited by one or more markings from other visualizations (see single click [Limit by Marking](#)) or by applying one or more of the many possible Spotfire filters.
- If coloring rules are defined, they are used to set the background color of gallery controls.

Lead Discovery ChemCharts

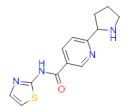
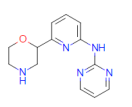
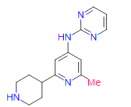
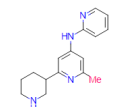
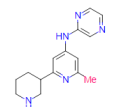
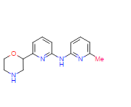
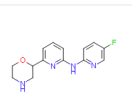
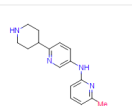
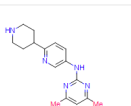
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Figure: Lead Discovery ChemCharts Gallery visualization.

Context menu

As with all the visualizations in Lead Discovery ChemCharts, much of the functionality of the Gallery visualization is accessed through the context menu, which is opened by right clicking anywhere in the visual. An example of the context menu for the Gallery visualization is shown in the next figure.

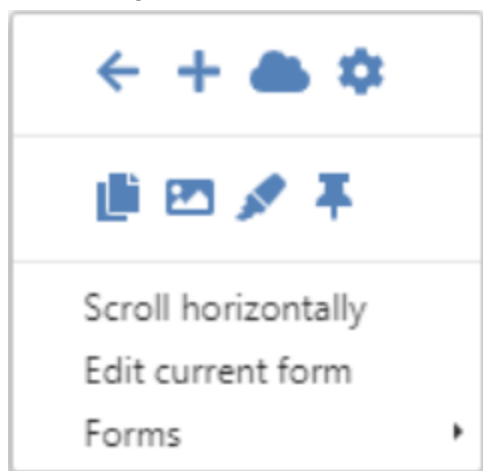











Figure: Lead Discovery ChemCharts Gallery visualization context menu.

The list below describes the function of each item in the context menu:

	Back: returns the user to the visualization 'home' page where the user can select a different visualization or data table to display in the current ChemCharts visualization.
	Add visualization: adds a new ChemCharts visualization to the current page. Used primarily in the web player.
	Web services: opens the web services dialog.
	Properties: opens the Properties dialog.
	Copy: The context menu Copy command will vary depending on the visualization in which it is contained. In most cases a tab delimited set of data will be copied on to the clipboard for the marked data in the visualization. In some cases the context menu Copy entry will be a sub menu, allowing the user to copy data to the clipboard in different formats.
	Tooltips: opens the tooltips control for the visualization.
	Limit by marking: toggles the limit by marking behavior of the visualization
	Fix item: toggle whether an item is fixed or unfixed (see Fixed items).
Scroll horizontally/vertically	Toggle between horizontal or vertical scrolling
Edit current form	Allows the user to edit the form that is current being used to display data using the Form Editor .
Forms	Opens the "Forms" submenu. Used to select a predefined form for display.

The following sections detail how to configure and interact with the Gallery visualization.

Create a Gallery visualization

Click the New Lead Discovery ChemCharts button  in the list of visualizations in Spotfire. A new Lead Discovery ChemCharts visualization will be added to the page. Select Gallery in the dropdown menu of available visualizations on the ChemCharts home page.

Sorting

Open the *Properties* dialog, select the Sorting page and use the controls to configure the sorting. Up to 5 columns can be used to sort the data. See the [Sorting](#) section for more information.

Coloring

Open the *Properties* dialog, select the Coloring page and use the controls to configure the coloring. See the [Coloring](#) section for more information.

Configuring Tooltips

Open the *Properties* dialog and select the Tooltips tab. Click the checkbox next to *Tooltips enabled* to enable or disable tooltips. Form based tooltips may be configured for use in a visualization. See the [Tooltips](#) section for more information.

Limit by marking

Limit by marking can be enabled or disabled by clicking the *Limit by marking* button on the left hand side. See single click [Limit by Marking](#) for additional information.

Form configuration

The current form used to display data can be edited by right-clicking on the visualization to produce the context menu and selecting Edit current form. The visualization will display the [Form Editor](#) where the user can add/remove and arrange the controls making up the form as they see fit. Once form editing is complete, click *Save and return* to apply changes to the form and return to the Gallery visualization, which should now be using the modified form.

Switching between forms

Multiple forms may be configured for visualizations that contain forms. See the [Form Editor](#) section for instructions on how to configure each form. To switch between forms, click the right mouse button to open the context menu and select the desired form from the Forms sub-menu.

Fixed items

Comparing items in a Gallery visualization may be aided through the use of fixed rows. Items may be fixed at the top of the Gallery visualization by right clicking over a row to open the context menu and selecting the Fix item menu option. Fixed items are duplicate copies with a fixed position at the top of the Gallery visualization.

Find

The gallery visualization has the same text search capabilities as found in the table visualization and works in a very similar way. See [here](#) for more details. The slight difference is that the highlighting of matches is not as exquisite as the table visualization and, as such, the entire gallery item is highlighted to indicate a match, rather than the exact cell.

MMP Filter Visualization

The Lead Discovery ChemCharts MMP Filter visualization is used to assist users in finding desired transformations in the results from the MMP Database Search web service. Upon retrieving results from an MMP Database Search, if the *Automatically configure visualizations* option is selected from the dialog, the MMP Filter visualization will be configured automatically along with additional visualizations for viewing the results.

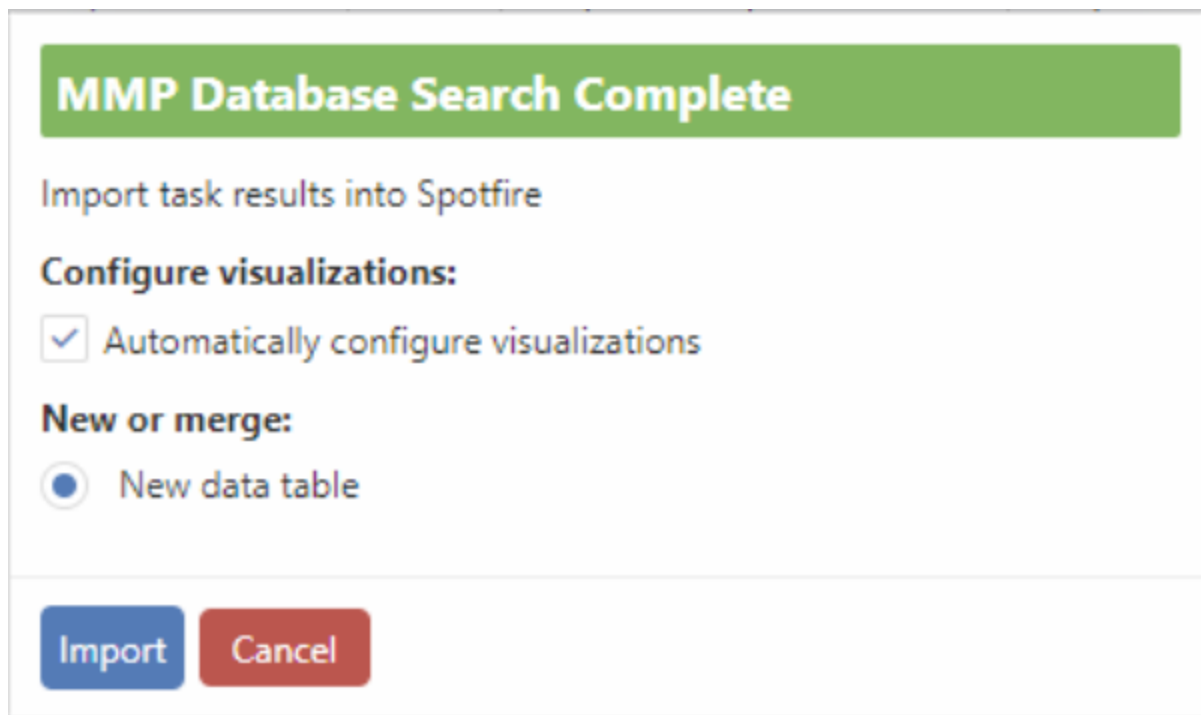


Figure: Dialog for retrieving results from an MMP Database Search service.

The MMP Filter visualization will display the query structure originally submitted to the MMP Database Search service. The results table will then be filtered by lassoing parts of the query structure, then clicking the *Filter* button. The results table contains a column of fingerprints of the query atoms and bonds affected by the transformation represented in each row of the results table. When the user clicks the *Filter* button in the MMP Filter visualization, a calculated column is created that contains a count of the fingerprint overlap between the lassoed atoms and bonds and the atoms and bonds affected by the transform represented in each row of the results table. Filtering and sorting the calculated column assists in identifying transforms of potential interest proximal to the lassoed atoms and bonds.

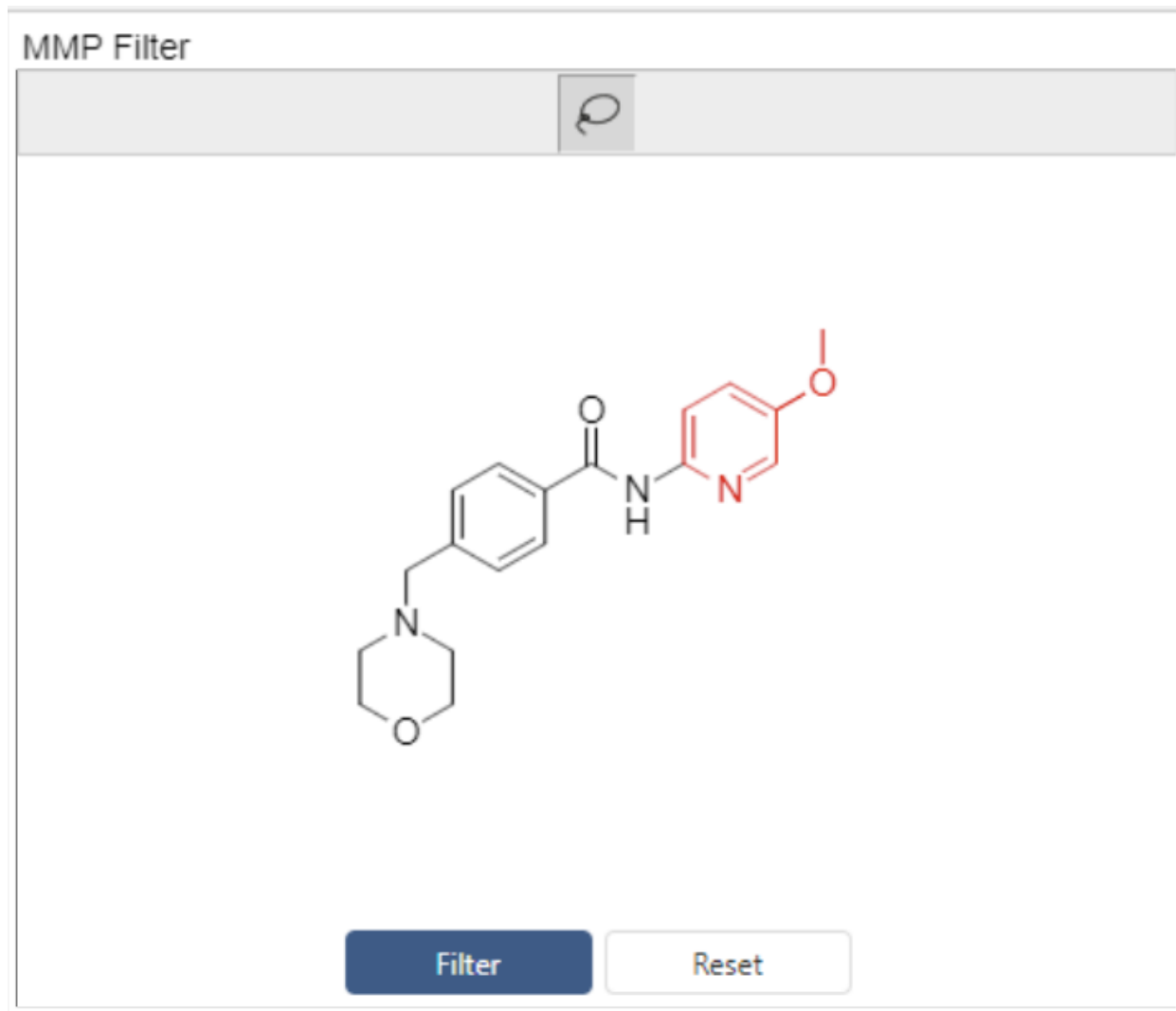


Figure: Applying a structure filter to the results from the MMP Database Search service.

Molecule Viewer Visualization

The Molecule Viewer visualization in Lead Discovery ChemCharts enables the interactive 3D display of small molecules and biopolymers in Spotfire. The Molecule Viewer visualization is best used in conjunction with a different visualization that allows the user to mark rows.

Molecules in marked rows will be displayed in the Molecule Viewer visualization. For molecules and/or biopolymers to be displayed correctly some configuration of the columns that contain these data may be required. See the [Configuration](#) section for details.

The 3D Molecule Viewer visualization has the following features:

- Molecules and biopolymers can be rotated, translated, zoomed etc.
- Typical display options for molecules and biopolymers e.g. coloring, cartoons, etc.
- Tiled layout to compare molecules side-by-side.
- Lock molecules such that they persist in the display regardless of marking.

A screen capture of the Molecule Viewer visualization is shown in the next figure. Note that the Molecule Viewer visualization is displaying molecules from a row marked in the Table visualization. The [Molecule Controls](#) panel is displayed on the left hand side. This contains options for altering the display of molecules currently visible in the 3D Molecule Viewer based on the marked row state of the data table. Clicking the checkboxes in the Locked column (denoted by the column header symbol) of the molecule controls will cause molecules to persist in the display regardless of the marked row state. When displaying superimposed molecules, locking a molecule used as a reference may be useful.

The controls under the name of each displayed column on the right hand side of the Molecule Controls alter the visible state and appearance of marked rows. The checkbox on the left of each displayed column controls the visible state. By unchecking the box, even if a row is marked, the structure contained in the column will no longer be visible. To re-enable visibility, simply click the checkbox again. The color picker to the right of the visible checkbox controls the color used to render carbons in the structure. Clicking the color picker will open a dialog that will allow the user to alter the color used to render carbon atoms for the structure. Note that this will not alter the color scheme for ribbons when displaying proteins or nucleotides. The center control shifts the display such that the geometric center of the structure will be placed at the center of the 3D Molecule Viewer.

The screenshot shows a software window titled "demo-charts-ld-760.dxp - TIBCO Spotfire (10.3.0 LTS, 64-bit RELEASE)". The main area displays a 3D protein structure with a ribbon representation, colored in shades of purple, yellow, and orange. On the left, there is a "Lead Discovery ChemCharts" panel with a search bar and a list of items, including "4K5Y_A". Below the 3D view is a data table with the following columns: ID, Structure, Genbank, DivisionCode, MoleculeType, SequenceLength, SequenceType, StrandTopology, Definition, Source, Genus, Species, ClassLevels, and RowId. The table contains two rows, with the first row (ID: 4K5Y_A) highlighted in green. The first row's definition is "Chain A, Crystal Structure Of Human Corticotropin-Releasing Factor Receptor 1 (CRFR1)". At the bottom, there is a navigation bar with various tabs like "Table", "Gallery", "Form", "SAR Map", "Sequence + Structure", "Superposition", "Blast", "Clustal", "Sequence", "MPO", "Distributions", "WS", "MMP Results", and a status bar showing "1,105 of 1,105 rows", "1 marked", "38 columns", and "proteins_1105".

ID	Structure	Genbank	DivisionCode	MoleculeType	SequenceLength	SequenceType	StrandTopology	Definition	Source	Genus	Species	ClassLevels	RowId
1		1...10...20... MFLTEEDKNSK...VZVAKVLRGH Domain 1 TM2_2	None	Protein	441	aa	Linear	Chain A, Crystal Structure Of Human Corticotropin-Releasing Factor Receptor 1 (CRFR1)	Unknown	Unclassified	Unknown	Unclassified	1
2		MFLTEEDKNSK...VZVAKVLRGH	None	Protein	443	aa	Linear	Chain A, Crystal Structure Of Human	Unknown	Unclassified	Unknown	Unclassified	2

Figure: A protein structure displayed in the 3D Molecule Viewer.

The 3D Molecule Viewer is able to display multiple 3D structures from appropriately configured columns simultaneously. This is useful for viewing the results of molecule superposition algorithms. In the following figure, the reference structure used in the superposition has the

carbons colored green for clarity, and the superimposed molecule uses a default gray color for carbon atoms.

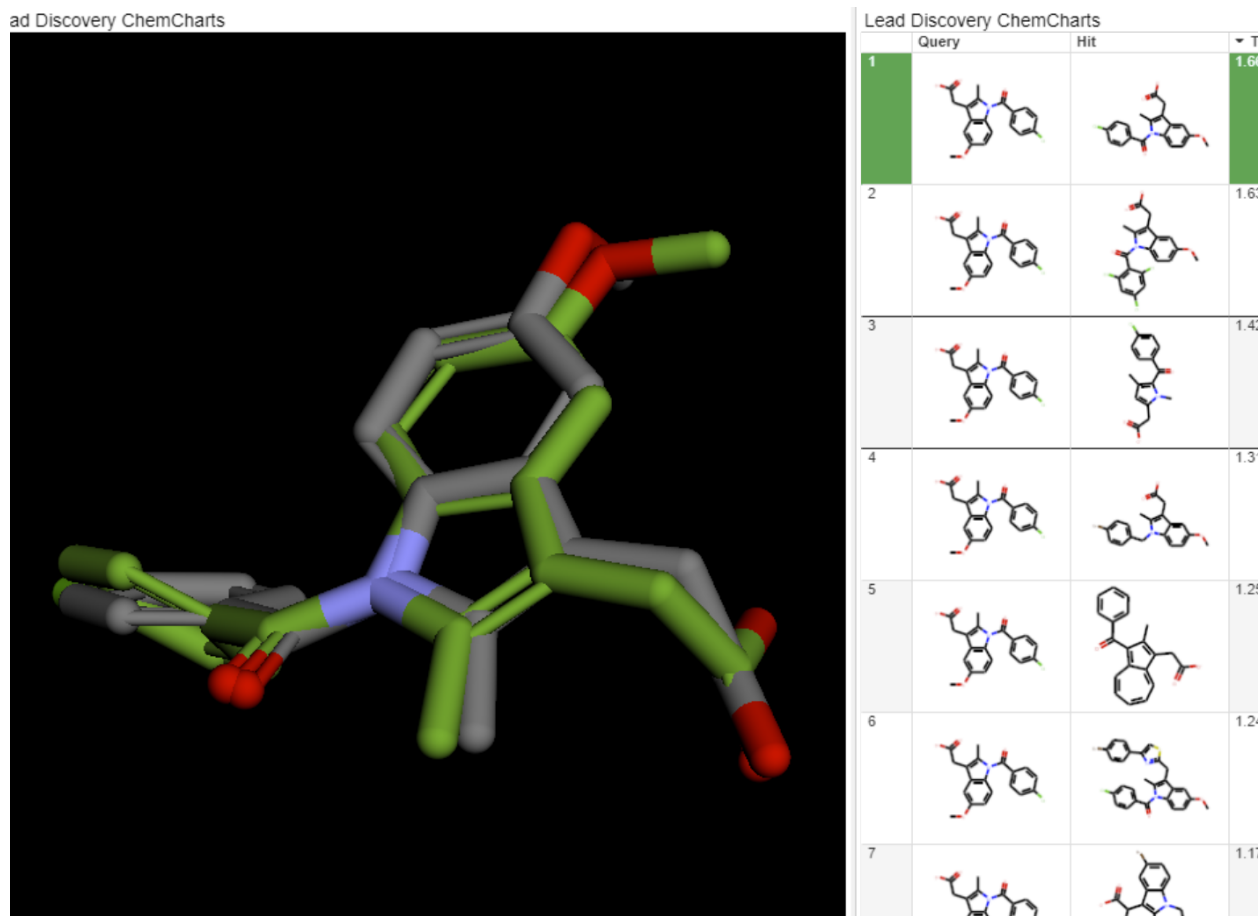


Figure: Display of superimposed molecules.





Context menu

As with all the visualizations in Lead Discovery ChemCharts, much of the functionality of the 3D Molecule Viewer visualization is accessed through the context menu, which is opened by right clicking anywhere in the visual. The context menu for the Molecule Viewer visualization is shown in the following figure.




Figure: The 3D Molecule Viewer visualization visualization context menu.

The following table describes the function of each item in the context menu.

	Back: returns the user to the visualization 'home' page where the user can select a different visualization or data table to display in the current ChemCharts visualization.
	Add visualization: adds a new ChemCharts visualization to the current page. Used primarily in the web player.
	Web services: opens the web services dialog.
	Properties: opens the Properties dialog.
Show/hide molecule controls	Toggles the open/closed state of the molecule controls panel.

The following sections describe the configuration and use of the Molecule Viewer visualization.

Create a Molecule Viewer visualization

Click the New Lead Discovery ChemCharts button  in the list of visualizations in Spotfire. A new Lead Discovery ChemCharts visualization will be added to the page. Select Molecule Viewer in the dropdown menu of available visualizations on the ChemCharts home page.

Display/hide molecules and or biopolymers

The Molecule Viewer visualization is used in conjunction with a second visualization to control the display of the Molecule Viewer. A [Table](#) visualization is appropriate to use in this case. Molecules that are contained in each row of the table will be displayed when their row is marked. Unmarking a row will remove molecules in that row from the display. For molecules and/or biopolymers to be displayed correctly, some configuration of the columns that contain these data may be required. See the [Configuration](#) section for details.

Rotate, translate and zoom


The list below describes the various mouse controls:

Rotate	Left mouse button + mouse move
Zoom	Mouse wheel or Shift + Left mouse button + mouse move
Translate	Middle mouse + mouse move button or Ctrl + left mouse button + mouse move


Measuring distances, angles and torsions

Distances, angles and dihedral angles (torsions) can be displayed. To start a measurement, right-click (or Ctrl + left-click) to select 1, 2, 3 or 4 atoms. The measurement is completed by clicking on the final atom twice. The atoms will be deselected on completion of the measurement. All atoms can be deselected by either a right-click (or Ctrl + left-click) in empty space. Measurements are removed by repeating the process used to add a measurement.

Molecule controls panel

To display the molecule controls panel, open the context menu (right click) and select *Show/hide molecule controls*. To hide the molecule controls panel, either toggle the *Show/hide molecule controls* option from the context menu, or click the Close molecule controls button  at the top right of the molecule control panel.

Lock/unlock molecules

[Open the molecule controls panel](#), select the Molecules tab and check/uncheck the checkboxes in the Locked column (denoted by the column header symbol ). This will cause molecules to persist in the display regardless of the marked row state.

Change the molecule color

[Open the molecule controls panel](#), select the Molecules tab and click the color control to the right of the visibility checkboxes under the column for the desired structure. The new color for the molecule can be selected from the color drop down that will appear. This new color is now used to color the carbon atoms for the structure. Note that this will not alter the color scheme for ribbons when displaying proteins or nucleotides.

Center on a molecule

[Open the molecule controls panel](#), select the Molecules tab and click center control for the molecule that is to be centered. The display is shifted such that the geometric center of the structure will be placed at the center of the 3D Molecule Viewer.

Change the column used to name rows in the molecule controls panel

The name used to identify each visible row in the 3D Molecule Viewer visualization is a configurable option. Open the *Properties* dialog and select the *Molecule viewer* tab. Select the column to be used as an identifier from the *Name column* dropdown menu.

Change the background color

Open the *Properties* dialog and select the *Molecule viewer* tab. The background color can be selected by clicking on the colored square next to Background color and selecting a different color from the color swatch.

Tiled display

Open the *Properties* dialog and select the *Molecule viewer* tab. Tiled display can be toggled by checking/unchecking the Tiled display checkbox. The number of columns of tiles that are displayed can be changed by entering the desired number in the Tiled column count text box. As more rows are marked, a new tile is added to the current row of tiles until the *Tiled column count* value is reached, after which, a new row of tiles will be added. Tile display is limited to a maximum of 6 tiles.

Slab

Open the *Properties* dialog and select the *Molecule viewer* tab. The near and far planes for the molecule viewer slab can be set using the range slider.

Protein cartoon settings

Cartoons (ribbon diagrams) that highlight the secondary structure can be displayed for proteins. In order to edit these settings, Open the *Properties* dialog and select the *Molecule viewer* tab. Here, the global protein cartoon settings can be configured. The display of protein cartoons can be toggled using the *Display cartoons/ribbons* checkbox. The cartoon style can be chosen using the *Cartoon/ribbon style* drop down and the opacity of the cartoon can be set via the *Cartoon/ribbon opacity* number box (1 is opaque, 0 is completely transparent). Note that setting the cartoon opacity to anything other than 1 may impact performance.

Configuration

Chemical structures may be imported as MDL Molfiles or SD files containing 3D coordinates using the Lead Discovery SDF file import. For structure columns to be recognized as displayable by the 3D Molecule Viewer, the *ContentType* for the column must be set to a recognized molecule format capable of containing 3D coordinates, such as "chemical/x-mdl-molfile". The *Dimension* property must also be set to the value "3".

Biopolymers in PDB or gzipped PDB format, hosted on web servers, may also be displayed by the 3D Molecule Viewer. Note that the biopolymers are not contained in the Spotfire data table directly, but referenced by URI (Uniform Resource Identifier) in order to minimize the data table size. To denote a column as a biopolymer URI column, the *ContentType* of the column should be set to "chemical/x-uri" and the *Dimension* property should be set to "3".

Columns imported from results of Lead Discovery Web Services will likely have the appropriate properties set to make them displayable by the 3D Molecule Viewer. Columns originating from other data sources, such as SDF or CSV import may need to have their properties set manually. To set column properties manually, open the Column Properties through the Spotfire Edit>Column Properties menu. Select the column from the list in the top half of the Column Properties dialog, then select the "Properties" tab in the middle of the dialog. Select the *ContentType* property and click the Edit button on the right hand side, and enter the appropriate

value for the ContentType. The Dimension property may be added by clicking the New button to the right of the properties listing. Enter "Dimension" as the property name, leave the Data type as "String" and enter the value "3" into the Default value field. An example is shown in the following figure:

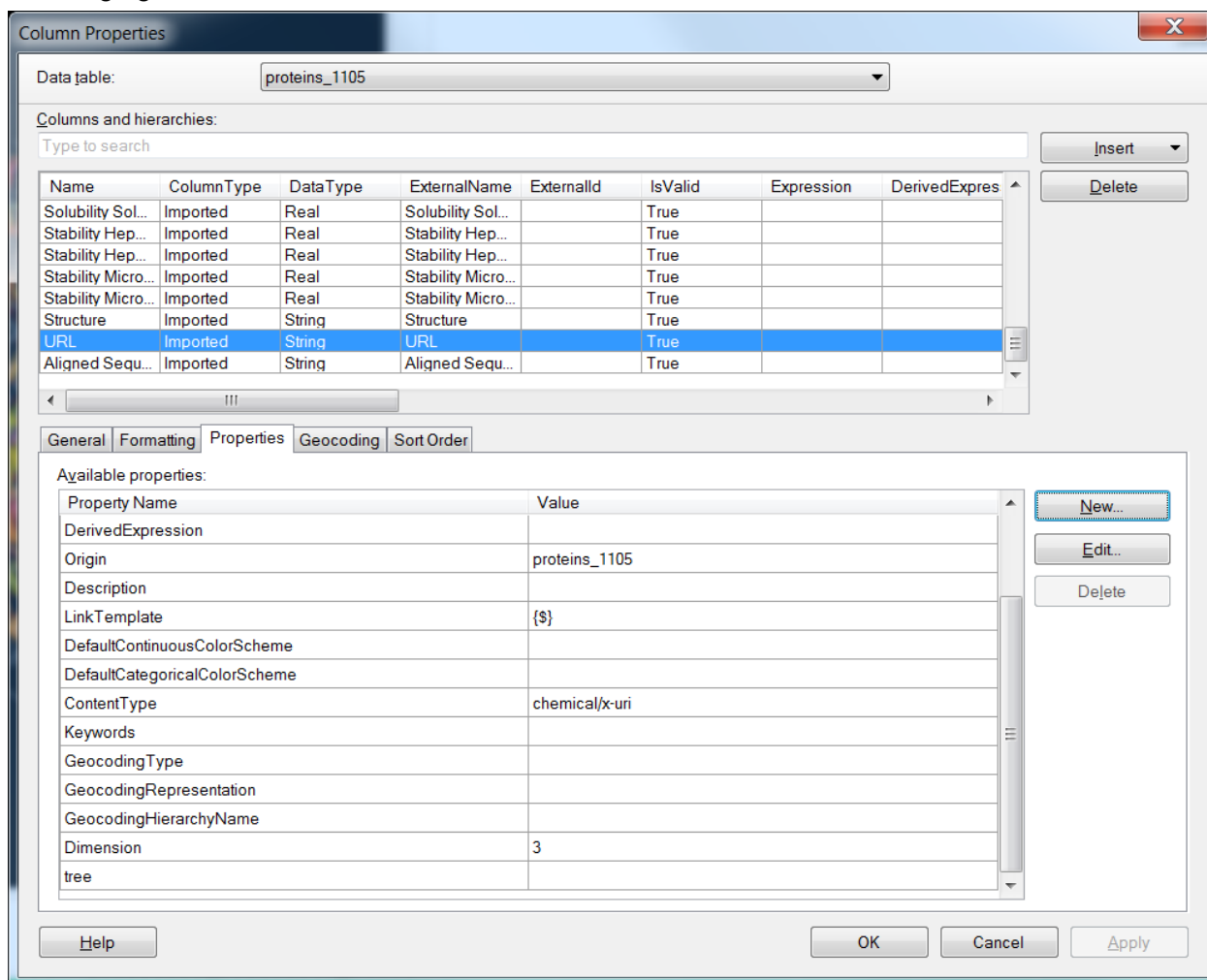


Figure: Editing properties using the Column Properties Dialog.

Once the properties are set correctly, the 3D Molecule viewer will display molecules for marked rows in the data table.

MPO Visualization

The Lead Discovery ChemCharts MPO (Multi Parameter Optimization) visualization can be used to visualize and filter numeric data using a Distribution visualization. In addition, the [Scoring](#) property page can be used in concert with the MPO to combine numeric data in a data table to create and edit calculated score columns. This feature provides the ability to create ranking functions by combining and scaling data in the data table.

An example of the MPO Visualization is shown in the next figure. Data from a data table are displayed in a Distribution visualization. Vertical axes are created for each numeric column in the data table. The axes can be placed in any order from left to right. The data from each row is then plotted as a distribution along each axis. In the figure below, distributions of the LogP, PSA, MW, HBA, HBD and MPO Score columns are shown in the MPO visualization. The displayed lines are marked and/or active rows. In the example below the light gray line is the marked row and the darker line is the active row.

Rows may be marked by clicking and moving the mouse to drag a selection rectangle. Rows are marked when the left-mouse button is released. The marked rows will appear as a parallel line plot overlaid on the distributions. Pressing the shift key while selecting with rectangles allows for multiple selections to be made on different axes.

Range filters can also be applied using the MPO visualization. This is shown in the following figure where a range filter has been applied to the HBA column/axis using the sliders. MPO filters alter Spotfire filters. Other visualizations on the same page as the MPO visualization will be subject to filter alterations.

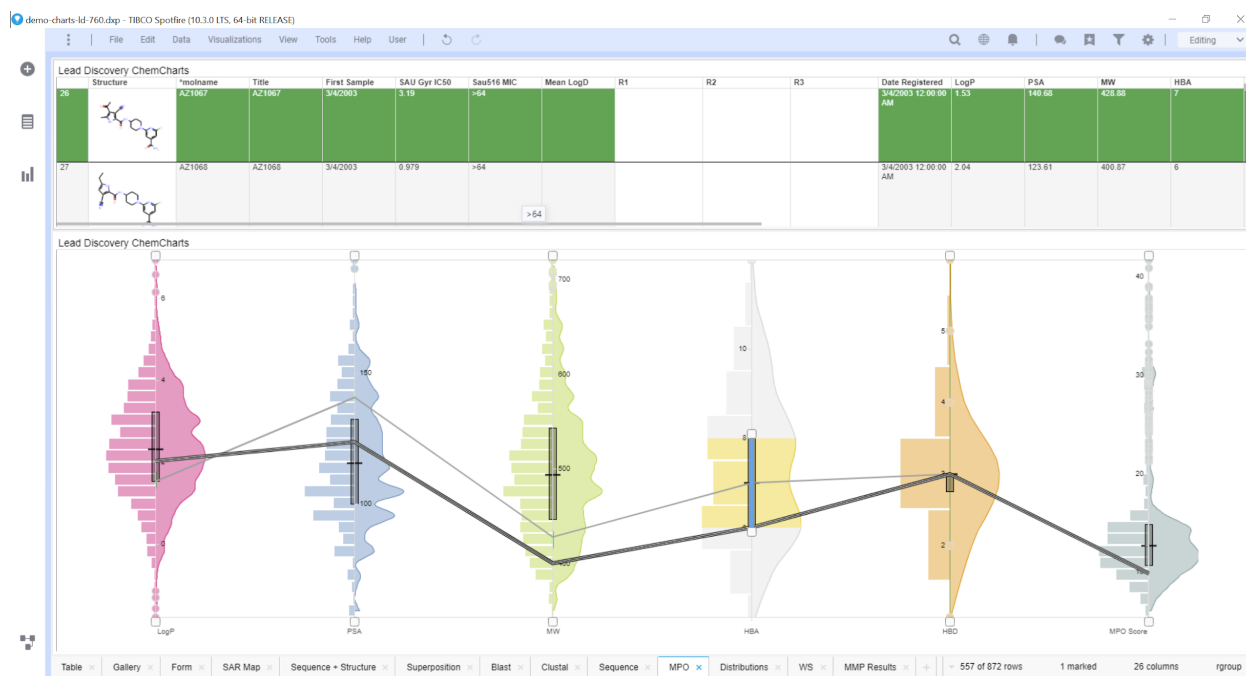


Figure: The MPO Visualization.

Context menu

Much of the functionality of the MPO visualization is accessed through the context menu, which is opened by right clicking anywhere in the visual. The context menu for the MPO visualization is shown in the following Figure.

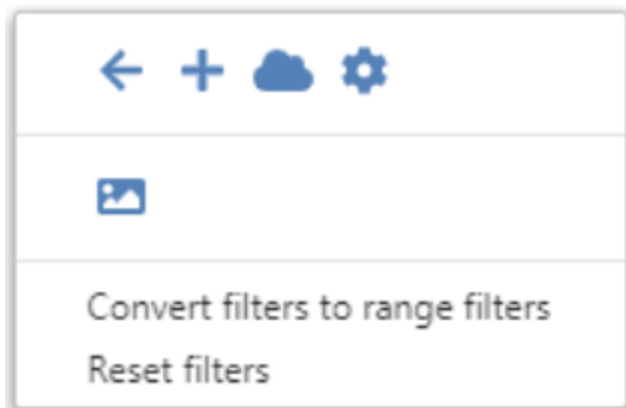








Figure: The MPO visualization context menu.

The list below describes the function of each item in the context menu:

	Back: returns the user to the visualization 'home' page where the user can select a different visualization or data table to display in the current ChemCharts visualization.
	Add visualization: adds a new ChemCharts visualization to the current page. Used primarily in the web player.
	Web services: opens the web services dialog.
	Properties: opens the Properties dialog.
	Tooltips: opens <i>Properties</i> dialog to the <i>Tooltips</i> tab.
Convert filters to range filters	Enables axis filters by changing filter types for associated axes to range filters.
Reset filters	Resets all filters controlled by the MPO visualization.

The following sections detail the configuration and use of the MPO visualization.

Create an MPO visualization

Click the New Lead Discovery ChemCharts button  in the list of visualizations in Spotfire. A new Lead Discovery ChemCharts visualization will be added to the page. Select Molecule Viewer in the dropdown menu of available visualizations on the ChemCharts home page.

Configure axes

The columns that appear as axes in the MPO chart can be configured using the Properties dialog. To display the Properties dialog, right click and select *Properties* from the context menu. Select the *Axes* page and use the column select box with the Add button to add new axes to the visualization. Once a column has been added for display, the minimum and maximum allowed values for the distribution may be adjusted using the min and max text boxes to the right of the column name in the Axis list. Distributions may be plotted with the base 10 Log function applied to column values. By default, the minimum and maximum axis values are displayed at the bottom and top of the chart respectively. Clicking the *Invert* checkbox inverts the axis such that the minimum value is at the top of the chart and the maximum value is at the bottom. The order of the axes can be adjusted by dragging and dropping the appropriate rows. The color for each of the distributions can also be configured by using the color picker for each axis.

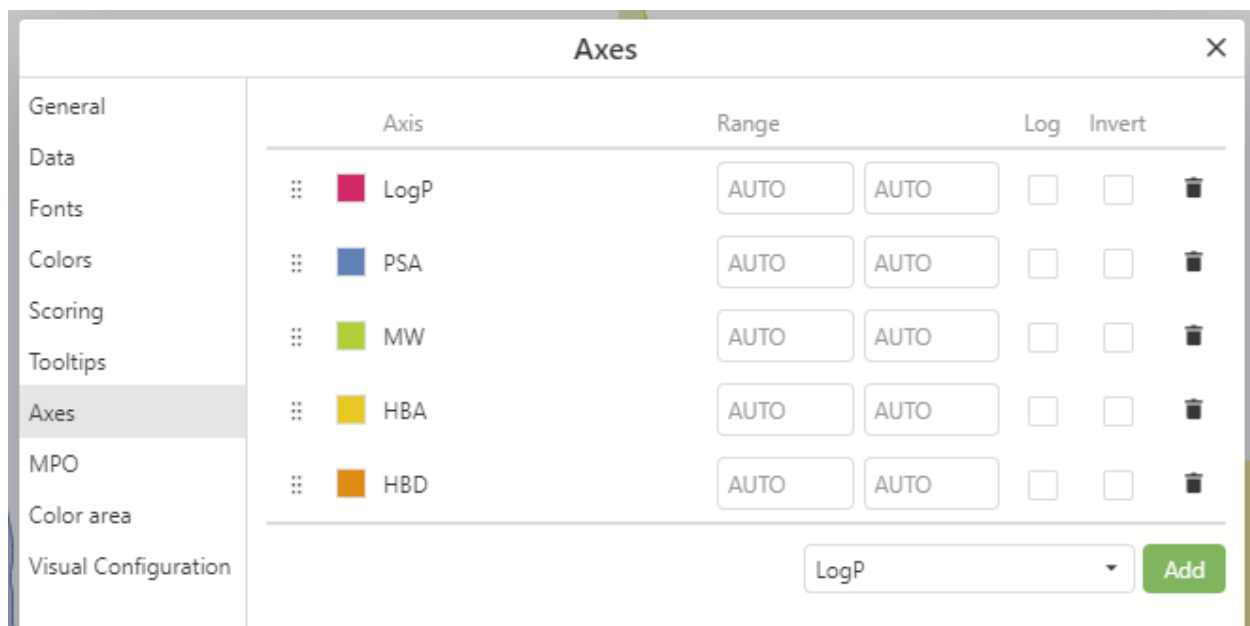


Figure Configuring the axes in an MPO visualization.

Color areas

Colored areas can be added to the MPO visualization. These are created by defining minimum and maximum bounds for each of the axes in the chart and assigning a color to the area defined by the bounds. An example is shown in the figure below.

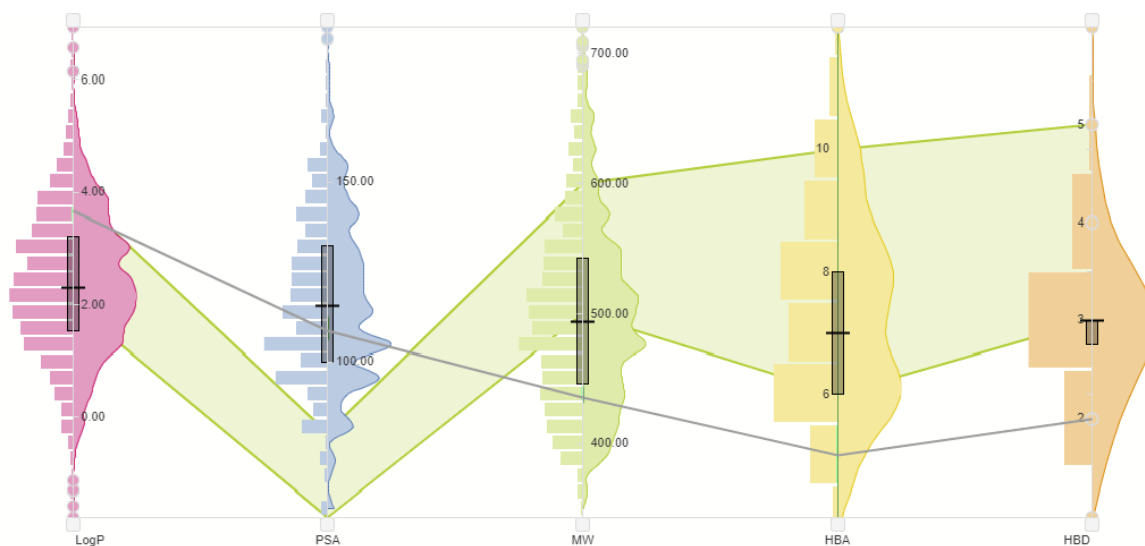


Figure Color area in the MPO visualization.

The color areas are configured in exactly the same way as the [Radar visualization](#).

Filter the MPO visualization

Filtering for the data displayed in the MPO visualization may be altered using the slider controls on each distribution. Slider controls will appear for columns that are numeric and that have the range filter type defined in the Spotfire *Filters* panel. To use the range filters, simply mouse over the slider thumbs on each axis and drag to the desired position. To reset all the filters, right click and select Reset filters. Changes to MPO visualization filters will be reflected in the filter panel and other visualizations on the same page as the MPO visualization, provided other visualizations are configured with the same data table as the MPO visualization.

Create a score column

See the [Scoring](#) property page documentation.

Multiple Sequence Alignment Visualization

The Lead Discovery ChemCharts Multiple Sequence Alignment (MSA) visualization is used to display aligned sets of biomolecule sequences. The MSA visualization contains many features that should be familiar to anyone that has viewed a sequence alignment e.g. the alignment can be scrolled horizontally (using either the scrollbar or a combination of ctrl + mouse wheel), the alignment position (or residue numbers) are displayed just above the sequences, the residues are colored according to a scheme. The Lead Discovery ChemCharts MSA visualization has a number of unique features: the alignment may be displayed with header or footer areas that show the annotations for a selected sequence, a sequence LOGO and/or box plots displaying population statistics for numeric data associated with the sequences grouped using sequence

motifs. Additionally it interacts with Spotfire in all the usual ways e.g. marking, limit-by-marking, filtering, active rows etc.

An example of the Sequence visualization is shown in the next figure:



Figure: The Multiple Sequence Alignment visualization. The header area is displaying the annotations for the marked sequence (in green). The center area displays the sequence alignment. The footer area is displaying population data for the 'Score' data where the data is grouped using motifs defined by a region of the sequence alignment - in this case a one residue length region labeled with the 'F' as it is the region associated with the footer. The left panel displays names for the sequences.

The Lead Discovery ChemCharts Multiple Sequence Alignment visualization interacts with Spotfire in an intuitive manner, for example:

- Left mouse click on a row will mark it.
- Hovering over a row will make it the active item and corresponding items will be highlighted in other visualizations in Spotfire (except in the WebPlayer).
- Rows can be sorted by the values in up to 5 columns.
- The data displayed in the MSA visualization can be limited by one or more markings from other visualizations (see Single Click Limit by Marking) or by applying Spotfire filters.

Context menu

As with all the visualizations in Lead Discovery ChemCharts, the configuration of the MSA visualization is accessed through the context menu which is opened by right-clicking anywhere in the visual. An example of the context menu for the Sequence visualization is shown in the figure below.

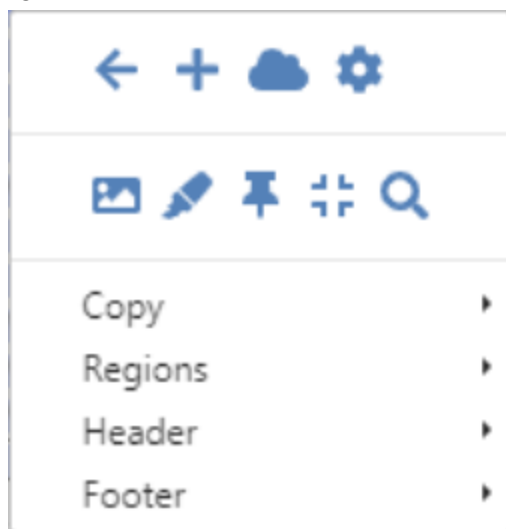











Figure: the MSA visualization context menu.


The table below describes the function of each menu item:

	Back: returns the user to the visualization 'home' page where the user can select a different visualization or data table to display in the current ChemCharts visualization.
	Add visualization: adds a new ChemCharts visualization to the current page. Used primarily in the web player.
	Web services: opens the web services dialog.
	Properties: opens the Properties dialog.
	Tooltips: opens the tooltips control for the visualization.
	Limit by marking: toggles the limit by marking behavior of the visualization
	Fix row: fixed rows persist in the sequence display regardless of scroll position. Fixed rows act as references when using differential color or character schemes.

	Active residue: toggles active residue selection in the sequence panel.
	Find: searches for text in a data table that matches a query.
Copy	Copy marked sequences to the clipboard.
Regions	Opens the <i>Regions</i> submenu.
Header	Opens the <i>Header</i> submenu.
Footer	Opens the <i>Footer</i> submenu.

The sections below detail how to configure and use the Multiple Sequence Alignment visualization.

Create a Molecule Viewer visualization

Click the New Lead Discovery ChemCharts button  in the list of visualizations in Spotfire. A new Lead Discovery ChemCharts visualization will be added to the page. Select *Multiple sequence alignment* in the dropdown menu of available visualizations on the ChemCharts home page.

Importing alignments

File format	Data type	Content type	Annotations
FASTA	String	chemical/x-sequence	No
Genbank	Binary	chemical/x-genbank	Yes (if included in the original file)
Antibody Numbering web service in Lead Discovery Web Services	Binary	chemical/x-genbank	Yes
Clustal (table) web service in Lead Discovery Web	Binary	chemical/x-genbank	Yes

Services			
----------	--	--	--

Table: Supported formats for importing alignments into Spotfire and the resulting column types.

Sequence display options

There are a number of options for coloring residues in the sequence alignment. There are 15 different common color schemes to choose from, and an additional 2 comparative coloring schemes where the similarities and differences to a reference sequence are displayed. Additionally, it is possible to display amino acid residues using the three letter codes instead of one letter codes in the sequence view.

The display options for sequences in the Sequence visualization can be set by selecting the *Properties* dialog from the [context menu](#). From the *Properties* dialog, navigate to the *Column renderers* page and choose the column that contains the sequences being displayed from the *Columns* dropdown menu. An example of this is displayed in the figure below.

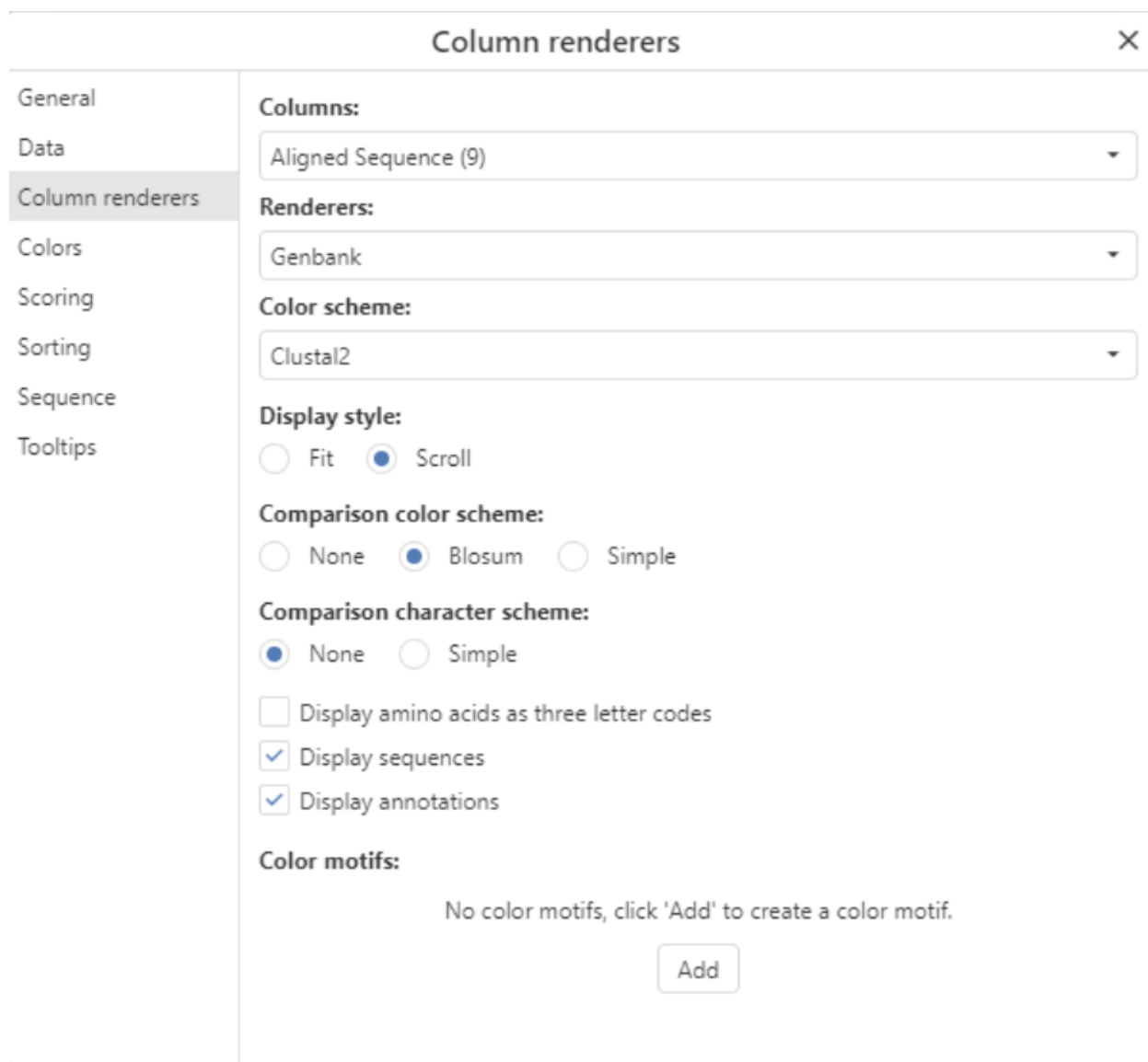


Figure: Configuring the sequence renderer through the Properties dialog.

Predefined color schemes may be selected from the *Color scheme* dropdown menu. If no color scheme is desired, select *Plain*. There are three options for comparison color schemes, that is, the coloring scheme applied to other sequences when a reference sequence is selected by [fixing](#) a row. Selecting *None* will remove coloring for non-reference sequences. The Simple color scheme displays differences in residues (when compared to the reference sequence) with a red background. The Blosum color scheme displays how commonly a residue replacement is observed, where blue indicates a common replacement and red indicates an uncommon replacement.

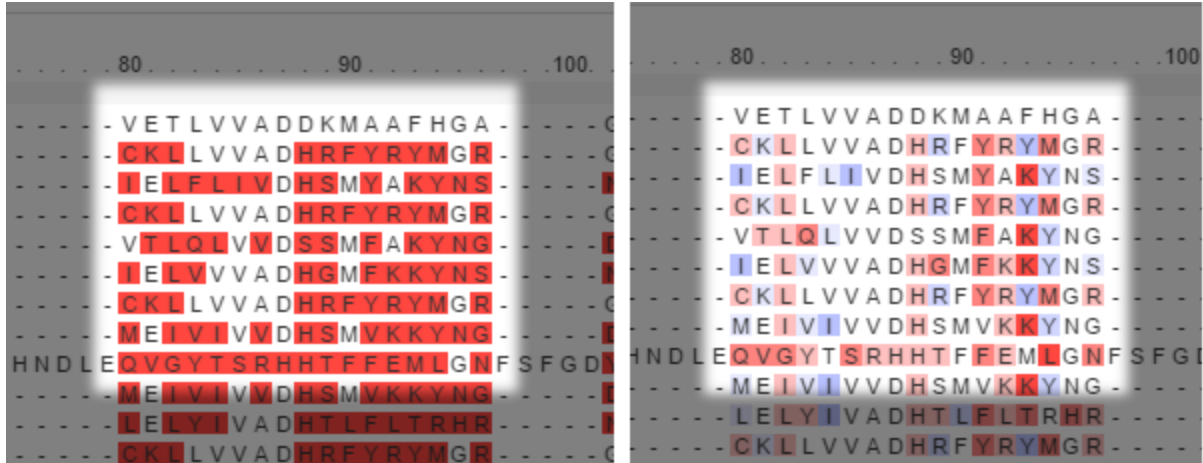


Figure: Comparative colors schemes in the Sequence visualization. The Simple scheme is on the left. The Blosum scheme is on the right.

The various color schemes available for nucleotides and proteins are illustrated below.

Nucleotide Color Schemes

	A	C	G	T	U	R	Y
Nucleotide	Green	Orange	Red	Blue	Blue		
Purine/Pyrimidine	Pink	Cyan	Pink	Cyan	Cyan	Pink	Cyan
UGENE	Yellow	Light Green	Blue-Gray	Pink	Pink		
UGNE Sanger	Light Green	Blue	Gray	Pink	Pink		

Amino Acid Color Schemes

	A	C	D	E	F	G	H	I	K	L	M	N	P	Q	R	S	T	V	W	Y
Bioedit	Teal	Brown	Red	Red	Teal	Orange	Pink	Green	Blue	Green	Green	Purple	Brown	Purple	Blue	Blue-Gray	Blue-Gray	Green	Green	Teal
Buried Index	Green	Blue	Light Green	Light Green	Teal	Teal	Light Green	Blue	Light Green	Teal	Teal	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Blue	Teal	Light Green
Cinema	White	Yellow	Red	Red	Pink	Brown	Cyan	White	Cyan	White	White	Light Green	Brown	Light Green	Cyan	Light Green	Light Green	White	Pink	Pink
Clustal	Orange	Green	Red	Red	Blue	Orange	Red	Green	Red	Green	Green	Light Green	Orange	White	Red	Orange	Orange	Green	Blue	Blue
Clustal2	Light Blue	Light Red	Pink	Pink	Light Blue	Orange	Light Blue	Light Blue	Red	Light Blue	Light Blue	Light Green	Yellow	Light Green	Red	Light Green	Light Green	Light Blue	Light Blue	Teal
Helix Propensity	Pink	Light Green	Gray	Pink	Gray	Light Green	Gray	Gray	Gray	Gray	Pink	Light Green	Light Green	Gray	Gray	Light Green	Light Green	Gray	Gray	Light Green
Hydrophobicity	Dark Red	Blue	Blue	Blue	Red	Blue	Blue	Purple	Blue	Red	Red	Blue	Dark Red	Dark Red	Purple	Purple	Purple	Purple	Purple	Red
Lesk	Orange	Green	Red	Red	Green	Orange	Pink	Green	Purple	Green	Green	Pink	Green	Pink	Purple	Orange	Orange	Green	Green	Green
MAE	Light Green	Light Green	Light Green	Light Green	Light Purple	Light Green	Purple	Light Blue	Light Orange	Light Blue	Light Blue	Light Green	Light Red	Light Green	Light Orange	Light Red	Light Red	Light Blue	Light Purple	Light Purple
Strand Propensity	Dark Purple	Brown	Blue	Blue	Light Green	Dark Purple	Dark Purple	Yellow	Dark Purple	Brown	Gray	Dark Purple	Blue	Dark Purple	Dark Purple	Dark Purple	Brown	Yellow	Light Green	Light Green
Taylor	Light Green	Yellow	Red	Pink	Light Green	Orange	Blue	Light Green	Purple	Light Green	Light Green	Purple	Yellow	Pink	Blue	Orange	Orange	Light Green	Light Blue	Light Green
Turn Propensity	Teal	Brown	Red	Gray	Teal	Red	Gray	Cyan	Gray	Teal	Teal	Red	Red	Teal	Gray	Red	Gray	Cyan	Gray	Brown
Zappo	Light Red	Yellow	Red	Red	Orange	Pink	Purple	Light Red	Purple	Light Red	Light Red	Light Green	Pink	Light Green	Purple	Light Green	Light Green	Light Red	Orange	Orange

Bioedit

Color	Residue
Cyan	A
Brown	C
Red	D, E
Dark Green	I, L, M, V
Orange	G
Light Blue	F, Y
Magenta	H
Dark Blue	K, R
Grey	P
Slate Blue	S, T
Violet	N, Q
Pale Green	W

Buried

Depending on the frequency of occurrence inside a globule, the amino acid residues are colored from light green (less frequent) to blue (most frequent).

C	I	V	L	F
M	G	A	W	S
H	T	P	Y	N
D	Q	E	R	K

Cinema

Category	Color	Residue
Polar positive	Cyan	H, K, R
Polar negative	Red	D, E
Polar neutral	Green	N, S, T, Q
Non-polar aliphatic	White	A, I, L, M, V
Non-polar aromatic	Magenta	F, W, Y
Conformationally special	Brown	P, G
Cysteine	Yellow	C

Clustal

Color	Residue
Orange	A, G, P, S, T
Red	D, E, H, K, R
Blue	F, W, Y
Green	C, I, L, M, V
White	Q

Clustal2

Category	Color	Residue
Hydrophobic	BLUE	A, I, L, M, F, W, V
Positive charge	RED	K, R
Negative charge	MAGENTA	E, D
Polar	GREEN	N, Q, S, T
Cysteines	PINK	C
Glycines	ORANGE	G
Prolines	YELLOW	P
Aromatic	CYAN	H, Y

Helix

Depending on helix propensity, the residues are colored from magenta (the highest helix propensity) to green (the lowest).

E	M	A	L	K
F	Q	I	W	V
D	H	R	T	S
C	Y	N	G	P

Hydrophobicity

Residues are colored based on their hydrophobicity. Most hydrophobic residues are red, most hydrophilic are blue.

Y	L	M	Q	A
F	P	V	S	T
W	R	C	D	E
G	H	I	K	N

Lesk

Category	Color	Residue
Small nonpolar	Orange	G, A, S, T
Hydrophobic	Green	C, V, I, L, P, F, Y, M, W
Polar	Magenta	N, Q, H
Negatively charged	Red	D, E
Positively charged	Blue	K, R

MAE

Color	Residue
Light Green	A, G
Green	C
Dark Green	D, E, N, Q
Light Blue	I, L, M, V
Lilac	F, W, Y
Blue	H
Orange	K, R
Pink	P
Red	S, T

Strand

V	I	Y	F	W
L	T	C	Q	M
R	N	H	A	S
G	K	P	D	E

Taylor

From Protein Engineering, Vol 10 , 743-746 (1997).

A	V	I	L
M	F	Y	W
H	R	K	N
Q	E	D	S
T	G	P	C

Turn

Residues with the highest turn propensity are red, with lowest are cyan.

N	G	P	D	S
C	Y	K	Q	W
T	R	H	E	E
A	F	L	V	I


Zappo

Property	Color	Residue
Aliphatic/hydrophobic	Pink	I, L, V, A, M
Aromatic	Orange	F, W, Y
Positive	Blue	K, R, H
Negative	Red	D, E
Hydrophilic	Green	S, T, N, Q
Conformationally special	Magenta	P, G
Cysteine	Yellow	C

Setting the name and/or sequence column

To set the data table column used as the display name for the sequences, or to change the sequence column, open the *Properties* dialog from the context menu and navigate to the Sequences page. The *Sequence column* dropdown menu is used to select the sequence column for display. The *Name area + column dropdown* menu is used to configure the source column for sequence identifiers.

Fixed rows

Comparing sequences in a MSA visualization may be aided through the use of fixed rows. Rows may be fixed at the top of the MSA visualization by double clicking the row, or by right-clicking over a row to open the context menu, and selecting the *Fix row*  menu option. Fixed rows can be removed by applying the previous steps to a currently fixed row.

Internal limit-by-marking

In addition to the limit-by-marking where the displayed data may be restricted to markings from other visualizations, the MSA visualization has an internal limit-by-marking mode. There are 3 areas of the MSA visualization where marking can potentially occur: the sequence area, the header and the footer. The internal limit-by-marking can be configured such that marking in one of the visualization areas will limit the contents displayed in the other two. For example, if the header area is displaying the sequence LOGO and the footer is displaying [distributions](#), then the

internal limit-by-marking could be configured so that marking the distribution plots in the footer area would result in only the marked row data being displayed in the sequence and header areas.

To configure the internal limit-by-marking, open the *Properties* dialog from the [context menu](#) and navigate to the *Sequence* page. Use the *Internal limit by* dropdown menu to select the limit-by-marking mode from the Internal limit by drop down. The choices are: None, Sequence marking, Header marking, or Footer marking.

Regions

Regions can be used to create motifs that group data in MSA distributions, or to hide uninteresting or irrelevant portions of the alignment. An example of regions added to an alignment is shown in the figure below.

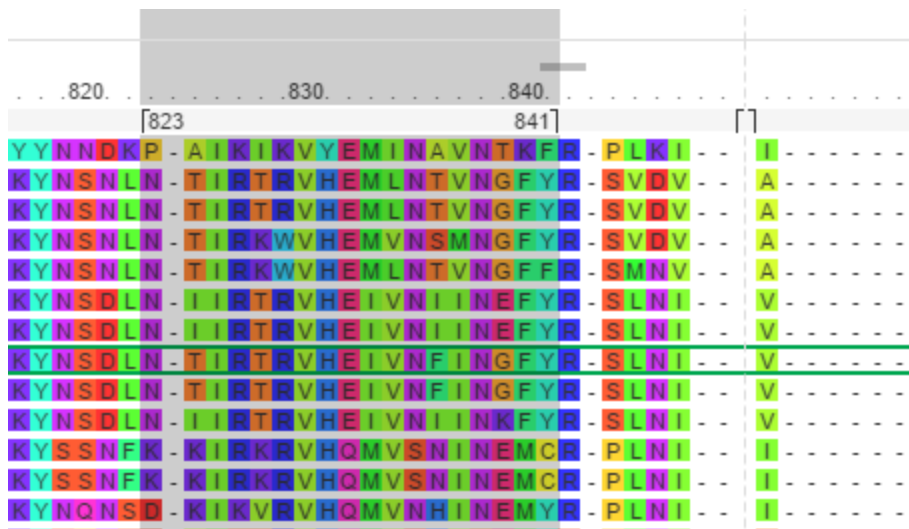


Figure: Sequence alignment that contains 2 regions. The region is on the left and is expanded (alignment position 823 to 841). Expanded regions are displayed as a shaded overlay. The region to the right is collapsed. Collapsed regions are displayed as a vertical dotted line.

Regions are displayed just below the sequence residue numbering. After a region has been added it can be moved or resized using the mouse (by left-clicking and dragging) as well as expanded and collapsed (by double clicking on the region).

At present there are 3 ways of adding a region to the alignment:

1. Add a region manually. In this case the new region is 1 residue long and will be created at the mouse position. To manually add a region, right-click where the region is to be added and selected Regions -> Add from the context menu.
2. Add a region using an annotation. In this case, the new region will be added with the position and length of the chosen annotation. To add a region from an annotation, right-click over the

annotation (either in the header or footer area) and select Regions -> Add region from annotation from the context menu.

3. Add a set of regions for all the areas of identity in the alignment. To add the identity regions, right-click and select one of All sequences, Visible sequences or Marked sequences from the Regions -> Add identity regions sub menu. The regions of identity will be determined using all the sequences (regardless of filtering), the visible sequences (taking into account filtering) or the marked sequences depending on the option selected.

Note that regions cannot be added where there are already regions present (i.e. regions are not allowed to overlap).

Regions may be removed by right-clicking on the region to remove and selecting Regions -> Remove from the context menu. Alternatively, all regions can be removed by selected Regions -> Remove all from the context menu.

If [distributions](#) are being displayed in either the header or footer areas, a region may be associated with the header and/or footer in order to provide sequence motifs that are used to group the data displayed in the distribution plots. To associate a region with the header or footer area, right-click on the region and select Regions -> Link region to header/footer. Note that this option will only appear if distribution plots are displayed in either the header or footer areas. After a region has been associated with a header or footer it will be labeled with an H or F respectively.

Region Properties

Regions can be assigned a name and a color. To edit these properties of a region, right click on the region and select Region -> Properties - this opens the region properties dialog. Here the user can edit the name, color, expanded/collapsed state, start and end indexes for all regions included in the visualization.

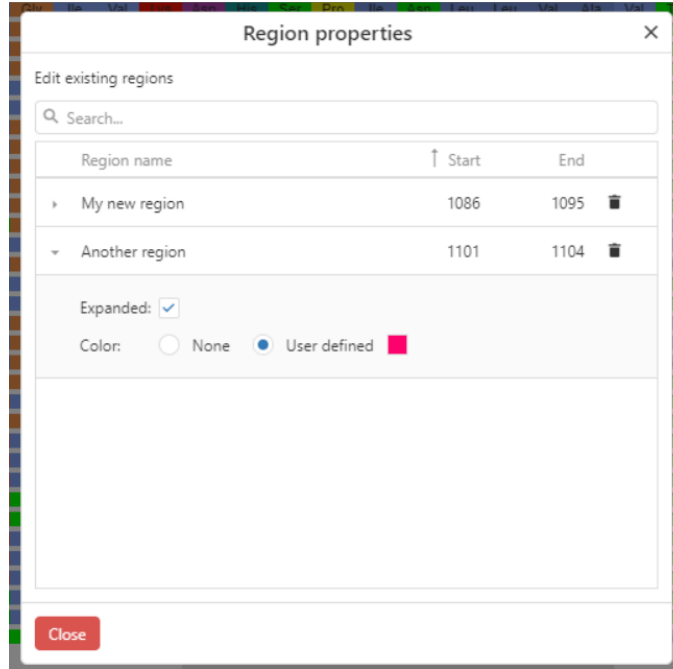


Figure: Editing region properties

Annotations

Annotations can be displayed in the header or footer for the first marked sequence as well as for each sequence in the main sequence area if the sequence column contains annotation data (see [Importing alignments](#)). The annotations are color coded according to type. Tooltips are available that will provide further details about the annotations if present. [Regions](#) may also be created from annotations.

To display annotations in either the header or footer area, right-click and choose Annotations from the Header or Footer sub menus of the Chart settings dialog. To display annotations in the main sequence area simply make the rows bigger by hovering over the space between the sequence names until the resize cursor appears and drag to resize.

LOGO

A LOGO view of the sequences can be displayed in either the header or footer areas. LOGO plots display the distribution of monomers at each position of the alignment. To display the sequence LOGO in either the header or footer area, right-click and select LOGO from the Header or Footer sub menus. When rows are marked, residues in the sequences contained in the marked rows will be displayed in color, with residues in rows not marked displayed in gray. An example is shown in the figure below.



Figure: Example of marking and the sequence LOGO. In this case only the top row is marked. Only the residues that are present in the marked sequences will appear colored in the sequence LOGO, the other residues are colored in gray.

The LOGO view can also be used to drive marking by selecting residues with a left mouse click. All sequences that contain the selected residue will be marked. This can be used in conjunction with the Ctrl key to extend/toggle selection. If the MSA visualization is in [internal limit-by-marking](#) mode, the LOGO view can control what is displayed in other areas of the MSA visualization.

Distributions

Distribution plots can be displayed in either the header or footer areas. Distribution plots are a method of displaying distributions of data associated with sequences. Data must be a numeric type that is associated with the sequences in the data table (e.g. activity data, stability data etc.) The data is grouped by a set of sequence motifs that are generated by adding a region linked to the distribution plot, whether it be in the header or footer. An example distribution plot in the MSA visualization is shown in the next figure.

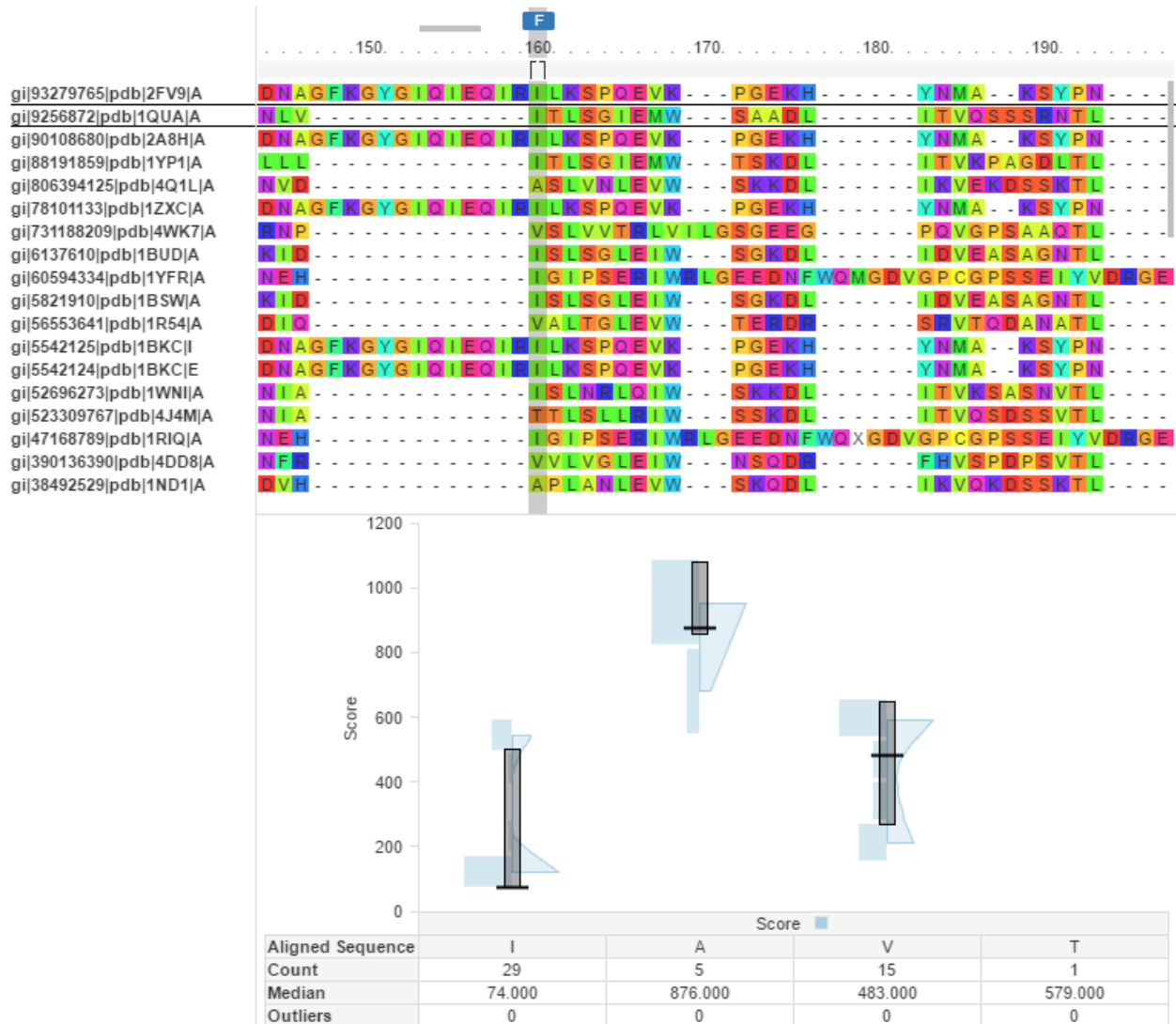


Figure: Example distribution plots in the MSA visualization. The region that is used to generate the sequence motif to group the data is marked with an 'F' (at position 160) as it is associated with the footer area. The distribution plot is displaying the distribution of values for the 'Score' column where the data is grouped by the single residue motifs created by the linked region. In this case there are only 4 different residues at position 160 in the alignment resulting in 4 distributions. In this case violin plots are being used to display the distributions.

The following steps are required to configure distributions in the MSA visualization:

1. Configure either the header or footer area to display distribution plots. This can be achieved by right-clicking and selecting Distributions from the Header or Footer sub menu on the context menu.
2. Create and link a region to the header or footer that contains the distribution plots. See the [regions](#) section for how to create a region. Once the region is created, right-click over the region and select *Link region to header/footer*.

There are three types of distribution plots that can be displayed; bar plots, notched bar plots, and violin plots. Bar and notched bar plots display the first and third quartiles with the median and include whiskers that indicate the position of $1.5 * IQR$ of the upper and lower quartiles. Notched plots additionally display the 95% confidence interval around the median. Violin plots display the first and third quartiles with the median as well displaying the actual distribution of the data. Outliers are displayed as small circles in all the distribution plots. Examples of the three distribution plots are shown below.

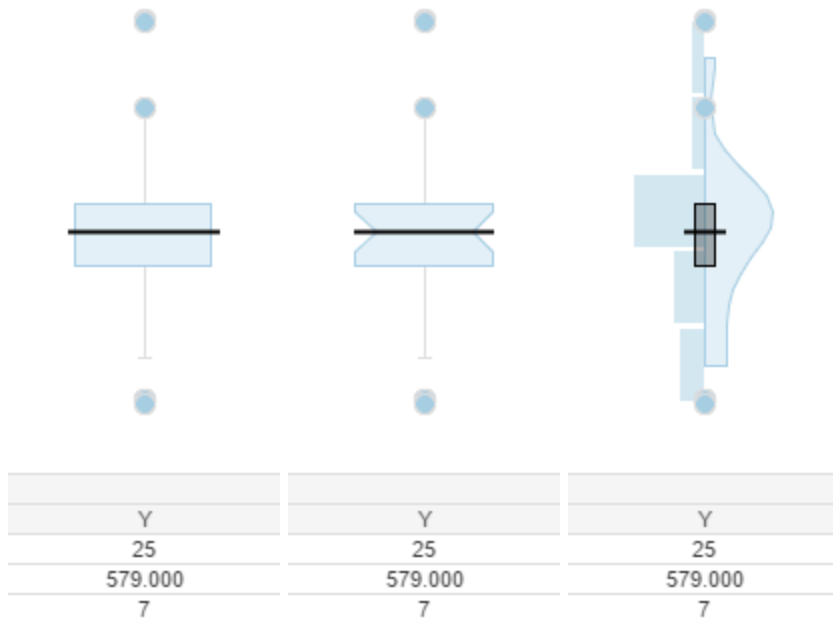


Figure: Examples of the different types of distribution plots. From left to right: bar, notched bar and violin.

To switch between chart types, open the *Properties* dialog from the context menu and navigate to the *Sequence* page. The header or footer may be configured by distributions display by selecting *Distributions* from the *Header area* or *Footer area* dropdown menus. After selecting an area for distributions display, three tabs will appear immediately beneath the dropdown menu. The distribution chart type can be selected from the *General* tab as shown below.

Sequence ✕

General

Data

Column renderers

Colors

Scoring

Sorting

Sequence

Tooltips

Sequence column:

Aligned Sequence (9)
▼

Name area + column:

Target Id

▼

Internal limit by:

None
▼

Header area:

LOGO
▼

Footer area:

Distributions
▼

General
Distributions
Statistics

Chart type:

Violin
▼

Figure: Selecting a distribution chart type for a footer area.

The data displayed in the distribution plots can be configured using the Distributions tab in the either the Header Panel or Footer Panel areas of the dialog e.g.

Sequence
×

General

Data

Column renderers

Colors

Scoring

Sorting

Sequence

Tooltips

Name area + column:

Target Id ▼

Internal limit by:

None ▼

Header area:

LOGO ▼

Footer area:

Distributions ▼

General
Distributions
Statistics

Display distributions for the following columns:

Score ✕

Display empty distributions

Single axis or one axis per column:

Single axis

Axis per column

Axis	Min	Max	Log	Invert
Score	60 ✕	1088 ✕	<input type="checkbox"/>	<input type="checkbox"/>

Figure: Selecting the data to be displayed in the distribution plots, note that multiple columns can be selected.

A wide range of statistics can be displayed in the table below the distribution plots. These can be configured using the Statistics tab in the either the Header Panel or Footer Panel areas of the dialog e.g.

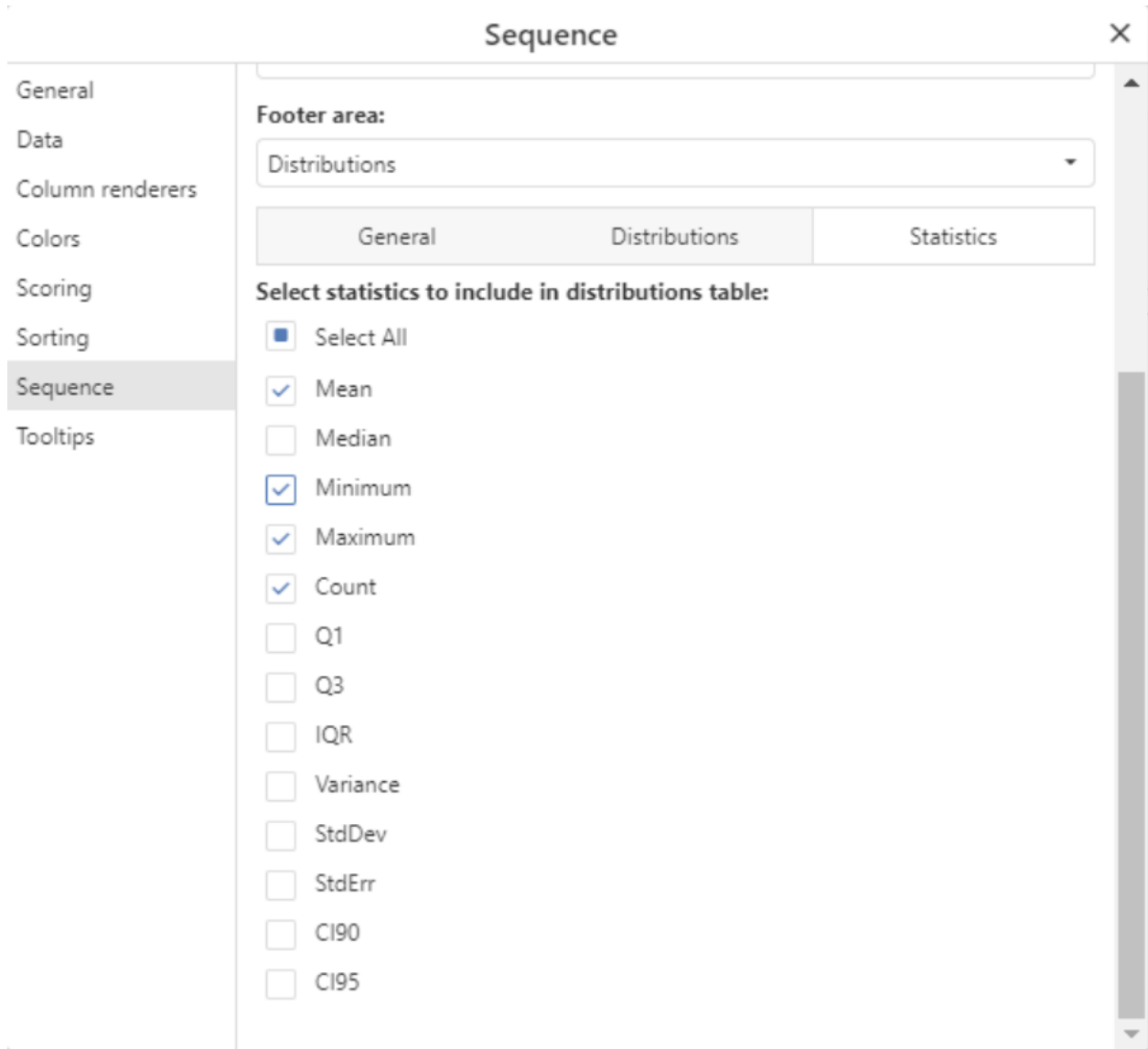


Figure 12: Selecting which statistics to display in the distribution plots.

The table below describes each of the statistics that can be added to the statistics table in the distribution plots.

Statistic	Description
Mean	Arithmetic mean of the dataset.
Median	The value separating the higher half of the dataset from the lower half.
Minimum	The minimum value in the dataset.

Maximum	The maximum value in the dataset.
Count	The number of values in the dataset.
Q1	The first quartile.
Q3	The third quartile.
IQR	The interquartile range.
Variance	The sample variance of the dataset.
StdDev	The sample standard deviation of the dataset.
StdErr	The sample standard error.
CI90	The 90% confidence interval of the dataset.
CI95	The 95% confidence interval of the dataset.

Marking is possible in the distribution charts. This is accomplished by drag selecting the region to be marked, this can be used in conjunction with the ctrl key to extend the selection. If the MSA visualization is in [internal limit-by-marking](#) mode, the distribution chart will respond to marking from other areas of the MSA visualization or can be used to drive marking.

Neighbor Properties Visualization

The Neighbor Properties visualization facilitates exploration of similarity relationships in sets of small-molecule chemical structures. It also helps to identify and visualize pairs of structurally related compounds that have large differences in associated properties. Activity cliffs are a noteworthy application for which the Neighbor properties visualization excels.

To use the Neighbor Properties visualization, a data table containing chemical structures (in SMILES or MOL format, CDX is not supported) and at least one column containing numeric properties is required. Following computation of near neighbors, the initial view of the results will display a grid of structures as shown in the following figure. By default the landing page shows the first 250 filtered structures in the data table. The landing page responds to Spotfire filters and the filters view may be used to rapidly identify compounds of interest. The following columns are added to the data table to facilitate filtering:

Neighbor transition counts	The column value is the number of near neighbors that are in a different category from the compound. If the compound is not in a category the value is 0. This column may be used to rapidly filter for activity cliffs
----------------------------	---

Upper neighbor counts	Given that the compound is in the high category the column value is the number of near neighbors that are also in the high category. If the compound is not in the high category or has no neighbors in the high category the value is zero. Use this column to identify clusters of high activity.
Lower neighbor counts	Given that the compound is in the low category the column value is the number of near neighbors that are also in the low category. If the compound is not in the low category or has no neighbors in the low category the value is zero. Use this column to identify clusters of low activity.

The upper and lower neighbor counts columns are exclusive in that, by definition, no compound may have a value greater than 0 in both columns.

This example initial view shows an HTS dataset of 165,000 compounds filtered to identify 68 compounds of high activity that have 2 or more neighbors also with high activity and at least 2 transition neighbors of low activity. Each compound is represented by a tabular card containing structure, identifier and one or two properties.

Lead Discovery ChemCharts

MOLECU... 250083 PRIMARY... 242.99

MOLECU... 334474 PRIMARY... 242.99

MOLECU... 334001 PRIMARY... 242.99

MOLECU... 311517 PRIMARY... 242.99

MOLECU... 334251 PRIMARY... 242.99

MOLECU... 334304 PRIMARY... 242.99

MOLECU... 250438 PRIMARY... 242.99

MOLECU... 334234 PRIMARY... 242.99

MOLECU... 334301 PRIMARY... 242.99

MOLECU... 311515 PRIMARY... 242.99

MOLECU... 254058 PRIMARY... 242.99

MOLECU... 333688 PRIMARY... 242.99

MOLECU... 333985 PRIMARY... 242.99

MOLECU... 334150 PRIMARY... 242.99

MOLECU... 334233 PRIMARY... 242.99

MOLECU... 333978 PRIMARY... 242.99

MOLECU... 140991 PRIMARY... 179.35

MOLECU... 334040 PRIMARY... 217.24

MOLECU... 254037 PRIMARY... 225.24

MOLECU... 344050 PRIMARY... 172.01

MOLECU... 250482 PRIMARY... 242.99

MOLECU... 334151 PRIMARY... 242.99

MOLECU... 254954 PRIMARY... 242.99

MOLECU... 334490 PRIMARY... 242.99

MOLECU... 334377 PRIMARY... 242.99

MOLECU... 334302 PRIMARY... 242.99

MOLECU... 334247 PRIMARY... 242.99

MOLECU... 253589 PRIMARY... 242.99

MOLECU... 334472 PRIMARY... 242.99

MOLECU... 254563 PRIMARY... 242.99

MOLECU... 334249 PRIMARY... 242.99

MOLECU... 254698 PRIMARY... 242.99

MOLECU... 334249 PRIMARY... 242.99

MOLECU... 150033 PRIMARY... 242.99

MOLECU... 254378 PRIMARY... 242.99

MOLECU... 334460 PRIMARY... 242.99

MOLECU... 334273 PRIMARY... 242.99

MOLECU... 334231 PRIMARY... 242.99

MOLECU... 334310 PRIMARY... 242.99

MOLECU... 250471 PRIMARY... 242.99

MOLECU... 333877 PRIMARY... 242.99

MOLECU... 254440 PRIMARY... 242.99

MOLECU... 257887 PRIMARY... 242.99

MOLECU... 253684 PRIMARY... 242.99

MOLECU... 253980 PRIMARY... 242.99

MOLECU... 254370 PRIMARY... 242.99

MOLECU... 334473 PRIMARY... 242.99

MOLECU... 257884 PRIMARY... 242.99

MOLECU... 333909 PRIMARY... 242.99

MOLECU... 257858 PRIMARY... 242.99

MOLECU... 334300 PRIMARY... 242.99

MOLECU... 380123 PRIMARY... 242.99

MOLECU... 330200 PRIMARY... 242.99

MOLECU... 314217 PRIMARY... 242.99

MOLECU... 314218 PRIMARY... 242.99

MOLECU... 254658 PRIMARY... 242.99

MOLECU... 334374 PRIMARY... 242.99

MOLECU... 380109 PRIMARY... 242.99

MOLECU... 254368 PRIMARY... 242.99

MOLECU... 182470 PRIMARY... 242.99

MOLECU... 254377 PRIMARY... 242.99

MOLECU... 253981 PRIMARY... 242.99

MOLECU... 312488 PRIMARY... 242.99

MOLECU... 254552 PRIMARY... 242.99

MOLECU... 253390 PRIMARY... 242.99

MOLECU... 314227 PRIMARY... 242.99

MOLECU... 314228 PRIMARY... 242.99

MOLECU... 254538 PRIMARY... 242.99

Filters

Type to search filters

MOLECULE_ID
117
509193

PRIMARY WT 21P (21PCT), DX BE.
-20.87
243.62

STDEV
0.00
77.33

COUNT
1
31

SMILES
Type to filter by text

NearNeighbors
Type to filter by text

Neighbor Transition Counts
2
10

Upper Neighbor Counts
2
10

Lower Neighbor Counts
0
10

2 filters changed

Neighbor Transition Counts: (2 << >>)

Upper Neighbor Counts: (2 << >> Up...)

68 of 165,036 rows 0 marked 9 columns

Figure: Initial view of Neighbor Property results.

After using filters to narrow the set of structures to those of potential interest, click on a structure to begin exploring its near neighbors. The view will change such that the selected structure is centered in the visualization with near neighbors arranged in concentric circles based on their similarity (such that the inner circle is the 10 nearest neighbors of the center structure and the outer ring comprises neighbors of the inner circle).

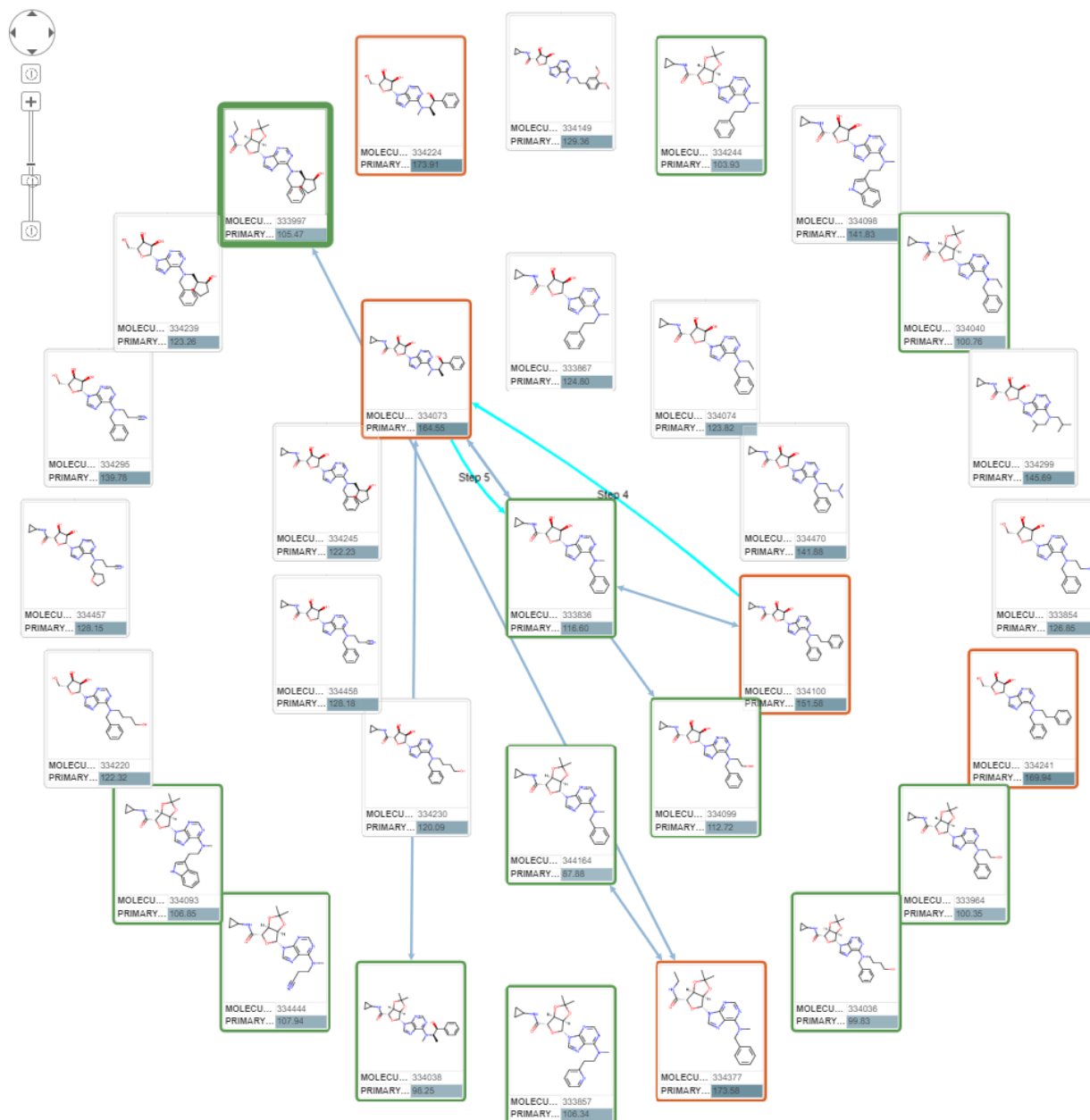


Figure: Viewing near neighbors and property differences.

Clicking on any visible structure will update the visualization with the selected structure becoming the new center with that structure's neighbors displayed in the concentric circles.

Context menu

Much of the functionality of the Neighbor Properties visualization is accessed through the context menu, which is opened by clicking the right mouse button anywhere in the visual. An example of the context menu for the Neighbor Properties visualization is shown in the figure below.

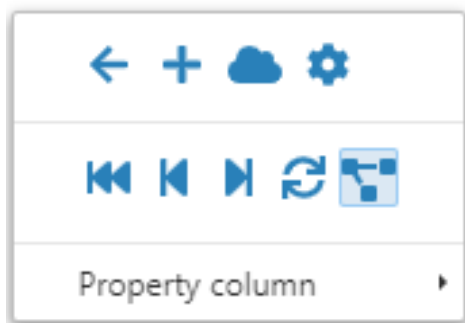












Figure: The Neighbor Properties context menu.


The table below describes the function of each context menu item:

	Back: returns the user to the visualization 'home' page where the user can select a different visualization or data table to display in the current ChemCharts visualization.
	Add visualization: adds a new ChemCharts visualization to the current page. Used primarily in the web player.
	Web services: opens the web services dialog.
	Properties: opens the Properties dialog.
	Reset to original layout: sets the visualization to the initial grid view of the data. This icon is not present if you are on the initial view.
	Previous layout: resets the visualization to the last selected structure or the grid view, depending on the selection history. This icon is not present if you are on the initial view.
	Next layout: resets the visualization to the next selected structure. This icon will not be present if you are on the final layout.
	Redraw current layout: resets the current layout to fill the visualization area, undoing zoom or translation changes.
	Display neighbor edges: toggles the gray lines indicating similarity

	relationships between neighbors.
Property column	Property column menu: allows the user to select the current property used for coloring.
	This option is only available when the context menu is activated over a structure. The structure will be selected and the visualization updated with the structure at the center. Additionally the row containing the structure will be marked replacing any marked selection in the datatable.

The following sections detail configuration and use of the Neighbor Properties visualization.

Create a Neighbor Properties visualization



Click the New Lead Discovery ChemCharts button  in the list of visualizations in Spotfire. A new Lead Discovery ChemCharts visualization will be added to the page. Select *Neighbor Properties* in the dropdown menu of available visualizations on the ChemCharts home page. If the data table has not been previously processed by the Neighbors Properties visual data a data function function will be called to calculate the nearest neighbors of each structure in the data table. The calculated nearest neighbors are encoded in JSON and added as a text column, called NearNeighbors, to the data table.

Depending on hardware, the data function will calculate neighbor lists for 150K compounds in under 10 minutes. For a larger number of compounds it may make more sense to calculate the neighbor lists asynchronously using the *Neighbor Properties* web-service.

If the data table currently configured for the visual doesn't contain the requisite information, the warning message "*Cannot find prerequisite columns for neighbor properties visual in current data table*" will be displayed.

Following the addition of the nearest neighbors a second data function is called to determine the counts columns used for filtering.

Exploring near neighbors

Clicking on any structure will update the visualization with the selected structure becoming the new center with that structure's neighbors displayed in the concentric circles. The visualization tracks the history of selected structures, such that the user can retrace a set of selections using the *Previous layout*  button from the [context menu](#). To undo all structure selections and revert the visualization back to the grid layout, click the *Reset to original layout*  button in the context menu. The position of the current display, whether grid or neighborhood, may be translated by clicking the left mouse button in whitespace within the visualization and dragging

to the desired new position. The display will update as the mouse is moved. The display may be made larger or smaller within the visualization either by mouse scroll, or using the navigation controls in the upper left corner.



Figure: Zoom and position control of the Neighbor Properties visualization.

Configuration

To alter the configuration, open the *Properties* dialog using the context menu and navigate to the *Neighbor properties* page.

Neighbor properties ✕

General	Nearest neighbors column:
Data	<input type="text" value="Molecule SMILES"/>
Colors	Property column:
Fonts	<input type="text" value="log SAU Gyr IC50"/>
Property columns	Second property label column:
Tooltips	<input type="text" value="Sau516 MIC"/>
Neighbor properties	ID column:
	<input type="text" value="External_ID"/>
	Fingerprint type:
	<input type="text" value="morgan"/>
	Outer ring size:
	<input type="text" value="20"/>
	<input checked="" type="checkbox"/> Show outer ring
	Structure depiction:
	<input checked="" type="checkbox"/> Align structures to center node (may impact performance)
	Edge labels:
	<input type="checkbox"/> Use change delta for transition edge labels
	Edge colors:
	Transition edge color <input type="text" value=""/>
	Neighbors edge color <input checked="" type="radio"/> None <input type="radio"/> User defined <input type="text" value=""/>
	Path edge color <input type="radio"/> None <input checked="" type="radio"/> User defined <input type="text" value=""/>
	Node borders:
	<input type="checkbox"/> Use column colors for node borders
	Categories:
	high <input type="text" value="75"/> <input type="text" value="Percentile"/> <input type="text" value=""/>
	low <input type="text" value="25"/> <input type="text" value="Percentile"/> <input type="text" value=""/>
<input type="button" value="Apply"/> <input type="button" value="Apply and close"/>	

Figure: The Neighbor properties page.

By default, the near-neighbors calculation is performed using compounds from the first structure column in the data table. If the data table contains multiple structure columns then the *Nearest*

neighbors column setting can be used to change the structure column used in the near neighbors calculation. Changing the Nearest neighbor column will result in the current stack of compound concentric views being discarded.

The Property column is used for coloring the border around structures and drawing arrows indicating large property differences between structures in the neighborhood display. The column may be changed using the *Property column* dropdown menu, or the *Property column* dropdown menu in the [context menu](#). The cutoff value used for coloring structure borders is specified in the *Thresholds* section. The upper bound above which a color is applied is configured on the line beginning with *upper*. The box on the far right of the *upper* line is a color control used to select the color that indicates rows with values exceeding the upper threshold value. The lower bound below which a color is applied is configured on the line beginning with *lower*. The border color that indicates row values falling below the lower threshold may be selected using the color control on the far right of the line. Color rules may be used as an alternative to the threshold border color scheme. Checking the box next to *Use column colors for node borders* will color the borders surrounding structures using a color rule defined for the selected Activity column.

An optional *Second property label column* may be selected. Values from that column will be included as an additional row on each compound card.

By default each compound in the visual is labelled its data table row number. Alternatively, an *ID column* may be selected and values from that column will be used as the compound label.

The near-neighbors lists that the visual uses are calculated using fingerprint types from RDKit. The fingerprint type (that defaults to Morgan) may be modified using the drop-down menu in the *Fingerprint type* section. Changing the fingerprint type will result in a new near-neighbors calculation and the current compound stack will be discarded.

The number of compounds shown in the outer ring is customized in the *Outer ring size* section. Increasing the number of compounds in the outer ring pull more compounds into the visual. Unfortunately, if a large number of compounds are present in the outer ring, the geometric constraints of displaying items in a circular ring mean that an increasing amount of white space is present in the visual. Depiction of the outer ring may be turned off using the checkbox.

The *Structure depiction* section contains a single option to align structures to the center compound. Selection of this option may result in a delay in rendering the neighbors visual. Furthermore, the identified alignment constraints may occasionally result in distorted structure depiction for the neighbor compounds.

Controls to alter the edge coloring and appearance are found in the *Edge colors* section. Transition edge color is used to indicate compounds that are structurally similar to each other, with one structure of the pair having an associated activity value below the lower threshold and

the other structure above the upper threshold. The *Transition edge color* is applied to the arrow in the neighborhood view that indicates an activity transition. The color may be altered using the color picker located to the right of *Transition edge color*. Neighbor edges indicate similar pairs of structures. The default neighbor edge color is gray, although it may be altered by selecting the *User defined* radio button and selecting a color with the color control that will appear on the right of the *Neighbors edge color* line. Each structure selected resulting in a neighborhood view is referred to as a step in the exploration path. When structures present in a neighborhood view were selected in previous steps, an edge (arrow) will be drawn between the structures with text indicating the *Step #* appearing next to the midpoint of the edge. Path edges coloring may be hidden by selecting the *None* radio button on the *Path edge color* line. The path edge color may be altered by selecting the *User defined* radio button and selecting an alternate color using the color control located on the far right of *Path edge color*. It is often the case that no paths will be present in a neighborhood view.

By default up to 5 property columns are shown in the *Property column* dropdown menu, or the *Property column* dropdown menu in the [context menu](#). To modify either the columns available or the order of the columns in either dropdown menu navigate to the *Property columns* page in the *Properties* dialog and move the desired columns into the *Chosen* panel in the required order.

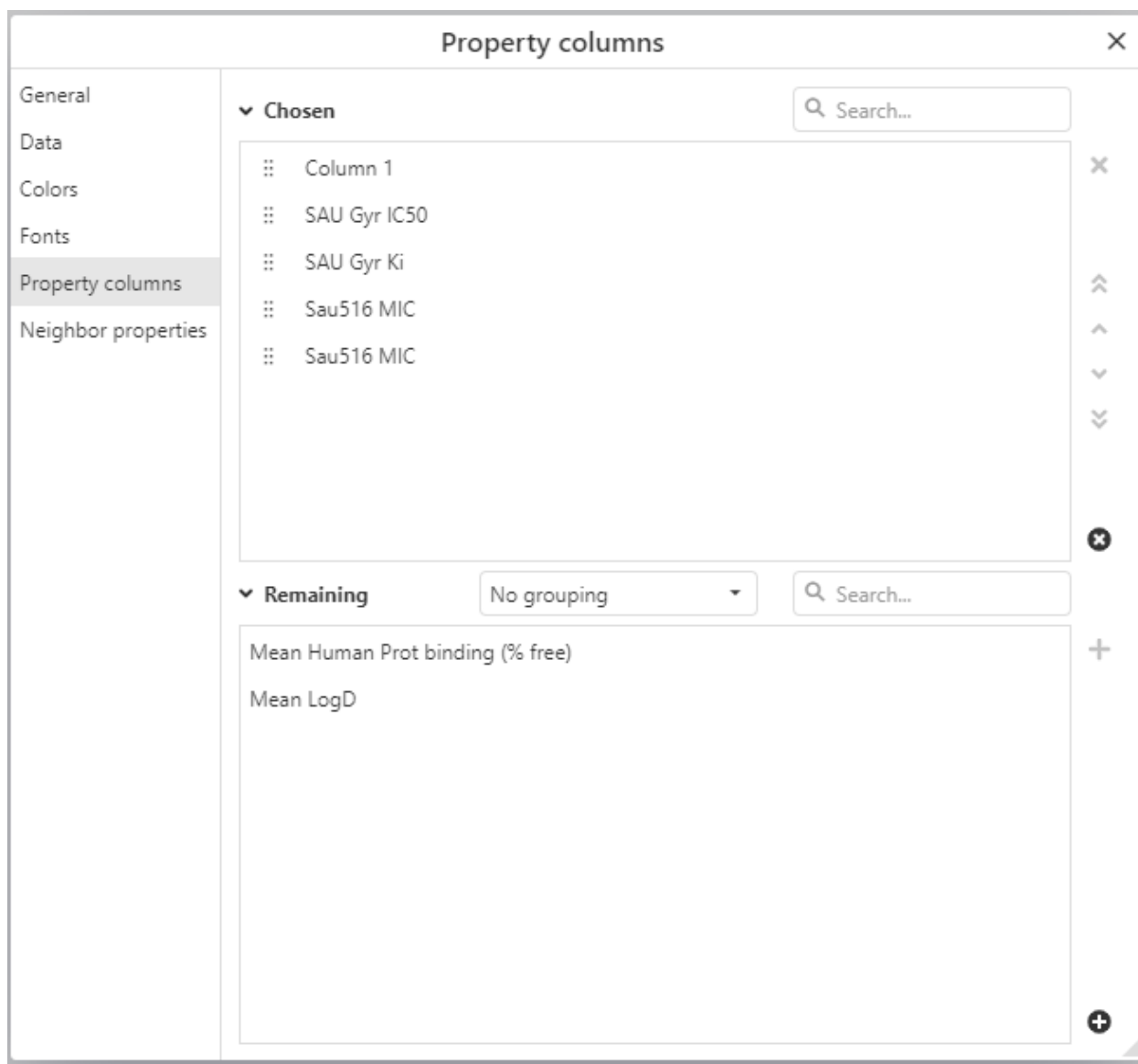


Figure: The Property columns page

Unlike other ChemCharts properties, modification of the neighbors property setting is not performed immediately (because modifying the visual can be time consuming). The *Apply* and *Apply and close* buttons are used to apply changed properties to the visual.

The column colors and tooltip settings defined in the properties pages are used to color properties in the neighbor property structure cards and define the tooltip used in the neighbors visual as shown in the figure below.

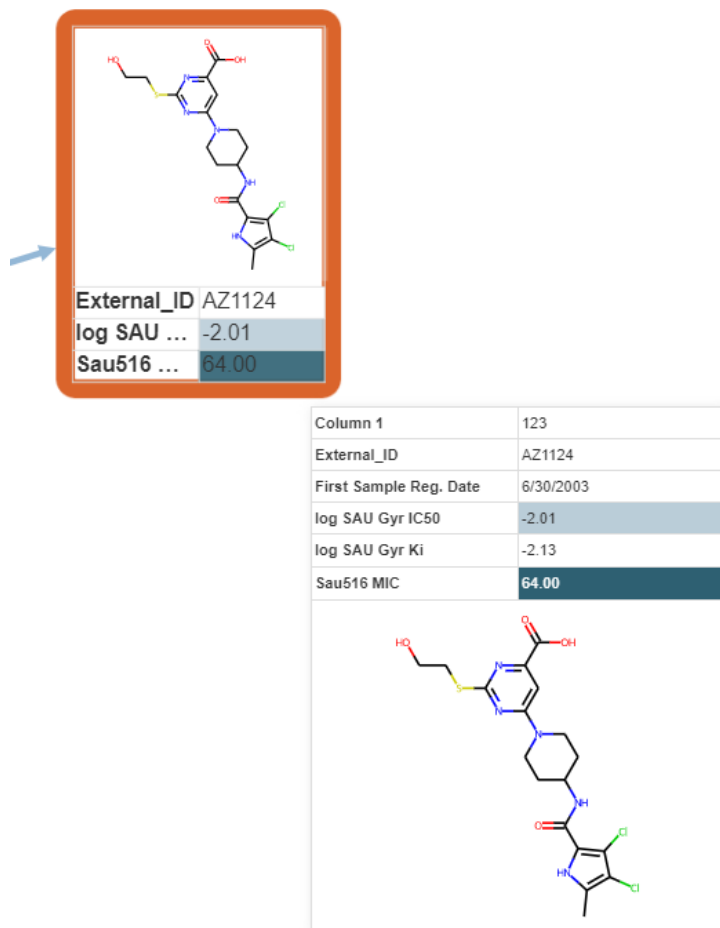


Figure: Neighbor property node coloring and form-based tooltip

Radar Visualization

The Radar visualization (also known as a spider, web or polar chart) is used to display data from 3 or more quantitative columns in a data table. Each axis starts from the same point at the center of the chart. The axes are distributed at equal angle increments around the origin at the center of the chart. Each item plotted on the chart is represented as a polygon formed by joining the points for the item on each axis.

The Radar visualization is used in conjunction with a second visualization (such as a Table or Gallery visualization) where the Radar visualization displays data from items that a user either marks or makes the active item (usually by hovering the mouse over the desired item). As the user marks items or changes the active item in the other visualization, the Radar visualization will update to display the data for these items. Some of the important features of the Radar visualization are provided below:

- Hovering over the label for an item or the item polygon, will highlight the item and make it the active item. The active item will be highlighted in other open visualizations in Spotfire.
- Up to 10 items can be displayed in a radar visualization.
- Axes can be added, removed or modified.
- The column from the underlying data table used to label the items can be configured.
- Trellis display is possible.

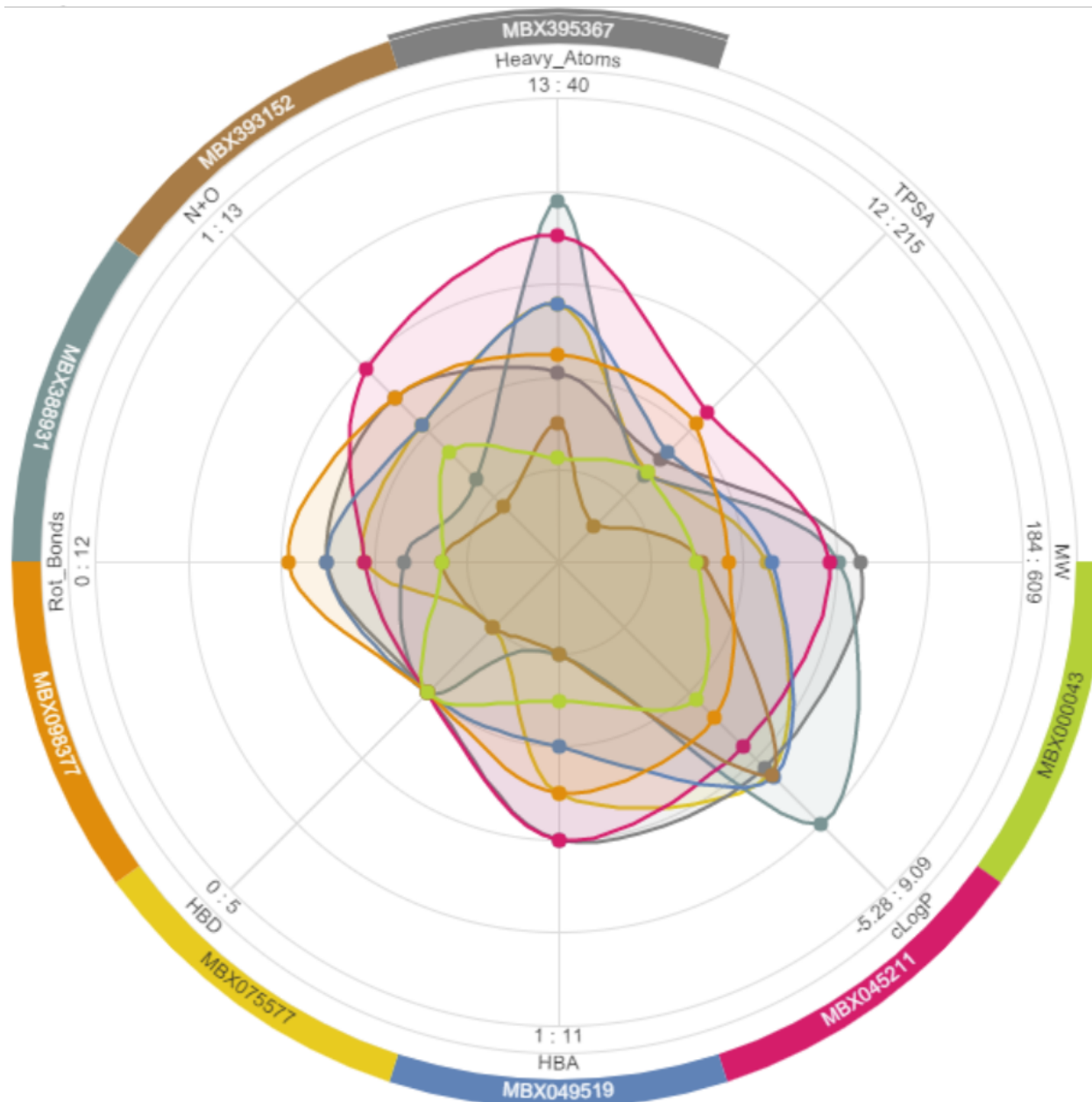


Figure: Lead Discovery ChemCharts Radar visualization.

As evident from the previous figure, the items that are displayed in the radar visualization are plotted as shapes where each vertex is a point on an axis. The lines connecting the points can

either be straight or curved. Each item is given a unique color and the legend for each item is displayed around the border of the radar chart. The title for each axis is displayed as well as the minimum and maximum values.





Context menu

Much of the functionality of the Radar visualization is accessed through the context menu, which is opened by clicking the right mouse button anywhere in the visual. An example of the context menu for the Radar visualization is shown in the figure below.




Figure: The Radar visualization context menu.

The table below describes the function of each context menu item:

	Back: returns the user to the visualization 'home' page where the user can select a different visualization or data table to display in the current ChemCharts visualization.
	Add visualization: adds a new ChemCharts visualization to the current page. Used primarily in the web player.
	Web services: opens the web services dialog.
	Properties: opens the Properties dialog.

Create a Radar visualization

Click the New Lead Discovery ChemCharts button  in the list of visualizations in Spotfire. A new Lead Discovery ChemCharts visualization will be added to the page. Select *Radar* in the dropdown menu of available visualizations on the ChemCharts home page. A radar chart should appear. If there are fewer than 3 numeric columns in the underlying data table, a 'Cannot draw Radar with less than 3 axes' warning will be displayed. To see what columns are available to display in the radar visualization navigate to the Axes page in the *Properties* dialog.

Add a new axis


To add a new axis, open the Properties using the [context menu](#) and navigate to the Axes page. Use the column select box and the *Add* button at the bottom of the list of current axes, to add a

new row to the list. Use the *Axis* dropdown menu in the newly added row to change the data column. The min and max text boxes in the *Range* column may be used to set the bounds of the axis. Checking the *Log* checkbox will apply the base 10 Log function to values plotted in the Radar visualization. By default the axes are drawn with the minimum at the center of the radar chart and the maximum at the edge. Checking the *Invert* checkbox on an axis will invert the axis i.e. draw the maximum value at the center of the circle and the minimum value at the edge.

Ordering axes

The axes in the radar visualization can be ordered by dragging and dropping the appropriate rows in the *Axes* panel of the property dialog.

Remove an axis

To remove an axis, open the Properties dialog using the context menu and navigate to the *Axes* page. Click the Delete  button on the far right of the axis to be deleted.

Item label

It is possible to change the column from the data table that is used to label each of the items in the Radar visualization. Open the Properties using the [context menu](#) and navigate to the *Appearance* page. Select the column that will be used to provide labels for the items from the *Labels* dropdown menu.

Radar shapes

The shapes created by joining the points for each of the items can be displayed using straight or curved lines. Open the Properties using the [context menu](#) and navigate to the *Appearance* page. Check (or uncheck) the *Curved shapes* checkbox to produce the desired shapes.

Trellis

An alternative means of viewing multiple row values overlaid on a single Radar chart is to use a trellis view. Open the Properties using the [context menu](#) and navigate to the *Appearance* page. Check the box next to *Enable trellis* and configure the number of *Trellis columns* using the number box.

Color areas

Colored areas can be added to the Radar chart. These are created by defining minimum and maximum bounds for each of the axes in the chart and assigning a color to the area defined by the bounds. An example is shown in the figure below.

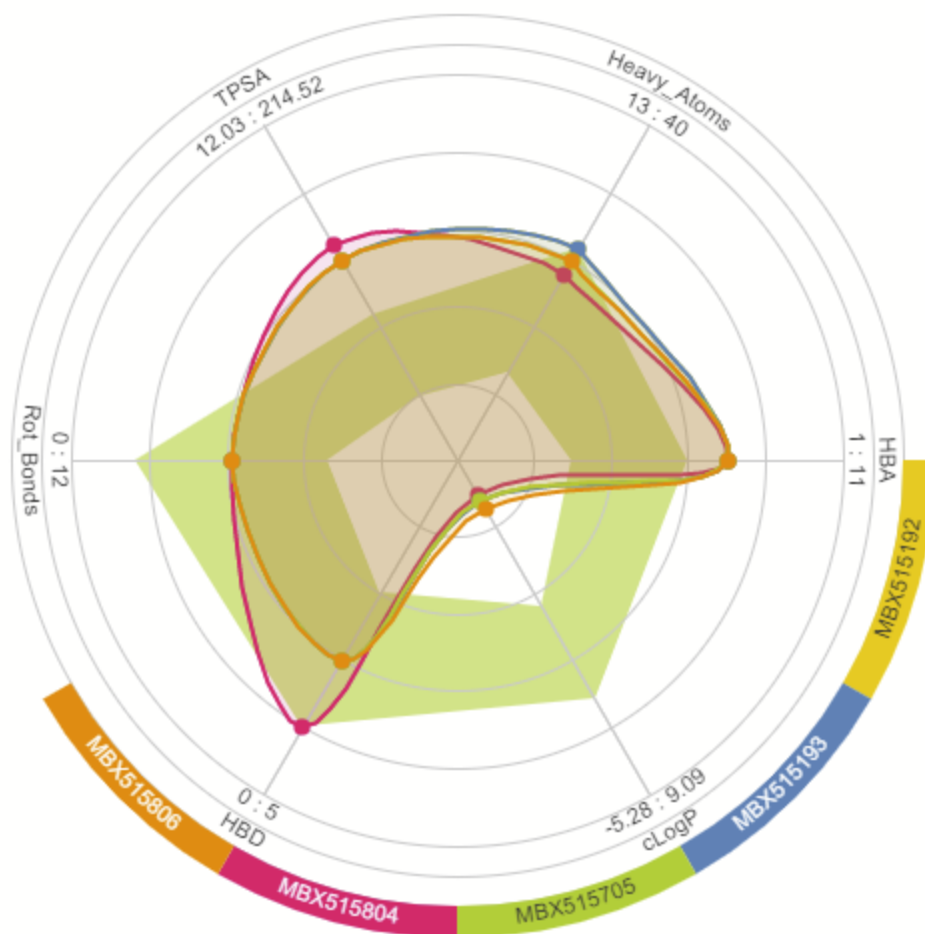



Figure Color area in the radar visualization.

To add a color area to the radar visualization open the property dialog and navigate to the *Color area* panel. Clicking the *Add* button will add a new color area to the visualization. Users can edit the color and name for the area, order the color areas (if there are more than 1) and remove it by clicking the  button on the right-hand side. The bounds for each axis defining the color area can be edited by selecting the desired color area and entering the minimum and maximum values.

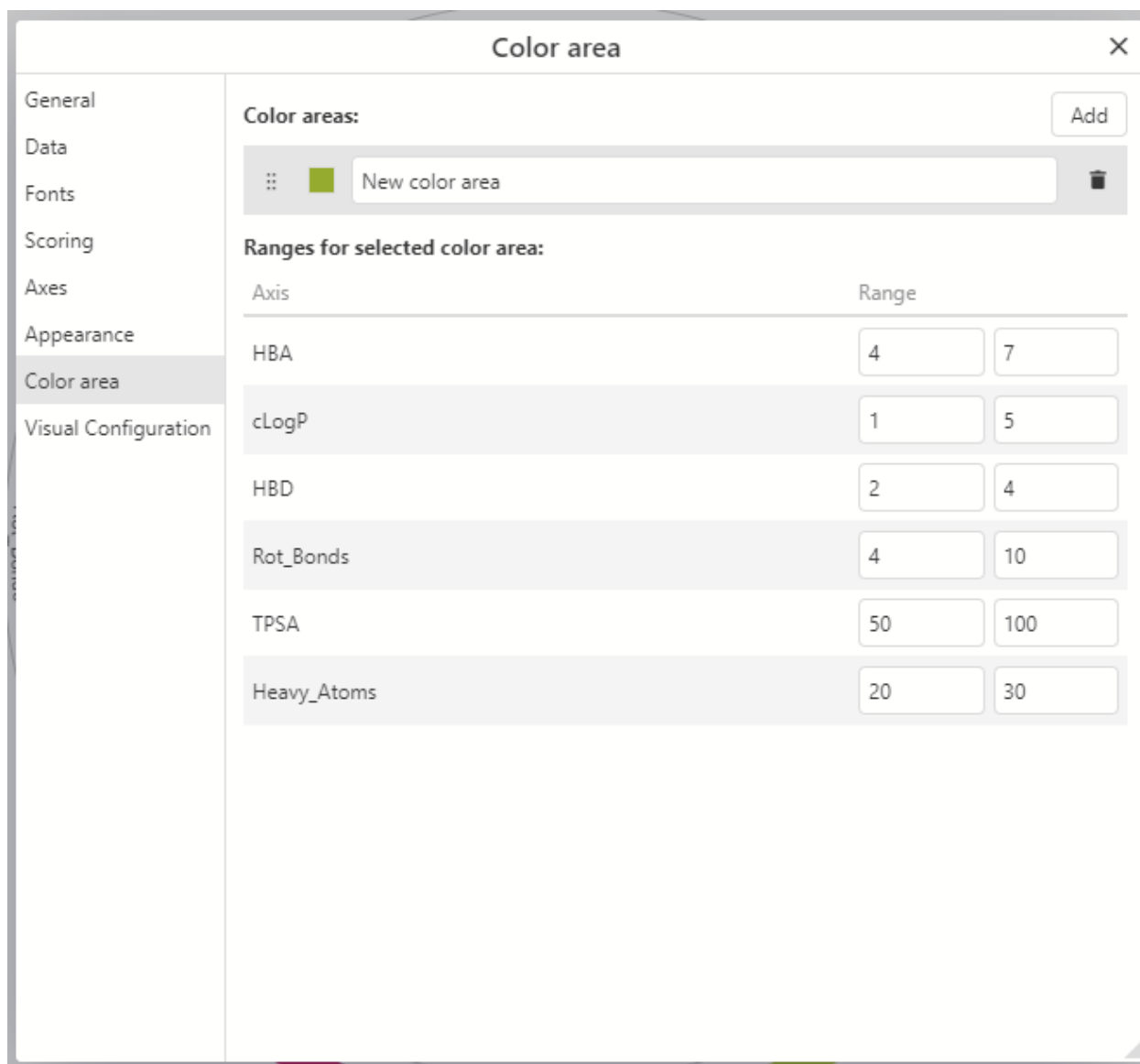


Figure Configuring a color area

SAR Map Visualization

The Lead Discovery ChemCharts SAR Map visualization is used to explore sets of molecules and their associated properties if the structures are related by a conserved core that has at least two variable positions. An R-Group decomposition must be performed prior to visualizing the data sets in a SAR Map visualization. The SAR map is created by listing all substitutions at a given position for the core along the x-axis and all the substitutions for another position for the core along the y-axis. The cells in the grid represent the molecules that contain the core and the R-Groups at the corresponding positions along the x and y axes. If there are more than 2 substitution positions around the core, it is possible to have multiple molecules (exemplars) contained in each cell. The grid is organized such that the cells containing the largest number of exemplars are displayed in the top-left corner of the grid.

An example R-Group decomposition for the first 3 molecules of a larger set is shown in a Lead Discovery ChemCharts [Table](#) visualization below.

Lead Discovery ChemCharts					
	Structure <MOLFIL...	Core	R1	R2	R3
1					
2					
3					
4					

Figure: Example results from an R-Group decomposition displayed in a Lead Discovery ChemCharts Table visualization. The core piperidine ring has 3 points of substitution, with the substitutions at the attachment points shown in the R1, R2 and R3 columns.

The SAR Map visualization created from the example decomposition shown above is displayed in the next screen capture. In this example R1 is plotted along the x-axis and R3 is plotted on the y-axis. The number of molecules that contain each instance of R1 and R3 is displayed in the cells within the SAR map. For example, there are 44 molecules in the highlighted cell where

R1 is and R2 is i.e. there are 44 variations in substitution at R2.

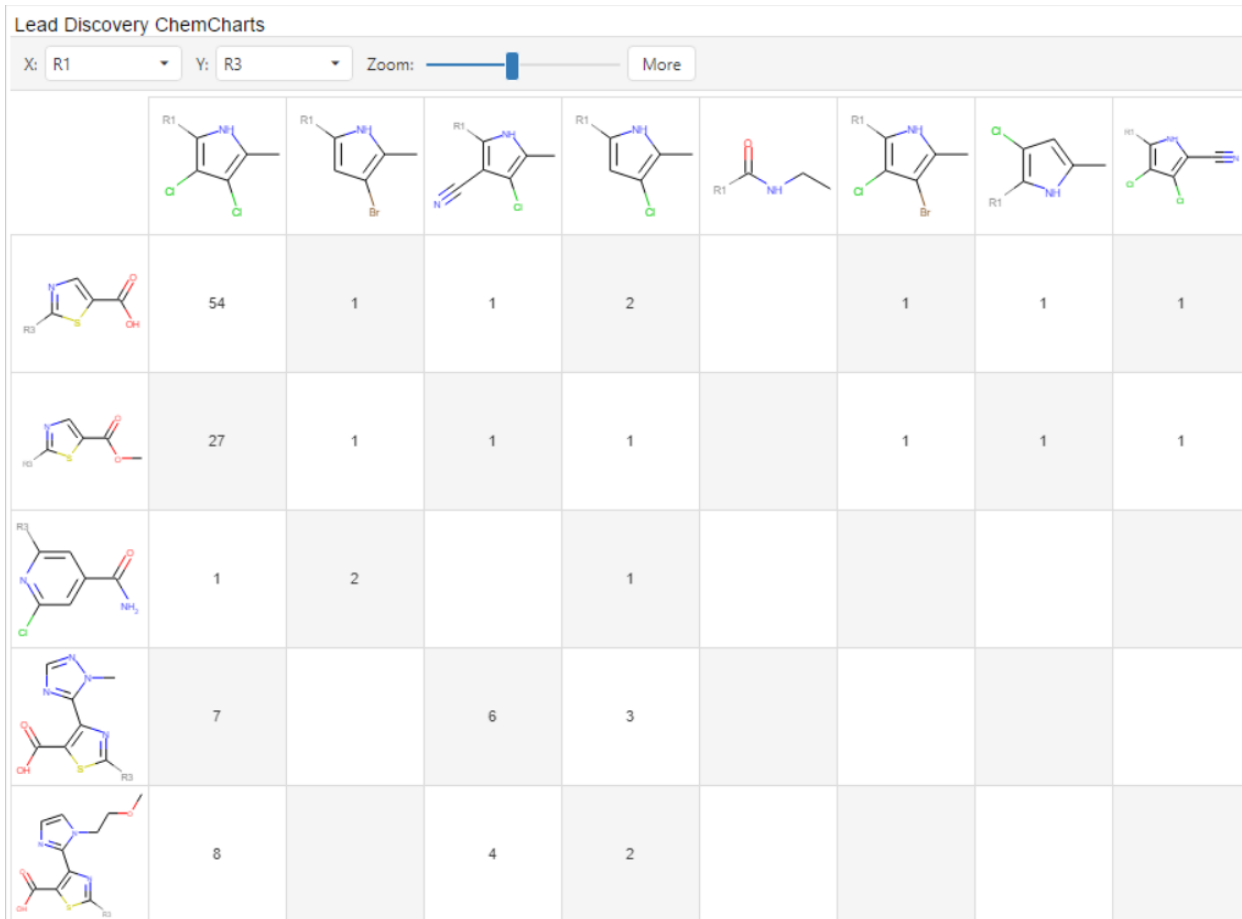


Figure: Example SAR Map visualization.

The SAR Map visualization interacts with Spotfire in an intuitive manner, for example:

- Marking a cell within the SAR map will mark all the corresponding items in other charts. In the example above, if the cell containing the 44 exemplars is marked and another visualization is open, the 44 corresponding items would be marked in the other visualization. Multiple cells can be marked or unmarked using mouse clicks in conjunction with the Ctrl key.
- Marking one of the R-Groups on the x and/or y axis will result in all the cells in the row or column being marked. As before, the marking is transmitted to any other open visualizations. Multiple rows and/or columns can be marked or unmarked using mouse clicks in conjunction with the Ctrl key.
- The SAR Map visualization responds to active item changes from other visualizations i.e. as items are highlighted (usually by hovering the mouse over a point or row) the corresponding cell which contains that item will be highlighted.
- The data displayed in the SAR Map can be limited by one or more markings from other visualizations (see [Limit by Marking](#)) or by applying one or more of the many possible Spotfire filters.

Viewing Exemplar Molecules

An effective technique to view exemplar molecules contained in a cell is to open another visualization in Spotfire, such as the Lead Discovery ChemCharts [Table](#) or [Gallery](#) visualization, and configure the associated visualization to only display marked items (see [Limit by Marking](#)). As cells in the R-Group grid are marked, the data in the other 'limit by marking' visualization will update to display the exemplar molecules and their associated data. If one of the R-Groups on either the x or y axis is marked, all the cells that contain that R-Group will be marked and the other 'limit by marking' visualization will update to display all the molecules that contain the selected R-Group.

Context menu

As with all the visualizations in Lead Discovery ChemCharts, much of the functionality of the SAR Map visualization is accessed through the context menu, which is opened by right clicking anywhere in the visual. An example of the context menu for the SAR Map visualization is shown in the figure below.

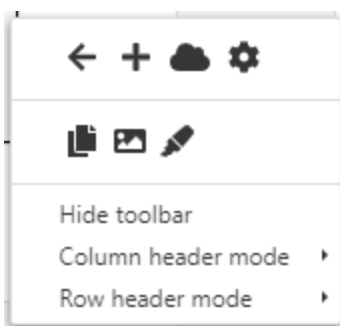









Figure: The SAR Map context menu.

The table below describes the function of each context menu item:

	Back: returns the user to the visualization 'home' page where the user can select a different visualization or data table to display in the current ChemCharts visualization.
	Add visualization: adds a new ChemCharts visualization to the current page. Used primarily in the web player.
	Web services: opens the web services dialog.
	Properties: opens the Properties dialog.
	Copy: opens the Copy dialog for copying specified content to the clipboard.

	Tooltips: opens the tooltips control for the visualization.
	Limit by marking: toggles the limit by marking behavior of the visualization
Hide toolbar	Hides the toolbar at the top of the SAR Map visualization.
Column header mode	Opens the column header submenu controlling the appearance of structures on the column header. Options are <i>None</i> , <i>Linear</i> , and <i>Offset</i> .
Row header mode	Opens the Row header submenu controlling the appearance of structures on the row header. Options are <i>None</i> , <i>Linear</i> , and <i>Offset</i> .

Cell renderer configuration

There are several options for data display in the SAR Map cells: count, text, and bar. To select a cell renderer, open the Properties dialog using the context menu and navigate to the SAR map page. Use the *Cell renderer* dropdown menu to select [Count](#), [Text](#), or [Bar](#). Additional configuration is required for Text and Bar cell renderers. After selecting the Text or Bar cell renderer, an additional dropdown multiselect menu will appear for configuring columns for Text or Bar cell renderer display. An example configuration is shown in the next figure.

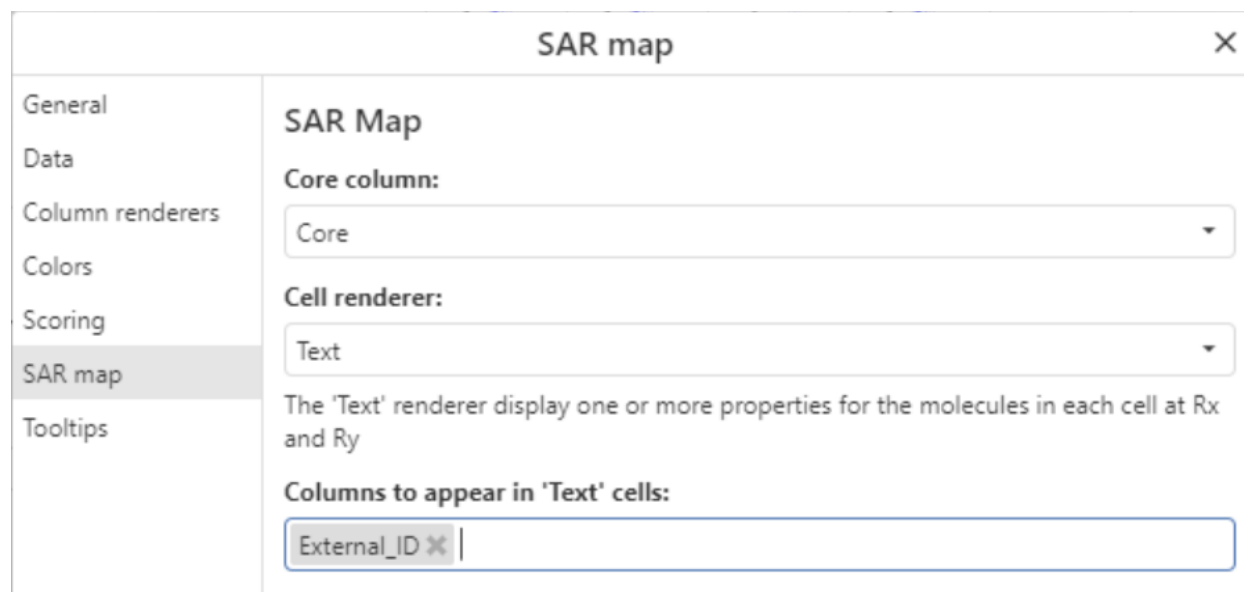


Figure: Configuring a Text cell renderer in the SAR Map.

Count cell renderer

The Count cell renderer is the default for the SAR Map. The Count cell renderer simply shows the number of exemplars represented by each cell. An example is shown in the next figure.

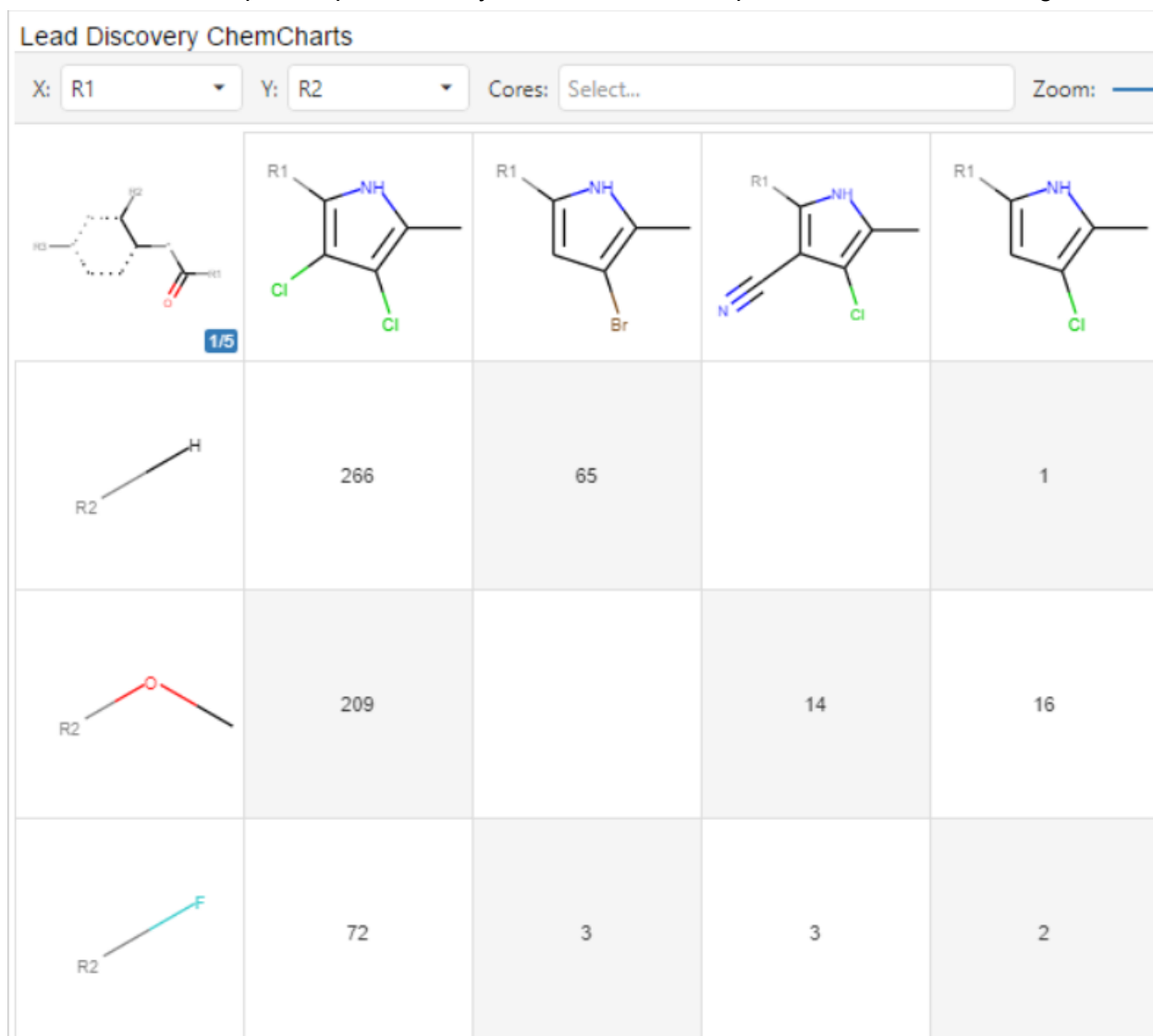


Figure: The SAR Map configured with a Count cell renderer.

Text cell renderer

SAR Map grid cells may be configured to display the exemplar count for each cell, and data values associated with each cell. After setting the renderer value to Text, select the columns of data associated with each exemplar to be displayed in the cell. The next figure is an example of the SAR Map configured with the Text cell renderer.

Lead Discovery ChemCharts

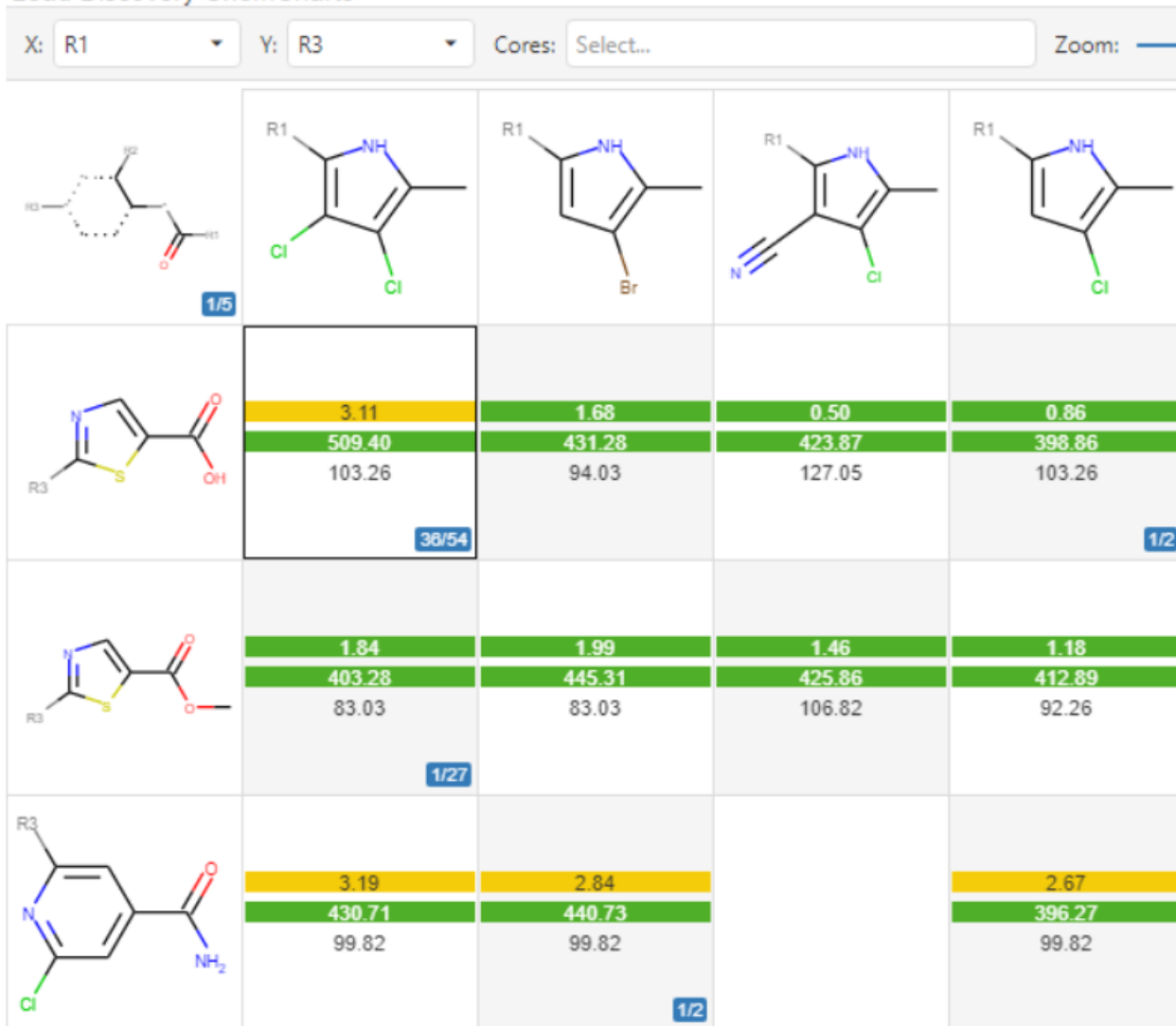


Figure: The SAR Map configured with a Text cell renderer.

Bar cell renderer

The cells within the SAR Map grid may be configured to display information about the properties and associated data for the population of exemplar molecules represented within the cells. This relies on configuring coloring rules for the properties of interest. For example, a coloring rule could be created for the molecular weight of the molecule where 0 to 500 is green, 500 to 550 is yellow and > 550 is red. Coloring rules can be created for any of the columns in the data table. Once coloring rules have been created, it is possible to display the number of molecules in each cell that belong to each color category. An example is shown in the figure below.

TIP: Coloring rules are configured in the *Colors* page in the *Properties* dialog. See the [Coloring](#) section for more information.

Lead Discovery ChemCharts

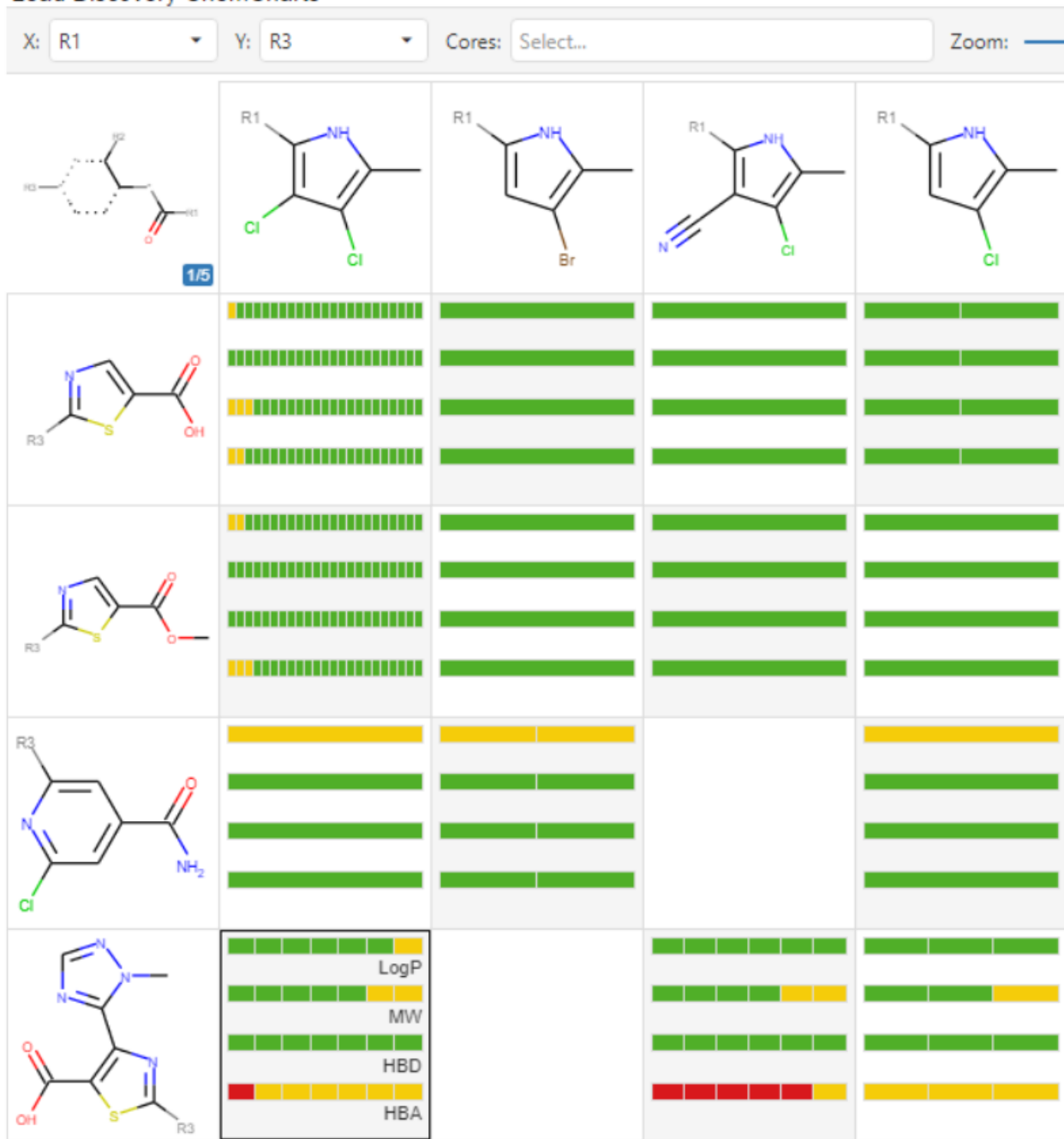



Figure: The SAR Map configured with a Bar cell renderer.

The following sections describe the configuration and use of the SAR Map visualization.

Create a SAR Map visualization

Click the New Lead Discovery ChemCharts button  in the list of visualizations in Spotfire. A new Lead Discovery ChemCharts visualization will be added to the page. Select *SAR Map* in the dropdown menu of available visualizations on the ChemCharts home page.

Tooltips

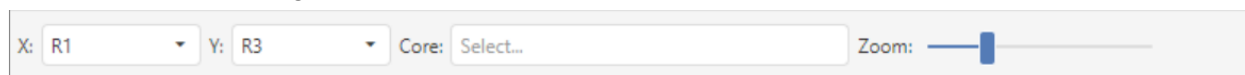
Molecule tooltips can be enabled or disabled in the *Tooltips* page of the *Properties* dialog, which may be opened using the [context menu](#). The *Tooltips enabled* checkbox controls whether tooltips are enabled or disabled. Advanced form-based tooltips are available by checking the *Use form-based tooltips* control. See the [Tooltips](#) sections for more information.

Limit by marking

Limit by marking can be enabled or disabled by clicking the toggle limit by marking button on the left hand side. See the [Limit by Marking](#) section for more information.

Change the R-Group axes

The control panel at the top of the SAR Map visualization provides facile access to select the structure column configuration for the X and Y axes.

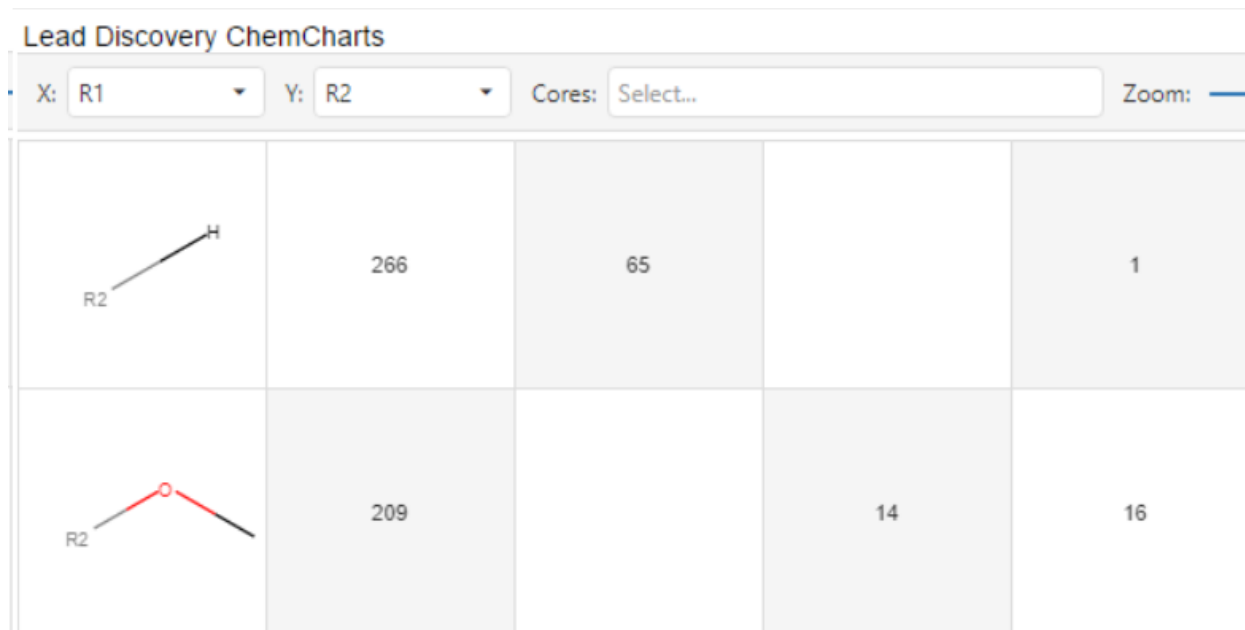



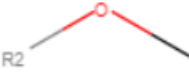
Configuring column or row headers

The column and row headers that display the R-Groups can be configured in one of three ways:

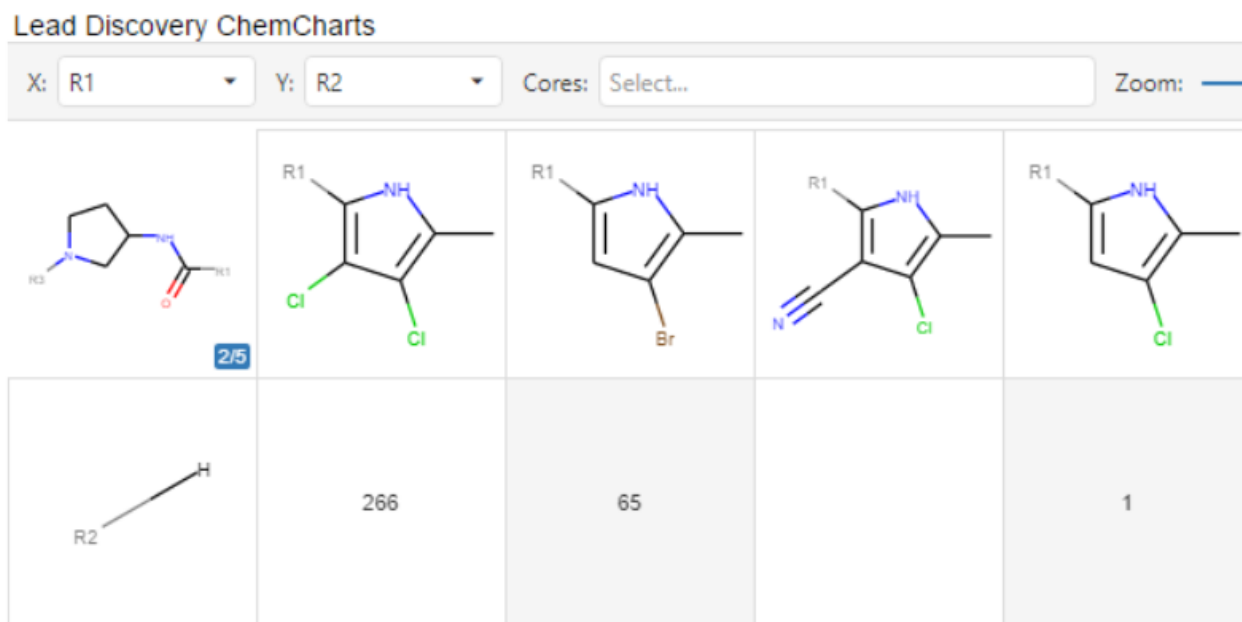
- None: Nothing is display for the header e.g.

Lead Discovery ChemCharts

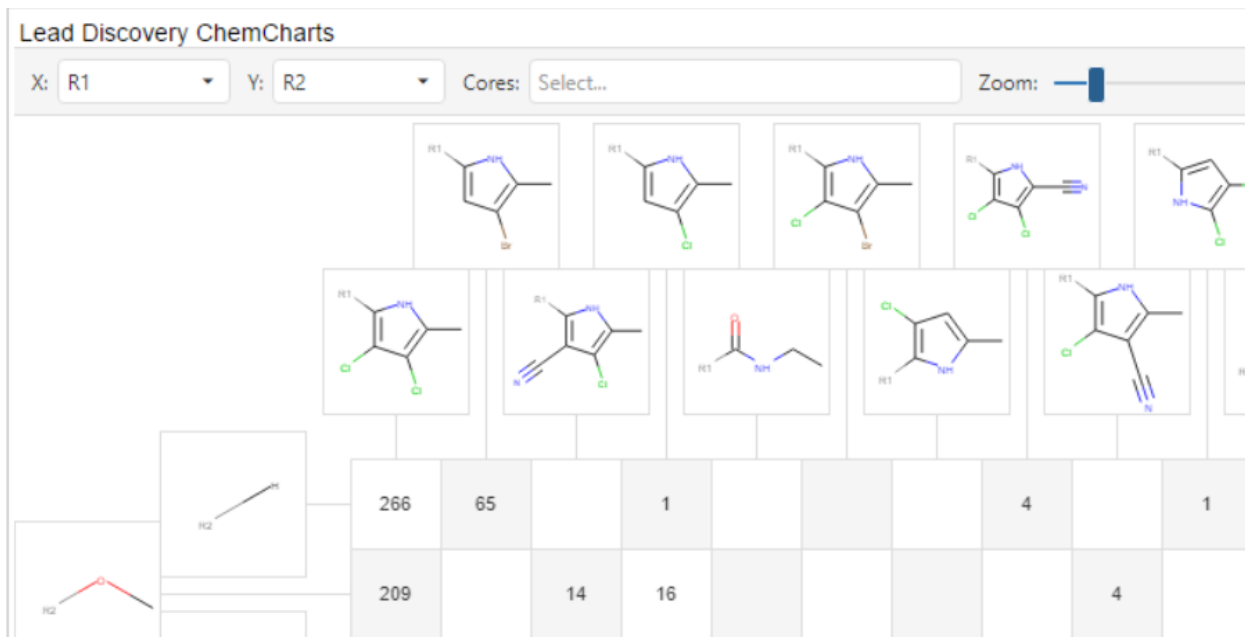


	266	65	1
	209	14	16

- Linear: The structures are displayed in a single column or row. e.g.



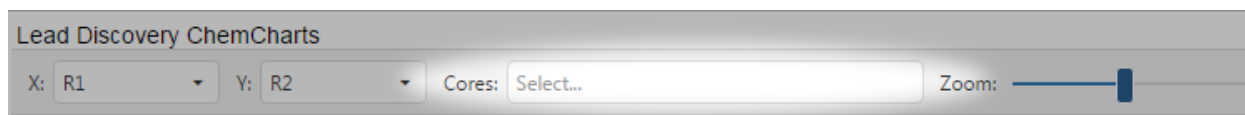
- Offset: The structures are displayed in two columns or rows and are offset to allow the display of larger structures e.g.



These options are all available from the context menu by right clicking and selecting one of the 3 modes from either the *Row header* or *Column header* submenus.

Limit the display using one or more cores

If the R-Group decomposition was created by using multiple cores it is possible to limit the display in the SAR Map by one or more of the cores. The cores must be present in the underlying data table for this to be possible. The core column is configured by opening the *Properties* dialog from the [context menu](#) and navigating to the SAR map page. Use the *Core column* control to select the column containing the core structures. After selecting the core column, the *Cores* menu in the top bar of the SAR Map will become enabled.



From the *Cores* dropdown menu it is possible to restrict what is displayed in the SAR map by checking or unchecking the core molecules. To remove the core filtering, open the *Properties* dialog from the [context menu](#) and navigate to the SAR map page. Select None in the *Core column* dropdown menu to remove the configured core column.

An example of Core selection is shown below.

Lead Discovery ChemCharts

X: R1 Y: R2 Cores: C0 X C1 X Zoom:

	259	65		4
	209		14	
	72	3	3	
	27		4	
	25		4	
	8		5	

Select All

Core 0

Core 1

Core 2

OK Cancel

Figure: Selecting cores from the Cores menu.

Structure Network Visualization

The Structure Network visualization assists in identifying structural and potentially synthetically interesting relationships within a set of compounds. For example, HTS data sets may be analyzed for common structural motifs found in active compounds. Structural analysis of any set of compounds that are related, yet not highly homologous, may be aided by the combination of the Core Decomposition web service and Structure Network visualization. The visualization is not intended for use with highly homologous structures such as in lead optimization, as it is unlikely to yield non-intuitive relationships.

To use the Structure Network visualization, a data table containing chemical structures must be submitted for preprocessing to the Core Decomposition Analysis web service. Upon returning results from the web service, selecting the *Automatically configure visualizations* option in the results dialog will configure the Structure network visualization to view the results. The initial display of the results is a tree-like network hierarchy representing the most common cores identified in the decomposition, with paths to the parent structures from which the cores were derived. The core nodes are arranged using a Sugiyama layout algorithm.

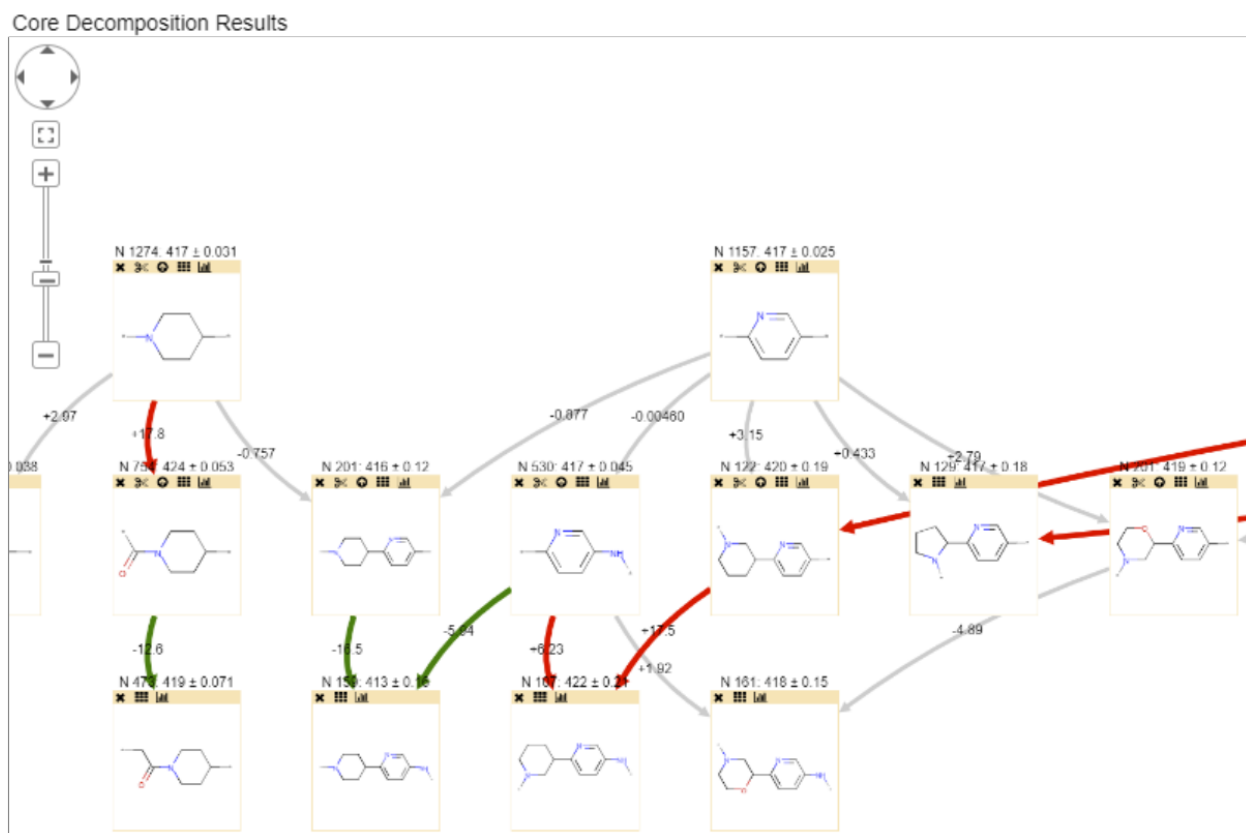


Figure: The Structure Network visualization.

The Core Decomposition Analysis web service decomposes sets of structures using either BRICS or Recap transformation rules. After one, two, and three BRICS transform rules are applied, the service builds a tree representing the most commonly observed cores found in the set of structures. The most commonly observed cores are arranged at the top of the Structure Network. The cores at the top of the visualization are commonly the smallest and most generic. The cores at the second and third levels moving downward in the display are more complex. Nodes displayed in the visualization may be expanded to inspect the structures from which the cores were identified. The arrows represent structural relationships between the cores. A core at the end of each arrow is a superstructure of the core at the arrow's origin. Activities of the parent structures for each node are compared using a standard two sample T-test comparing the parent activities (minus the child activities) with the child activities. Green arrows represent

transitions that improve activity (values are lower). Red arrows represent transitions where the activity declines (values are higher). The choice of arrow colors may be customized using the *Properties* dialog (see below).

Context menu

Much of the functionality of the Structure Network visualization is accessed through the context menu, which is opened by right clicking anywhere in the visual. An example of the context menu for the Structure Network visualization is shown below.

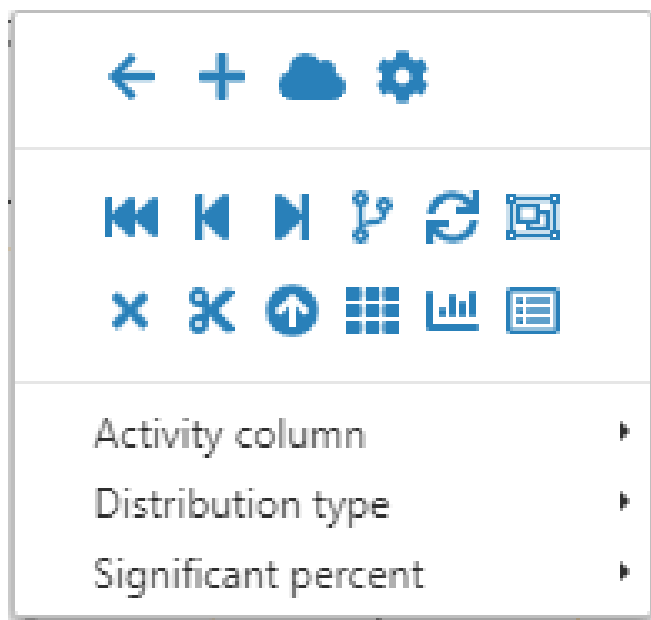

















Figure: The Structure Network visualization context menu.

The following table describes the function of each item in the context menu:

	Back: returns the user to the visualization 'home' page where the user can select a different visualization or data table to display in the current ChemCharts visualization.
	Add visualization: adds a new ChemCharts visualization to the current page. Used primarily in the web player.
	Web services: opens the web services dialog.
	Properties: opens the <i>Properties</i> dialog.
	Reset to original layout. This icon will not be present when viewing the original layout.

	Previous layout: undo the last change to the layout. This icon will not be present when viewing the original layout.
	Next layout: resets the visualization to the next selected structure. This icon will not be present if you are on the final layout.
	New layout: Recalculates node coordinates using Sugiyama layout (see description below).
	Redraw current layout: resets the current layout to fill the visualization area, undoing zoom or translation changes.
	Merge parent nodes: collapses nodes if the set of structures from which cores (nodes) are derived are identical.
Activity column	Dropdown menu for selecting the activity column.
Distribution type	Dropdown menu for selecting the distribution type: options are Two tailed, upper tail, and lower tail.
Significant percent	Dropdown menu for selecting the significant percent test used to color transition arrows. Options are 1, 5, 10 and 20 percent.

The following table describes additional operations that are available if the context menu is activated while the mouse is over a core node. Most of these operations are also available by clicking directly on the node icons at the top of a node (see below).


	Delete node: removes this node from the network.
	Delete child nodes: removes all nodes beneath this one. If this node has no parent it will also be removed. Will not be present if the node has no children.
	Move to root: removes all nodes except this node and its children from the layout. Will not be present if the node has no children.
	Toggle representative structure display: toggles the core display with a grid up to 12 diverse representative structures from the table that contain the core.
	Toggle histogram display: toggles the structure display with a frequency histogram of activity values for all compounds that contain the core.



Select structures in node: marks all rows in the data table that have structures which contain the core. Replaces any current marking in the data table.

The following sections describe the configuration and use of the Structure Network visualization.

Create a Structure Network visualization

Click the New Lead Discovery ChemCharts button  in the list of visualizations in Spotfire. A new Lead Discovery ChemCharts visualization will be added to the page. Select *Structure Network* in the dropdown menu of available visualizations on the ChemCharts home page. If the data table currently configured for the visual doesn't contain the requisite information, the warning message "Cannot find column containing structure network for current data table" will be displayed. Best practice is to automatically configure the Structure Network visualization when retrieving the results from a Core Decomposition Analysis web service task.

Exploring the structure network

The position network display may be translated by clicking the left mouse button in whitespace within the visualization and dragging to the desired new position. The display will update as the mouse is moved. The display may be made larger or smaller within the visualization either by moving the mousewheel, or using the navigation controls in the upper left corner.



Figure: Zoom and position control of the Structure Network visualization.

Node controls

The default node view displays a core and node controls. Nodes may be rearranged by clicking and dragging node positions with the mouse. Moving the mouse over a node will display a histogram of values drawn from the currently configured *Activity* column.

N 111: 398 ± 0.25

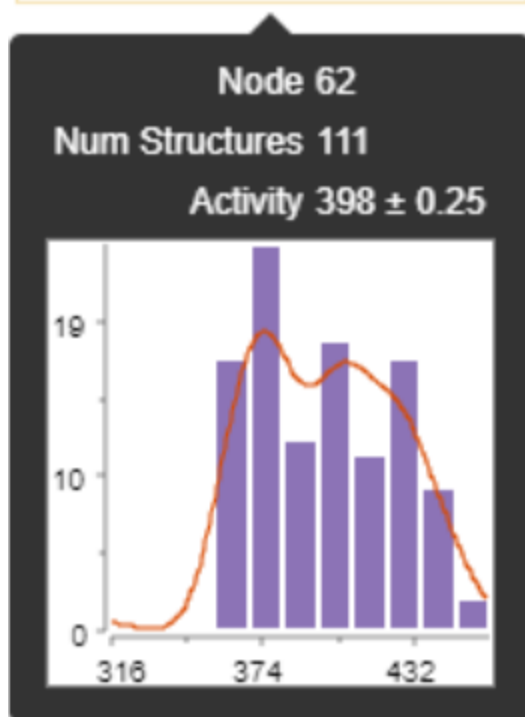
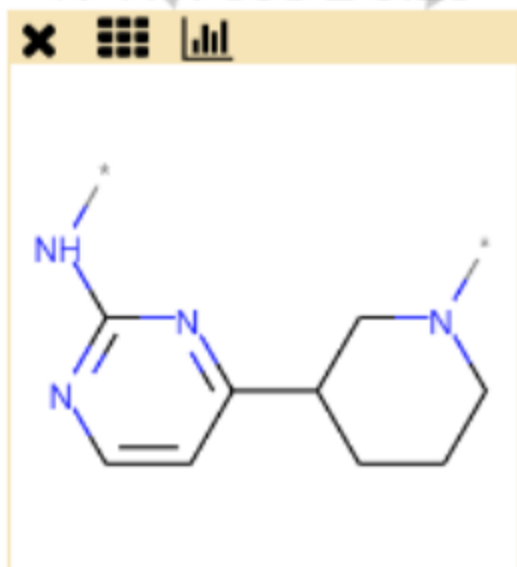



Figure: Node display with the mouse cursor hovering over the node. A histogram of activity values for structures from which the core was derived is displayed in the tooltip.

The histogram and structure display may be interchanged by clicking the  button.

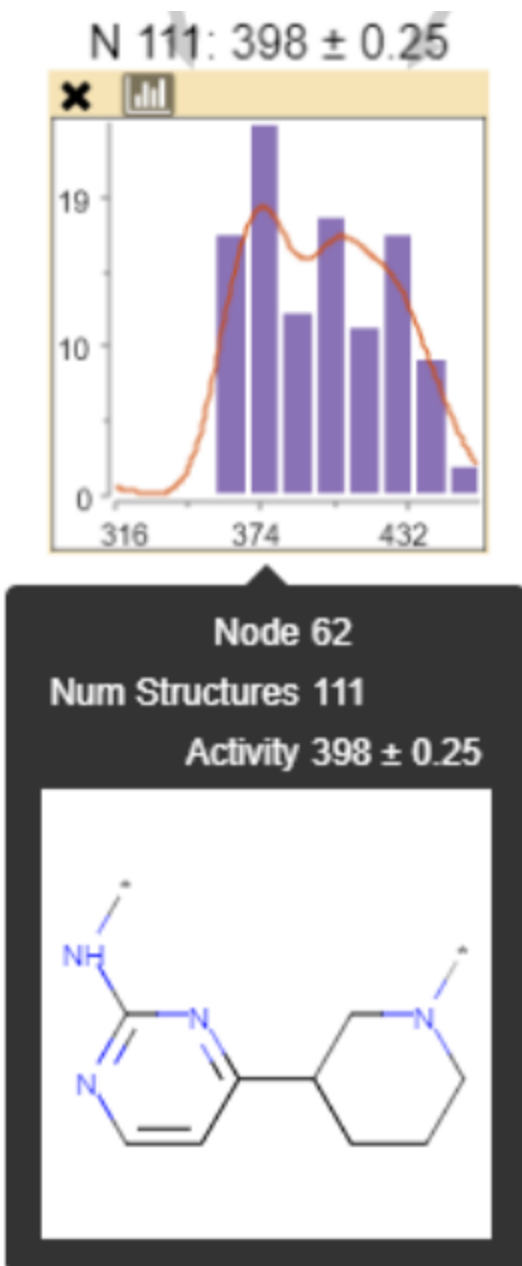



Figure: A node configured to with primary histogram display. The core structure is displayed in the tooltip.

A diverse set of up to 12 representative structures which contain a core may be inspected by clicking the  button. The node will be replaced by a grid view of the parent structures from which a node was derived. The core substructure is highlighted in each of the parent structures.

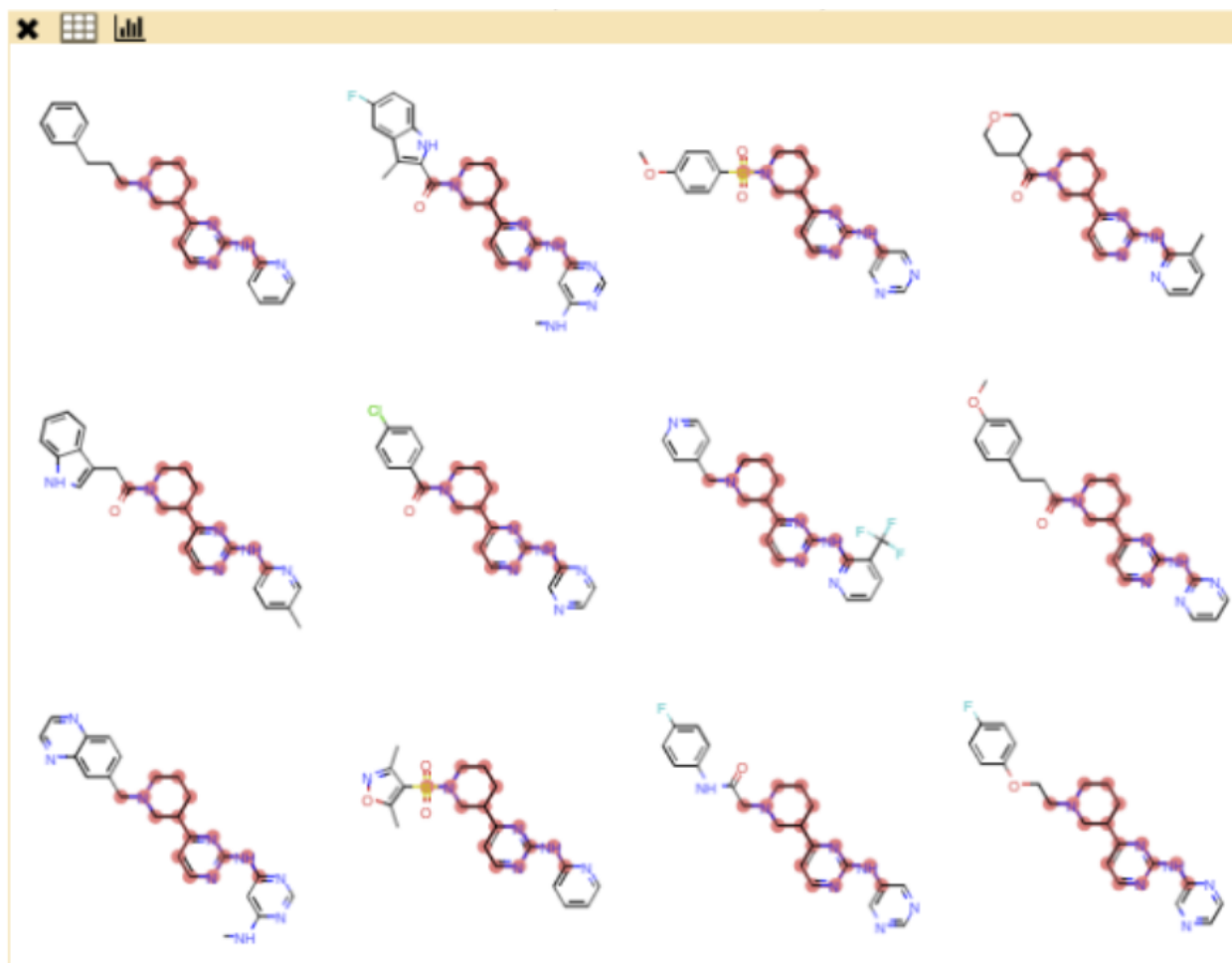



Figure: Grid display of a node's parent structures.

Clicking the  button will collapse the grid view back to the original core structure display.

Nodes may be removed from the network by clicking the close  button.

If the node has child nodes additional buttons will be available. The scissor and up-arrow icons perform the same operations as those for the context menu (when opened over a node).

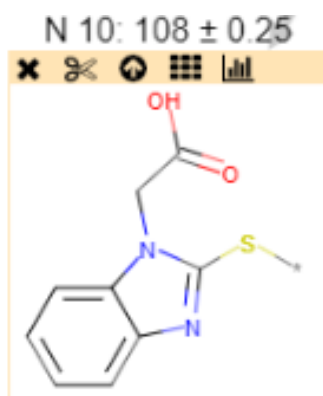


Figure: Buttons on a core node with children.

Edge information

Moving the mouse over an edge will display a combined histogram of parent and child activities (where the child activities are excluded from the parent activities) together with a summary of the T-test statistics.

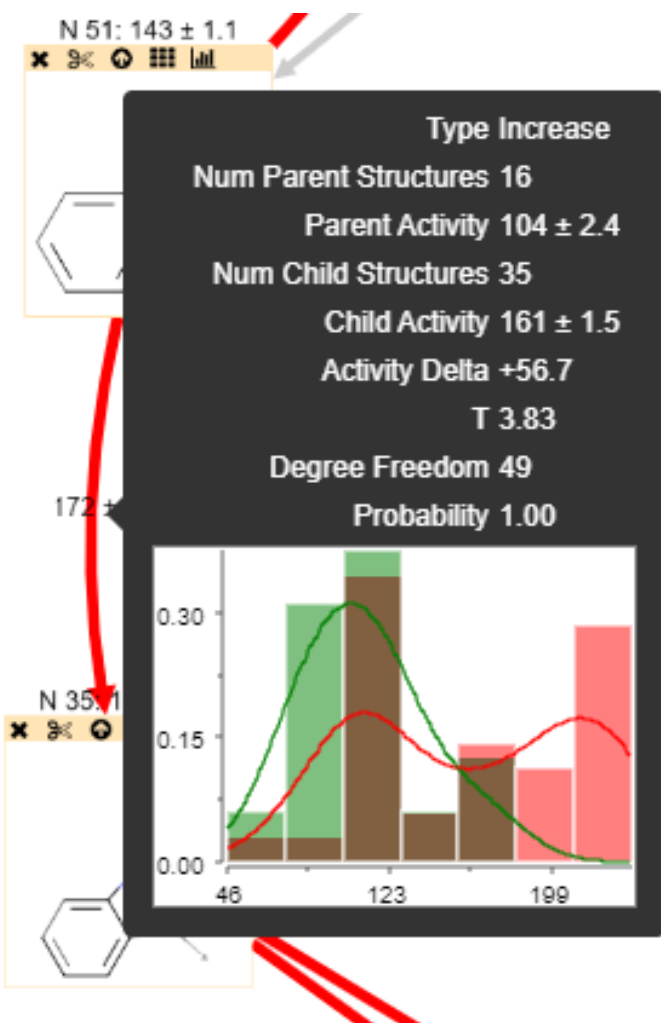



Figure: Edge information

Recalculating node coordinates.

As portions of the graph are deleted or representative structures are displayed the graph will appear disorganized as node coordinates are not updated. The new layout button, , from the context menu will recalculate a new layout for the displayed nodes using the Sugiyama layout algorithm.

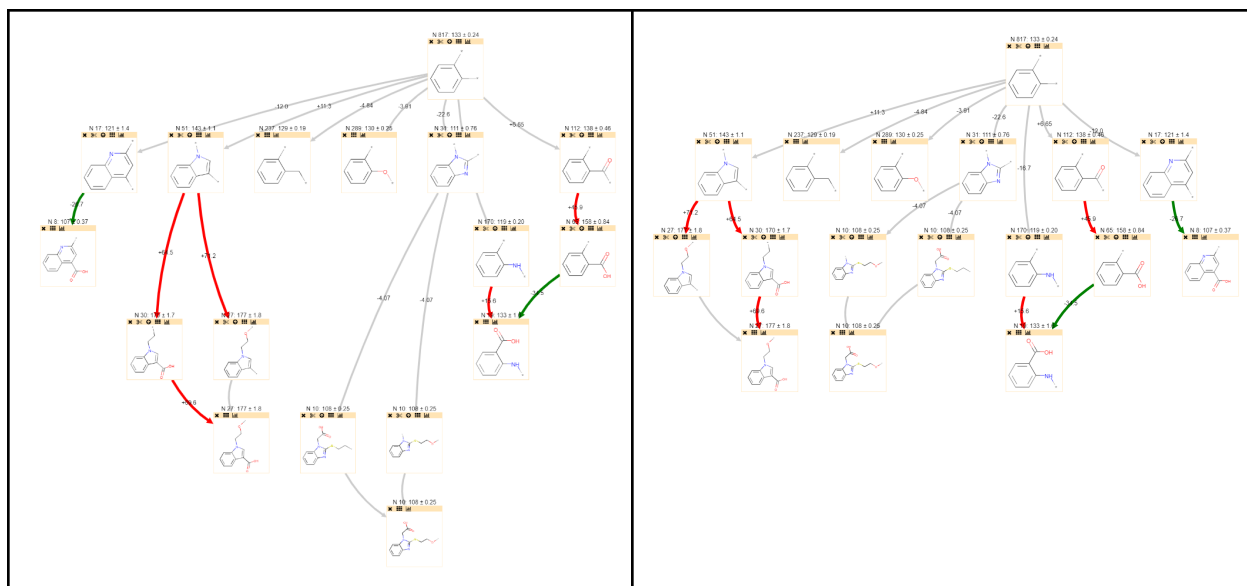


Figure: An edited graph before (left) and after (right) a new layout operation

Change edge colors

To alter edge colors, open the *Properties* dialog using the [context menu](#), and navigate to the *Structure network* page. Use the *Network edge color*, *Activity increase color*, and *Activity decrease color* controls to alter colors used for each of the respective edge types.

Table Visualization

The Lead Discovery ChemCharts Table visualization works in a similar fashion to any other table plot; data is presented in a table of rows and columns and the table can be used to compare values for a number of items:

- Left mouse click on a row will mark it.
- Hovering over a row will make it the active item and corresponding items will be highlighted in other visualizations in Spotfire (except in the WebPlayer).

- Rows can be sorted by the values in up to 3 columns.
- Columns can be added, removed and reordered.
- The data displayed in the table can be limited by one or more markings from other visualizations (see Single Click Limit by Marking) or by applying Spotfire filters.
- If color rules are defined, the background color of the table cells are colored accordingly.

The Lead Discovery ChemCharts Table visualization adds a number of features that are not currently available in Spotfire, such as:

- Resizable rows via mouse drag
- Molecule depiction
- Sequence depiction
- Molecule image and form-based tooltips
- Fixed rows
- Fixed columns
- Transpose table
- Column header filter indicators
- [Column header popups](#) with filter controls
- [Text search/find functionality](#)
- Facile tag column manipulation
- CheckBox marking

An example of the Table visualization is shown below.

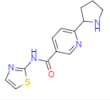
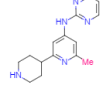
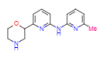
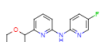
Lead Discovery ChemCharts														
Structure <MOLFILE>	Code	Salt	cLogP	HBA	HBD	Rot_Bonds	TPSA	Heavy_Atoms	MW	Name	StereoComment	N+O	Parent_MW	Salt_MW
	MBX000043	HCl	2.75	4	2	3	66.91	19	310.61	5-(pyrrolidin-2-yl)...	Mixture of Enan...	5	274.35	36.46
	MBX000205	HCl	1.76	6	2	3	71.96	19	293.76	N-(6-morpholin-2-yl)...	Mixture of Enan...	6	257.30	36.46
	MBX000230		1.32	5	2	3	62.73	20	269.35	N-(2-methyl-6-(methylamino)pyridin-3-yl)pyridin-2-amine	None	5	269.35	
	MBX000273		2.09	4	2	3	49.84	20	268.36	2-methyl-6-(piperidin-2-yl)pyridin-3-amine	Mixture of Enan...	4	268.36	
	MBX000274		0.88	5	2	3	62.73	20	269.35	N-(2-methyl-6-(piperidin-2-yl)pyridin-3-yl)pyridin-2-amine	Mixture of Enan...	5	269.35	
	MBX000277		1.93	5	2	3	59.07	20	270.34	N-(6-methylpyridin-2-yl)pyridin-2-amine	Mixture of Enan...	5	270.34	
	MBX000278		1.94	5	2	3	59.07	20	274.30	N-(5-fluoropyridin-2-yl)pyridin-2-amine	Mixture of Enan...	5	274.30	

Figure: The Lead Discovery ChemCharts Table visualization.










Context menu




Much of the functionality of the Table visualization is accessed through the context menu, which is opened by right clicking anywhere in the visual. An example of the context menu for the Table visualization is shown below.



Figure: The Table visualization context menu.


The following table describes the function of each item in the context menu:

	Back: returns the user to the visualization 'home' page where the user can select a different visualization or data table to display in the current ChemCharts visualization.
	Add visualization: adds a new ChemCharts visualization to the current page. Used primarily in the web player.
	Web services: opens the web services dialog.
	Properties: opens the <i>Properties</i> dialog.
	Copy: opens the <i>Copy</i> dialog for copying specified content to the clipboard.
	Export: export selected data to tab delimited text file or Excel. Structures loaded into the data table in MOL format are automatically converted to SMILES on export to tab-delimited text. When exporting to Excel depictions will be created for structures, anchored to the cell containing the structure.
	Tooltips: opens the tooltips control for the visualization.
	Transpose: toggles between regular and transpose table layout.
	Limit by marking: toggles the limit by marking behavior of the visualization.

	Fix row or column: this item only appears when the context menu is opened from a row or column header.
	Tags: opens the <i>Properties</i> dialog to the <i>Tags</i> page for configuring tag columns.
	Configure column: allows the user to change the ContentType of a column by selecting from a list of known content types.

The following sections describe the configuration and use of the Table visualization.

Create a Table visualization

Click the New Lead Discovery ChemCharts button  in the list of visualizations in Spotfire. A new Lead Discovery ChemCharts visualization will be added to the page. Select *Table* in the dropdown menu of available visualizations on the ChemCharts home page.

Add or remove columns

See the [Columns](#) section in [Configuring Visualizations](#).

Change column order

The order in which columns are displayed can be altered in one of two ways:

- Left click a column header (or row header, if transposed) and drag the column or row to the desired position.
- Open the Properties dialog using the [context menu](#), select the Columns page and reorder the columns in the Selected Columns list on the right hand side. See the [Columns](#) section in [Configuring Visualizations](#).

Change column and row dimensions

Columns and rows can be resized by moving the mouse pointer to the right edge of a column heading (to resize a column) or the bottom edge of a row heading (to resize a row). The mouse pointer should change to indicate column or row resizing is possible. Adjust the column width or row height by holding down the mouse button and moving the mouse horizontally or vertically respectively.

TIP: If a column (or row, if the table is transposed) containing a molecule depiction is being resized, holding down the shift key whilst resizing will maintain a square aspect ratio for the cells.

Change column header dimensions

Column headers may be resized vertically to display long column names as wrapped text when using standard table view. To increase column header height, mouse over the bottom of the

rectangle in the upper left corner of the table. The mouse pointer should change to indicate resizing is possible. Click and drag the mouse vertically to resize column headers.

Change a column renderer

In some cases there are multiple possible renderers available for columns (notably for columns that contain molecules and sequence data). To configure the renderer for a column open the visualization properties dialog, select the Columns page and set the renderer (and configure any settings the renderer may have) for the selected column. See the [Columns renderers](#) section in [Configuring Visualizations](#) for more details.

Grouping columns

Beginning with the 4.3.0 release of Lead Discovery ChemCharts, related columns may be grouped, or have an additional hierarchical layer of organization. When enabled, column groups will appear as group headers immediately above column headers.

Lead Discovery ChemCharts

Compounds						Properties
Structure	Code	Salt	Name	StereoComment	Parent_MW	
1 	MBX000043	HCl	6-(pyrrolidin-2-yl)-N-(1,3-thiazol-2-yl)pyridine-3-carboxamide	Mixture of Enantiomers	274.35	
2 	MBX000205	HCl	N-[6-(morpholin-2-yl)pyridin-2-yl]pyrimidin-2-amine	Mixture of Enantiomers	257.30	

Figure: Appearance of grouped columns in standard vertical layout.

In transpose mode, groups will appear vertically to the left of row headers.

Lead Discovery ChemCharts

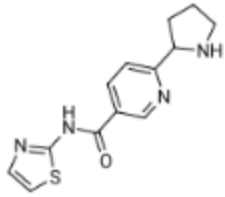
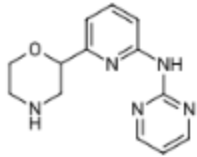
	1	2	
Compounds	Structure <MOLFILE>		
	Code	MBX000043	MBX000205
	Salt	HCl	HCl
	Name	6-(pyrrolidin-2-yl)-N-(1,3-thiazol-2-yl)pyridine-3-carboxamide	N-[6-(morpholin-2-yl)pyridin-2-yl]pyrimidin-2-amine
	StereoComment	Mixture of Enantiomers	Mixture of Enantiomers
Properties	Parent_MW	274.35	257.30
	MW	310.81	293.76
	Salt_MW	36.46	36.46
	cLogP	0.75	1.18
	HBA	4	6
	HBD	2	2
	Rot_Bonds	3	3
	TPSA	66.91	71.96
Data	Heavy_Atoms	19	19
	N+O	5	6
	Structure search ...	False	False
Structure search ...	False	True	
Form cell	{"b6e4d3f0-621b-4c81-aa1d ...	{"b6e4d3f0-621b-4c81-aa1d ...	

Figure: Appearance of grouped columns in transpose layout.

To configure column groups, open the *Properties* dialog, select the *Columns* tab, then check the *Group columns* checkbox.

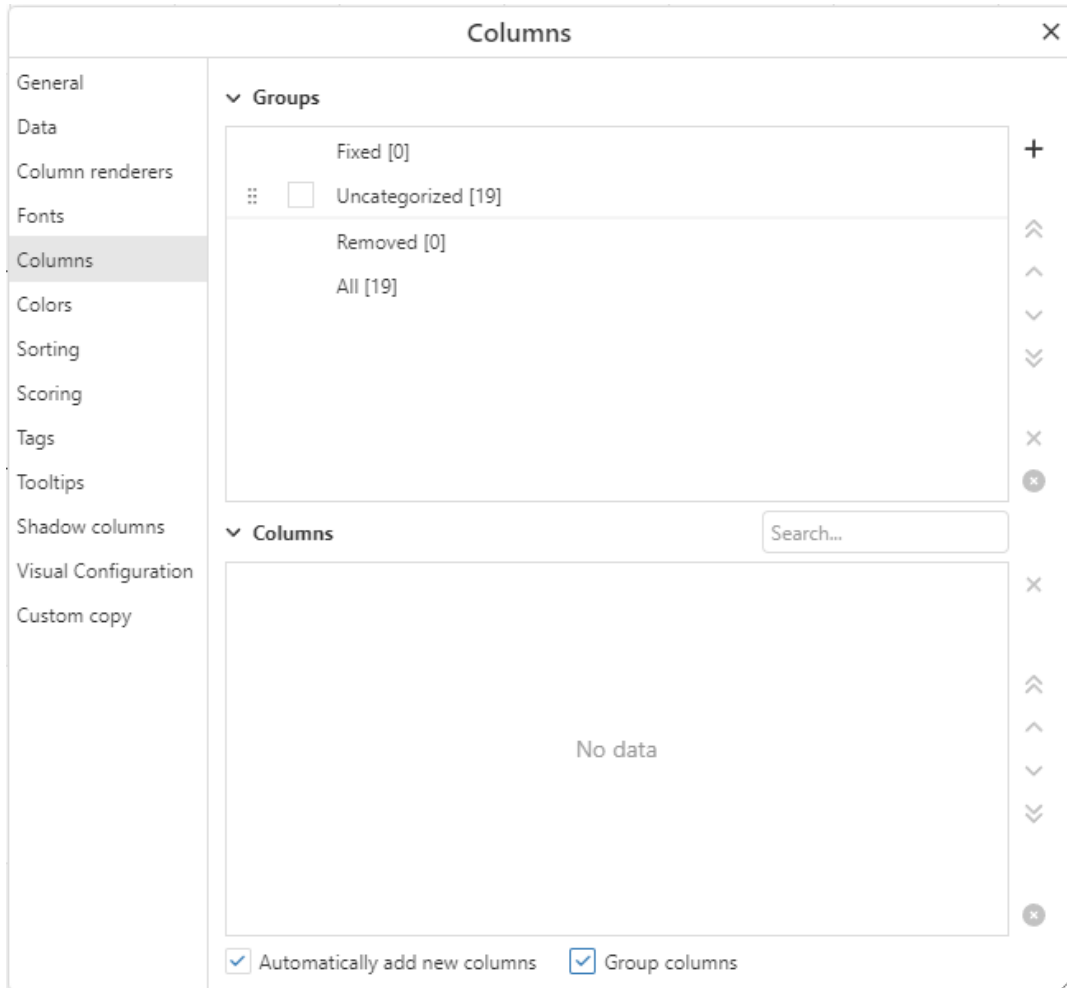




Figure: Initial appearance of Columns tab after Group columns has been enabled.

Upon enabling column groups, the *Chosen* and *Remaining* columns selectors become *Groups* and *Columns* selectors. Four default groups will appear, and are unable to be removed: Fixed, Uncategorized, Removed, and All. The Uncategorized group, if populated, will be visible in the group header section of the table. Columns that were fixed prior to enabling column grouping are not automatically added to the Fixed group. The configuration of fixed columns in grouped and ungrouped modes are distinct. To add a new group, click the **+** button in the upper right corner of the *Columns* dialog, and enter the name (and optionally the color) of the new group.



Figure: Adding a new column group.

The new group will appear in the Groups selector. The order of appearance of groups in the group header may be altered by clicking the  icon next to the group name and dragging and dropping the group to alter its position in the list.

Groups may be populated with columns two different ways. Click on either the *All* or *Uncategorized* groups in the *Groups* selector to display the list of associated columns in the *Columns* selector. Next, in the *Columns* selector, click on the current group assignment to the right of the desired column to expose a dropdown list (see the next Figure) of selectable groups. Selecting a different group will alter the column's group membership. The other approach to changing a column's group membership is to left mouse click on the  icon to the left of the column name and drag and drop the selected column up to the desired group in the *Groups* selector. Using either method of altering group membership, the *Groups* and *Columns* selectors will automatically update to reflect the change.

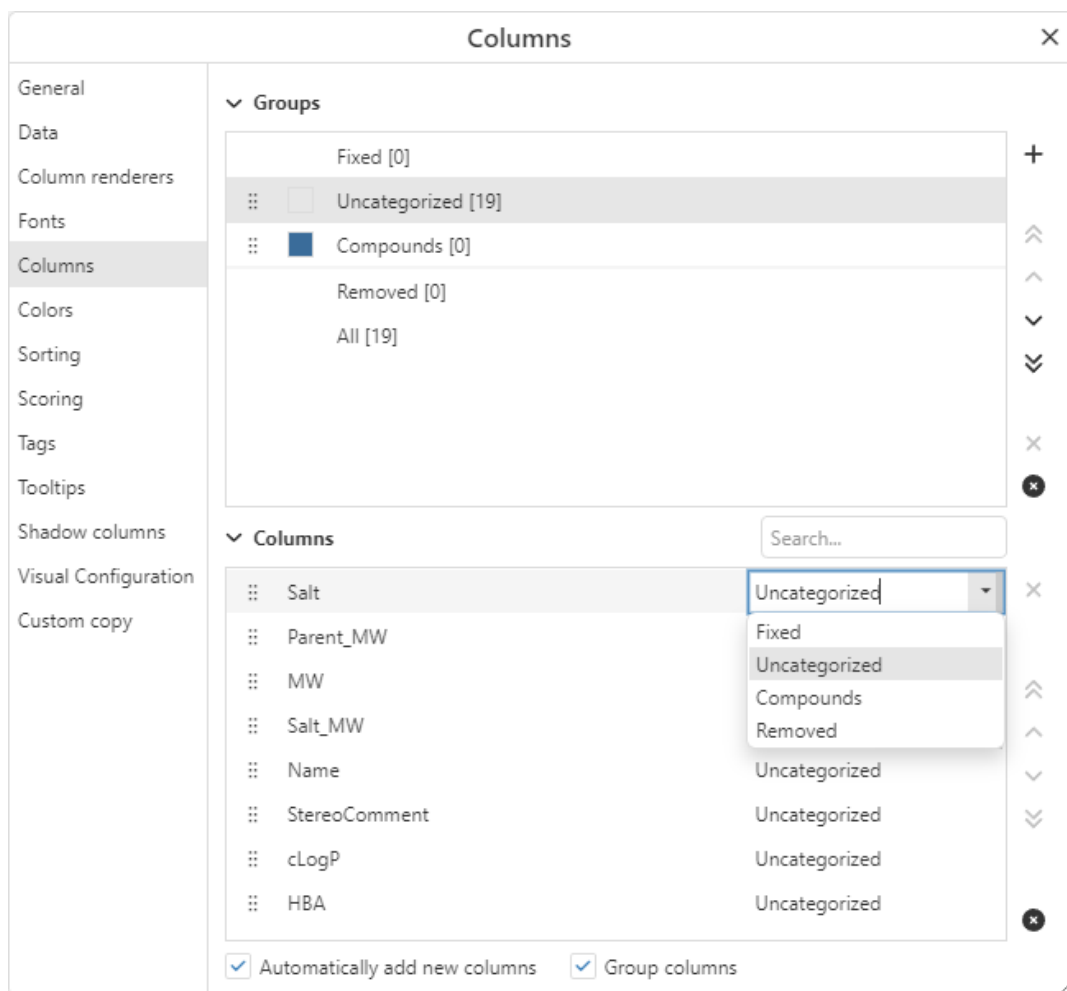


Figure: Configuring column groups.

Sorting

There are 2 ways to apply sorting to the table:

- Click the header of the column (or row, if the table is transposed) that is to be used to sort the table. Repeatedly clicking the same heading will cycle through the following sort states; ascending, descending, unsorted.
- Open the *Properties* dialog from the [context menu](#), select the Sorting page and use the controls to configure the sorting. Up to 5 columns can be used to sort the data. See the [Sorting](#) page in the [Configuring Visualizations](#) section for more information.

Coloring

Open the *Properties* dialog from the [context menu](#), and navigate to the *Coloring* page. Use the controls to configure the coloring. See [Coloring](#) in the [Configuring Visualizations](#) for more information.

Tooltips

See the [Tooltips](#) section in [Configuring Visualizations](#)

Limit by marking

Limit by marking can be enabled or disabled by clicking the *Limit by marking* item in the [context menu](#). See [Limit by Marking](#) in [Configuring Visualizations](#) for more information.

CheckBox Marking

An additional type of marking, called checkbox marking, is supported in the ChemCharts Table visualization. Standard marking, controlled by left mouse clicks or dragging rectangles, tends to be volatile due to inadvertent clicks. A secondary marking is also useful in that it may be used to affect marking interactions on separate charts without switching the marking configured for a table visualization. To configure a checkbox marking, open the *Properties* dialog, navigate to the *Data* tab, and select a marking from the *CheckBox marking* dropdown.

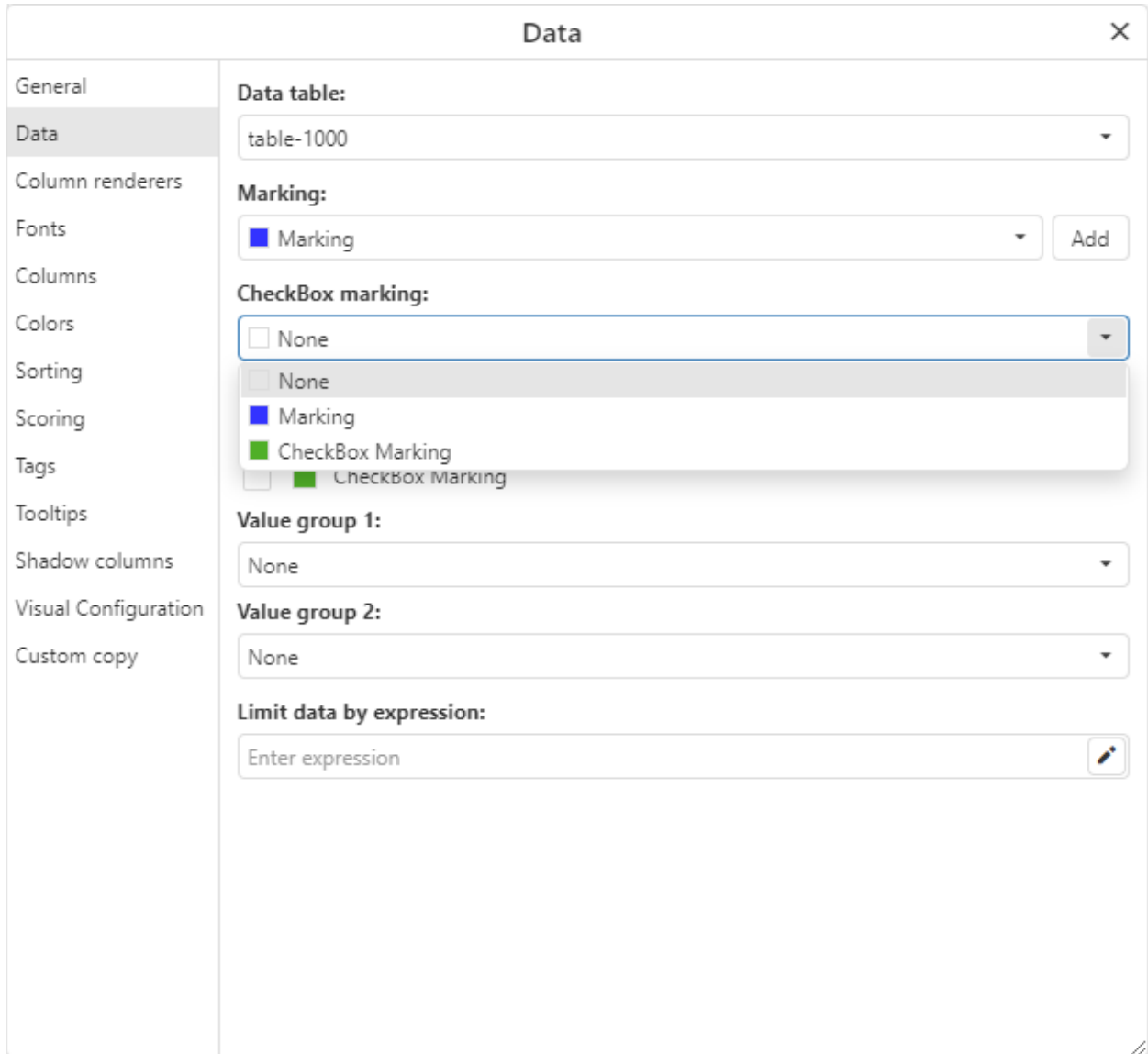


Figure: Configuring a CheckBox marking

With a checkbox marking configured, checkboxes will appear in the row headers (or column headers in transpose view). Clicking the left mouse button inside a row header will mark that row using the configured checkbox marking. When a row is marked with the checkbox marking, the row header will be colored with the checkbox marking color, and the checkbox in the row header will be checked.

	Code
<input type="checkbox"/>	1 MBX000043
<input checked="" type="checkbox"/>	2 MBX000205
<input type="checkbox"/>	3 MBX000230

Figure: Checkbox marking example applied to the second row of a table.

To clear a checkbox marked row, simply click again using the left mouse button. *Shift* and *Ctrl* key modifiers have the same effect on both standard and checkbox marking. To either mark or clear all rows of a checkbox marking, hover over any row header and click the right mouse button to open the row context menu and click the desired *Check all* or *Uncheck all* button.

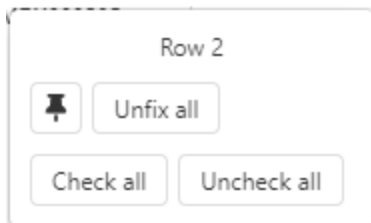


Figure: CheckBox marking context menu

Transpose table

The table can be transposed - rows are displayed as columns and columns are displayed as rows. This is accomplished by clicking the right mouse button to open the [context menu](#) and selecting the *Transpose* menu item. To switch back to the standard table display, open the context menu and select the *Untranspose* menu item. Repeatedly clicking this button will toggle the table from transposed to standard orientation. In transpose mode columns can be resized, but they will all be sized the same - much like when resizing rows when the table is not transposed.

TIP: If the table is transposed, the mouse scroll wheel will scroll the table horizontally instead of vertically. If the alt key is pressed while scrolling using the mouse scroll wheel, the table will be scrolled vertically if transposed or horizontally if not transposed.

Fixed rows

Comparing row values in a Table visualization may be aided through the use of fixed rows. Rows can be fixed at the top of the Table visualization (or on the left in Transpose view) by double clicking the row header (or column header in Transpose view), or by right clicking over a row to open the [row header popup](#) and clicking the *Toggle fixed/unfixed row* button. Note that fixed rows will still appear in the scrollable rows section of the table. Fixed rows are duplicate copies with a fixed position at the top of the Table visualization.

Fixed columns

Maintaining column visibility may be desirable while horizontally scrolling a table viewed in standard layout. The analogous feature for a Transpose table view is to persist rows while scrolling vertically. Fixing columns in the standard table view will persist fixed columns on the left hand side of the Table. Fixing rows in a Transpose view will persist fixed columns on the top of the table. Note that if columns are fixed in standard view, once transposed, the original fixed columns become fixed rows in Transpose view. The reverse is true as well. Columns may be fixed on the left of the Table visualization (or at the top in Transpose view) by double clicking the column header (or row header in Transpose view), or by right clicking over a column header to open the [column header popup](#) and clicking the *Toggle fixed/unfixed column* button.

Text alignment and wrapping

Columns containing textual data may have their appearance altered by configuring the *Text* renderer. Open the *Properties* dialog using the [context menu](#), and navigate to the *Column renderers* page. Select the column to configure from the *Columns* menu. Select *Text* from the *Renderers* dropdown menu, if necessary. The Text renderer has options for horizontal and vertical alignment. Text in cells is wrapped by default, although this may be disabled using the *Wrap text* checkbox. Note that the selection for horizontal alignment will be applied to the column header as well for the standard table display. The selection for vertical alignment is applied to the column header when the table is Transposed.

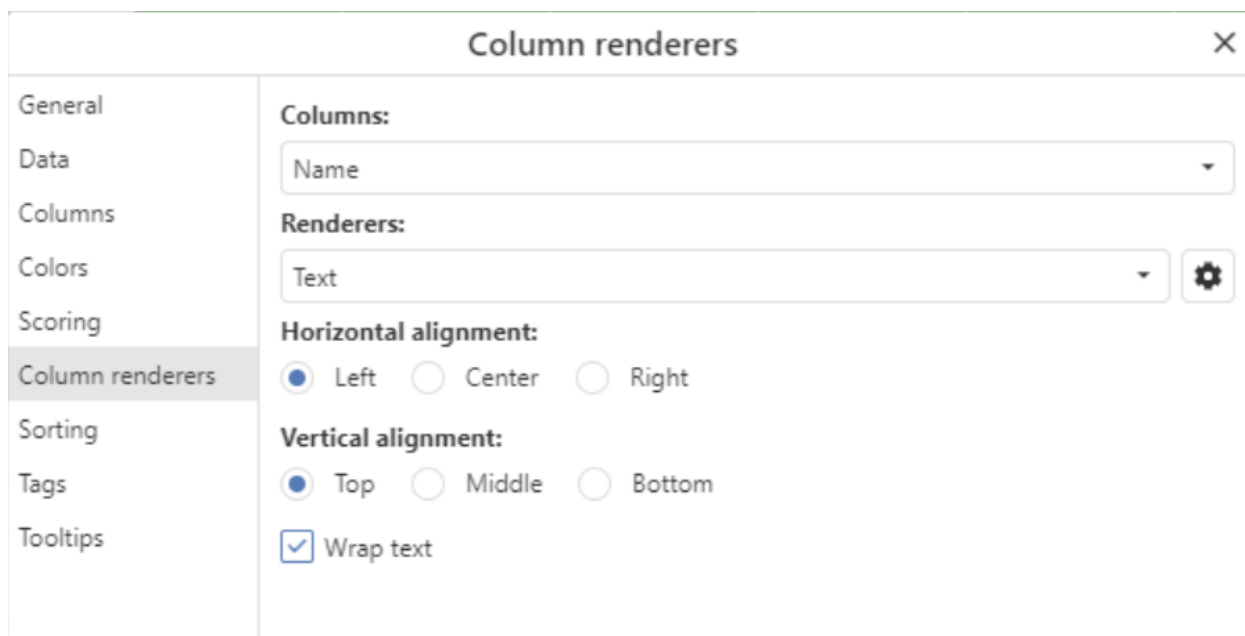


Figure: Configuring alignment for a text column.

Find

The table visualization has text search capabilities akin to those found in web-browser or applications like Excel. To use the table find either use the keyboard shortcut Ctrl + F (assuming the visualization has keyboard focus) or right-click to bring up the context menu and select the *Find* menu item. This should display the find toolbar at the bottom of the table. This is shown in the figure below.



Figure: The find toolbar. The controls from left to right are: search text box, toggle button for regular expressions, search up, search down, mark matches and a multi column select box that allows the restriction of the search to a subset of the displayed columns.

Typing the search text into the provided text box will trigger the find. The figure below shows the results of a find after 'en' was entered into the search box. Cells that contain matching text are highlighted in yellow. The current matching cell is highlighted in a darker shade of yellow. Pressing return will move the search on to the next match. This is functionally the same as clicking the *Find next* button. To search in the opposite direction, click the *Find previous* button.

	Parent_MW	MW	Salt_MW	Name	StereoComment	cLogP	HBA	HBD
12	272.33	272.33		5-(4-fluorophenyl)-4-(piperidin-3-yl)pyrimidin-2-amine	Mixture of Enantiomers	2.08	4	2
13	272.33	308.79	36.46	5-(3-fluorophenyl)-4-(piperidin-3-yl)pyrimidin-2-amine	Mixture of Enantiomers	2.08	4	2
14	288.78	288.78		5-(4-chlorophenyl)-4-(piperidin-3-yl)pyrimidin-2-amine	Mixture of Enantiomers	2.54	4	2
15	269.35	305.81	36.46	N-(3-methylpyridin-2-yl)-4-(piperidin-3-yl)pyrimidin-2-amine	Mixture of Enantiomers	2.16	5	2
16	282.39	318.85	36.46	4-[2-(piperidin-3-yl)ethyl]-N-(pyridin-2-yl)pyridin-2-amine	Mixture of Enantiomers	3.24	4	2
17	283.38	319.84	36.46	N-{4-[2-(piperidin-3-yl)ethyl]pyridin-2-yl}pyrazin-2-amine	Mixture of Enantiomers	1.86	5	2

X
Searching all columns

Figure: Example of table visualization find functionality. The yellow highlighted cells contain matches for the query. The darker yellow cell is the current match.

By toggling the regular expression button, users can take advantage of the power of regular expressions instead of simple case insensitive substring searches.

The mark matches button will mark every row that contains a cell that matches the query.

By default the text search is carried out over all the columns in the table. This can be quite inefficient for very wide tables. It is possible to restrict the columns that are searched by selecting a subset from the multi column select box on the right hand side of the find toolbar. This is shown in the figure below where the same text search is performed ('en'), but now the search is limited to the 'Name' column.

	Parent_MW	MW	Salt_MW	Name	StereoComment	cLogP	HBA	HBD
12	272.33	272.33		5-(4-fluorophenyl)-4-(piperidin-3-yl)pyrimidin-2-amine	Mixture of Enantiomers	2.08	4	2
13	272.33	308.79	36.46	5-(3-fluorophenyl)-4-(piperidin-3-yl)pyrimidin-2-amine	Mixture of Enantiomers	2.08	4	2
14	288.78	288.78		5-(4-chlorophenyl)-4-(piperidin-3-yl)pyrimidin-2-amine	Mixture of Enantiomers	2.54	4	2
15	269.35	305.81	36.46	N-(3-methylpyridin-2-yl)-4-(piperidin-3-yl)pyrimidin-2-amine	Mixture of Enantiomers	2.16	5	2
16	282.39	318.85	36.46	4-[2-(piperidin-3-yl)ethyl]-N-(pyridin-2-yl)pyridin-2-amine	Mixture of Enantiomers	3.24	4	2
17	283.38	319.84	36.46	N-{4-[2-(piperidin-3-yl)ethyl]pyridin-2-yl}pyrazin-2-amine	Mixture of Enantiomers	1.86	5	2

en

✖
✱
↑
↓
✎
Name ✖
✕

Figure: Example of table visualization find functionality where the search is restricted to a single column (in this case the 'Name' column).

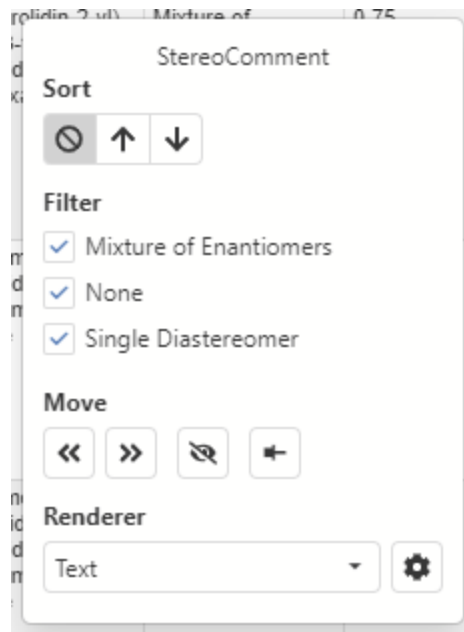
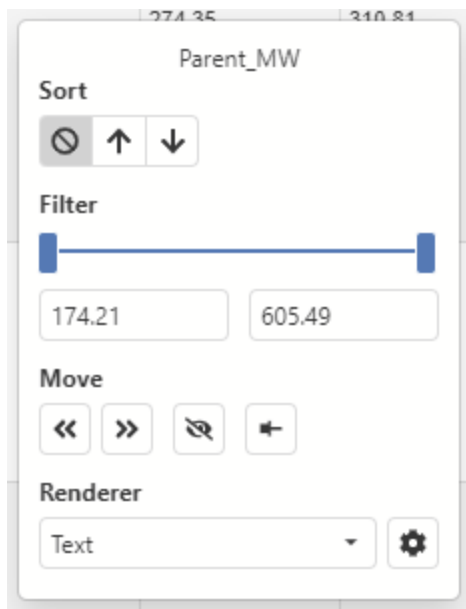
Column header popups

Right-clicking on a column header will display a column header popup. This contains the following functionality:

- Buttons to sort and clear sorting from the column
- A filter control that allows filtering the table based on the contents of the column without using the Spotfire filter panel. Note that filter controls will only appear for non-binary column types and only if the filter type for the column is a range filter, checkbox filter or list box filter.

- Buttons to move the column to the far-left or far-right as well as hide or fix/unfix the column. Fixing a column locks the column on the left-hand side of the table such that it is always displayed regardless of scroll position.
- Select box that allows switching between renderers for the column as well as a button that will open the properties dialog on the column renderer panel for the chosen column for further renderer configuration.

Clicking outside the column header popup will close the popup. The figure below shows a few examples of column header popups.



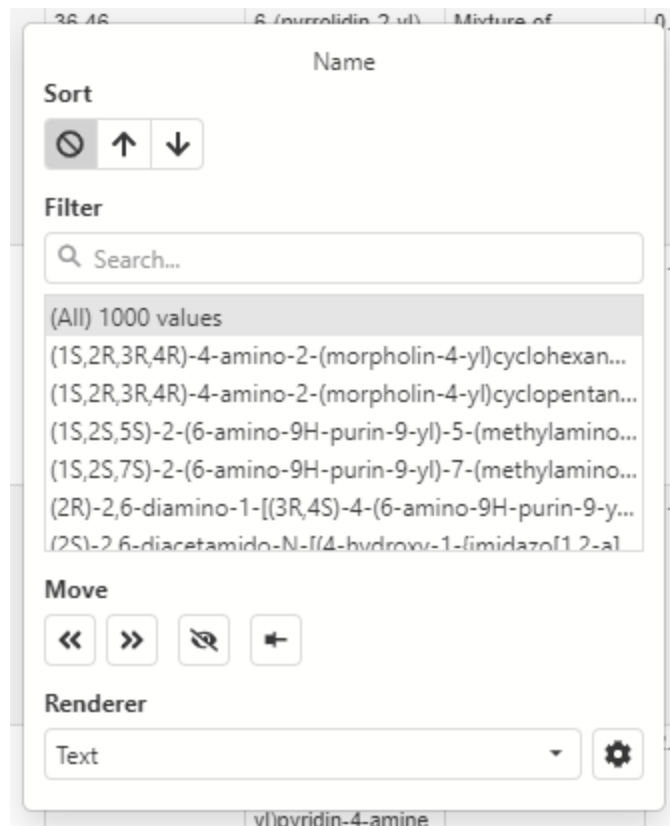


Figure: Example column header popups for various column/filter types.

Row header popups

Right-clicking on a row header displays a popup that allows the user to fix or unfix a row. Fixing a row effectively duplicates it and locks it to the top (or the left, if transposed) of the table. It will not be filtered and is always displayed regardless of scroll position.

Column finder

For very wide tables containing hundreds of columns it can be difficult to locate a particular column. To make this easier the table visual includes a column finder popup that can be accessed by right-clicking on the top-left corner of the table. This popup will display a searchable list of all the columns currently displayed in the table. Clicking on one of the column names will scroll the table to the selected column. Clicking outside of the popup will close it. The 'Find column' popup is displayed in the figure below.

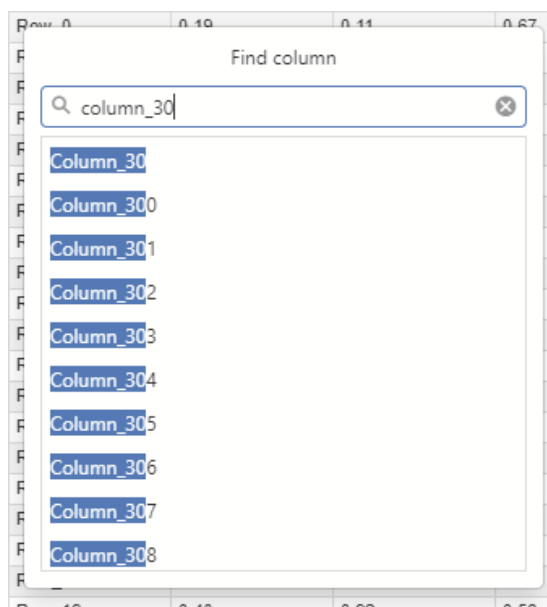


Figure: The Find column popup.

Form cell columns

It is possible to add one or more 'form cell columns' to a ChemCharts table visualization where the arrangement of the data displayed is defined using the [Form editor](#). A form cell column is added to a data table as a dummy calculated column that contains no data. The data shown in the form is taken from other columns in the data table. As a result, form cell columns are not included in any [Find](#) operations. An example is shown in the figure below.

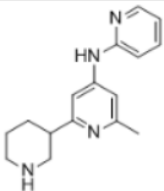
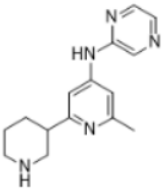

	Form cell column		Name	StereoComment	Rot_Bonds	TPSA	
3		Code	MBX000273	Mixture of Enantiomers	3	49.84	
		Salt					
		MW	268.36				
		cLogP	2.09				
		HBA	4				
		HBD	2				
4		Code	MBX000274	Mixture of Enantiomers	3	62.73	
		Salt					
		MW	269.35				
		cLogP	0.88				
		HBA	5				
		HBD	2				
5		Code	MBX000277	N-(6-methylpyridin-2-yl)...	Mixture of Enantiomers	3	59.07

Figure: Example form cell column. The form comprises a molecule [image control](#) as well as a [column data control](#).

Adding a form cell column

Form cell columns are added to a data table by right-clicking in the table visualization and selecting the 'Create new ChemCharts column...' () icon from the context menu. This will open a dialog where the user can enter the name for the new column. The column is added with a rudimentary form configuration.

Editing form configurations for a form cell column

The form configurations for a form cell can be edited in exactly the same way as any of the other forms that appear in ChemCharts (see [here](#)). To edit the form either go to the [Column renderers](#) section of the [Properties dialog](#), choose the column to be edited and click 'Edit forms' or right-click on the column header for the form cell column and click 'Edit forms'. In either case the form editor will be opened and users can edit the form used in the form cell column just like any other form in ChemCharts.

Note that multiple forms can be configured for a form cell column. Users can switch between them easily using the column header popup and selecting the desired form. An example is shown below.

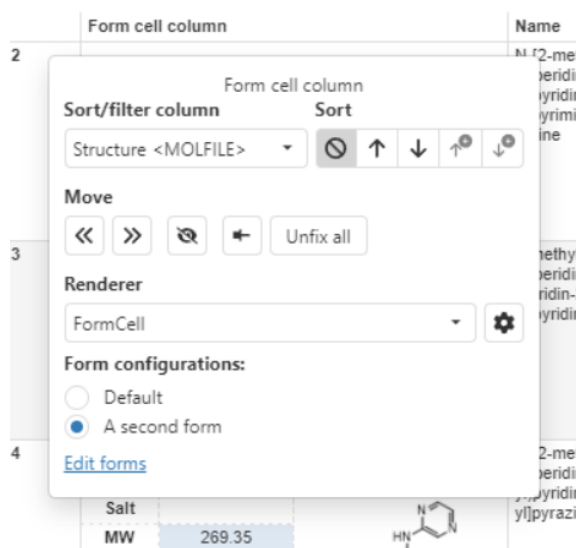


Figure: Switching between two form configurations via the column header popup menu.

Editable tables

The table visualization has an editing mode in which users can edit a data table in a somewhat-similar fashion to Excel. The changes are stored as a set of transformations that are applied to the original data table.

In editing mode users can simply double-click a cell to edit the content. Data type specific editors are used in each cell to edit the data. For example, if the cell contains text or numbers,

users can type to edit the data whereas a molecule sketcher is used to edit molecules in cells containing chemical structures. Rows can be added or removed. Columns can be added, removed or renamed. Tabular data can also be pasted into existing columns and rows.

Two conditions must be met for a data table to be editable:

1. The 'Store data' data table property on the General tab of the 'Data Table Properties' dialog must be set to 'Linked (individual settings per source)'.
2. One or more columns must be configured in the 'Key columns for linked data' property on the General tab of the 'Data Table Properties' dialog. This ensures that each row can be identified uniquely.

Enabling/disabling edit mode

To enable editing, right-click to produce the table visualization context menu and select 'Edit > Enabled editing'. If the 2 conditions required to allow data table editing are met, the table visual will switch into edit mode and the column and rows header will be colored to indicate that the visual is in edit mode.

If condition 1 is not met a dialog will be displayed offering the user 2 options (see figure below). The first option is to make a copy of the data table which will result in the 'Store data' property being configured correctly to allow editing on the copied data table. If this option is chosen, the table visualization will switch to view the duplicated data table. This is the recommended approach to creating an editable table. The second option is to manually configure the 'Store data' property using the 'Data Table Properties' dialog (this is only available in Analyst).

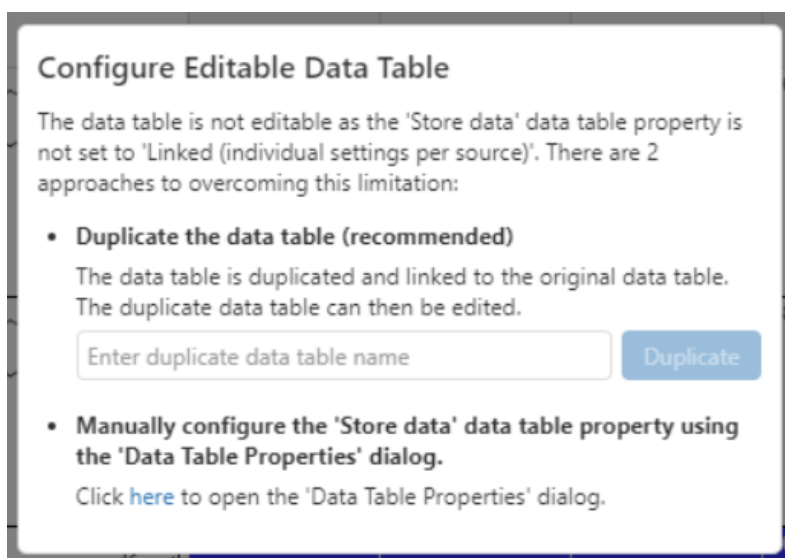


Figure: Editable table configuration solution dialog (condition 1)

If condition 2 is not met a dialog will be displayed allowing the user to configure the 'Key columns for linked data' property using the 'Data Table Properties' dialog (again, this is only available when using Analyst).

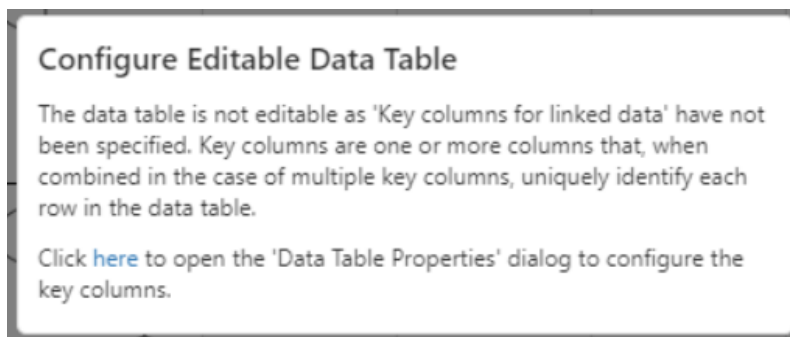


Figure: Editable table configuration solution dialog (condition 2)

To disable editing, right-click to produce the table visualization context menu and select 'Edit > Disable editing'. The table visual will revert to its normal state and cells will not be editable. It is strongly recommended to disable edit mode before saving the Spotfire document.

Editing cell data

Once the table is in edit mode, double-clicking a cell will open a cell editor. The nature of the cell editor depends on the column data type. The text and date editors both appear in place of the cell being edited. The molecule editor is a dialog containing a sketcher. Once a cell editor is open (other than the molecule editor) users can use the arrow keys to move focus to other cells.

The table below shows a list of the different cell editors and the data types for which they are used.

Cell editor	Data types	Example
Text editor	String, Integer, LongInteger, Real, SingleReal and Boolean data types (note the boolean data type only allows values true and false)	

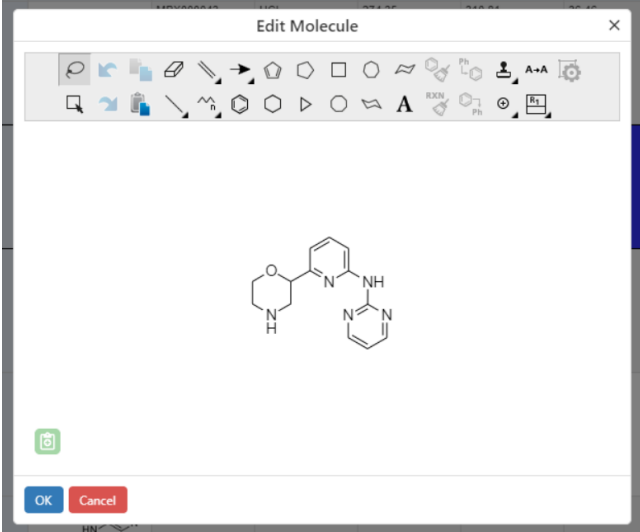
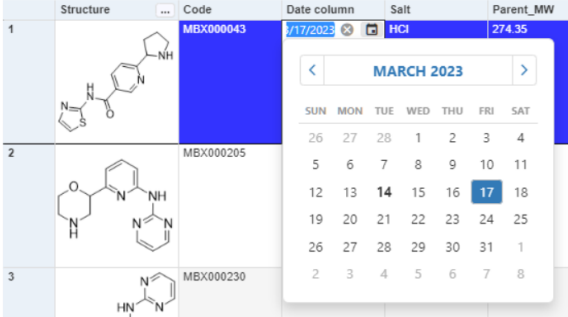
Molecule editor	String or binary data types with a chemical renderer set	
Date editor	Date and DateTime	

Figure: Cell editors and data types

As data is strongly typed in Spotfire data tables, the cell editor displays errors if the user attempts to enter data of the wrong type for the column. An example is shown in the figure below.

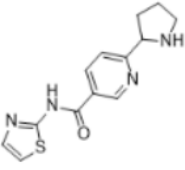

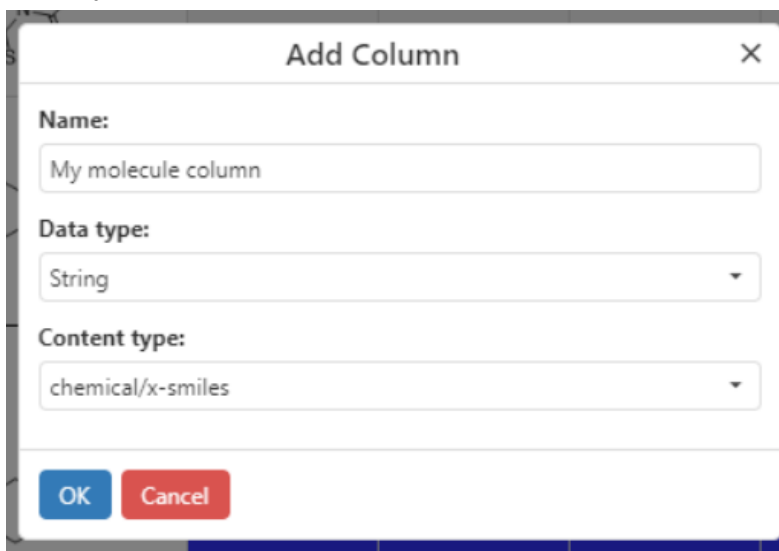
	Structure	Code	Date column	Salt	Parent_MW	MW
1		MBX000043	3/17/2023	HCl	This is wrong	310.81
2		MBX000205		HCl	Number required	293.76

Figure: Data validation. An error is being displayed here as the the user attempted to entered a string value in a numeric column

Adding columns

Columns can be added to the data table by right-clicking to produce the table visualization context menu and selecting 'Edit > Add column...'. This will produce the 'Add Column' dialog (see the figure below). Here the user must enter a name and select a data type for the column. Optionally a content type can be set (note, this allows the creation of new molecule columns should a molecular content type be chosen). Clicking OK will add the new column to the data table and it will be displayed in the table visualization.



The image shows a dialog box titled "Add Column" with a close button (X) in the top right corner. It contains three input fields: "Name:" with the text "My molecule column", "Data type:" with a dropdown menu showing "String", and "Content type:" with a dropdown menu showing "chemical/x-smiles". At the bottom are "OK" and "Cancel" buttons.

Figure: Adding a new column. Note the data type is string and the content type chemical/x-smiles. The resulting column will therefore be a molecule containing column that is editable as such.

Deleting columns

Deleting columns is accessible via the column header popup. Right click on the column header for the column that is to be deleted to produce the column header popup menu. If the table is in editing mode users can click the trash can icon to remove the column (see the figure below). A dialog will appear requesting confirmation.

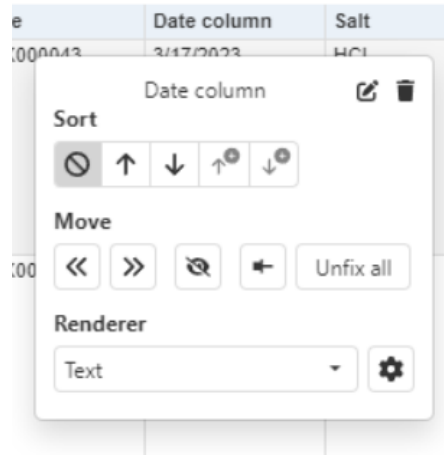


Figure: Column header popup menu when the table is in edit mode. Clicking the trash can icon will delete the column.

Editing column names

Editing the column name is accessible via the column header popup. Right click on the column header for the column that is to be renamed to produce the column header popup menu. If the table is in editing mode users can click the edit icon (next to the trash can icon) to rename the column (see figure below). Once the new column name has been entered press return or click the tick button. To cancel the column name edit, click the cross (cancel) button.

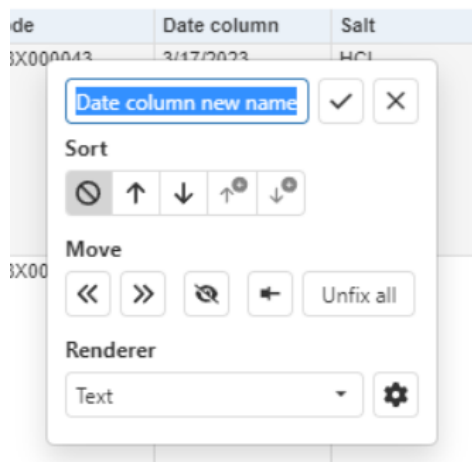


Figure: Column header popup menu when the table is in edit mode and the user is renaming a column.

Adding rows

In order to add empty rows to the data table, right-click to produce the table visualization context menu and select 'Edit > Add rows > 1 or 5 or 10'. This will add the indicated number of rows to the bottom of the data table. Note any columns that are defined as 'Key columns' will contain an

auto generated value in the new rows to ensure that each of the added rows can be uniquely identified.

Deleting rows

Rows can be deleted by right-clicking and selecting 'Edit > Delete rows > Marked... or Filtered...'. Alternatively right-clicking a row header and clicking the trash can button will delete the indicated row.

Pasting data

To paste tabular data from the clipboard into the editable data table, first the user must copy tabular data from another source (such as Excel) onto the clipboard. Then, position the mouse over the cell in the table visualization at which the data should be pasted, right-click and select 'Edit > Paste > Paste cells...'. An example is shown in the figure below.

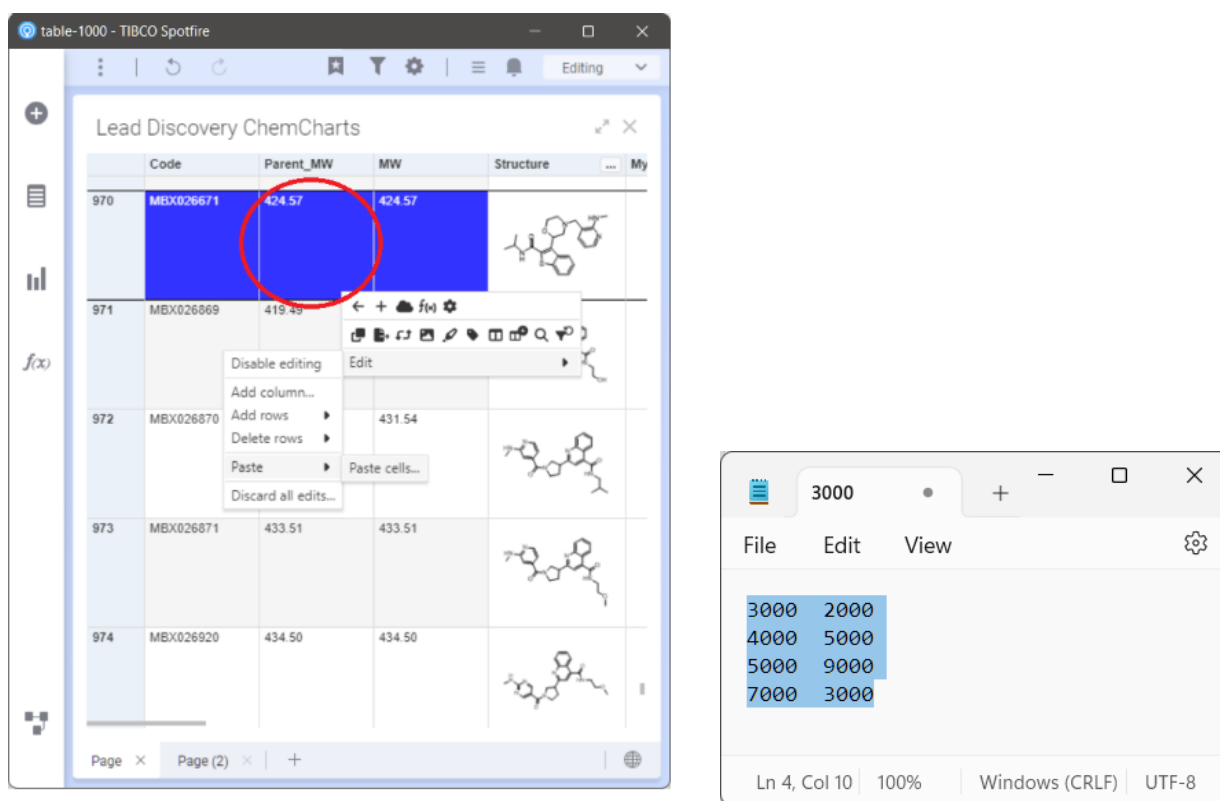


Figure: The user is going to paste the tab separated values from Notepad into the Parent_MW and MW columns in the table visualization. The values from Notepad are first copied to the clipboard, the user must then right-click over the cell in the table at which the paste should begin (this is highlighted by the red-circle). Then choose Edit > Paste > Paste cells to bring up the Paste dialog.

The paste dialog previews how the data will be pasted into the data table. Users can select from a variety of delimiters that will affect how the data is pasted into the data table. An example is shown in the figure below.

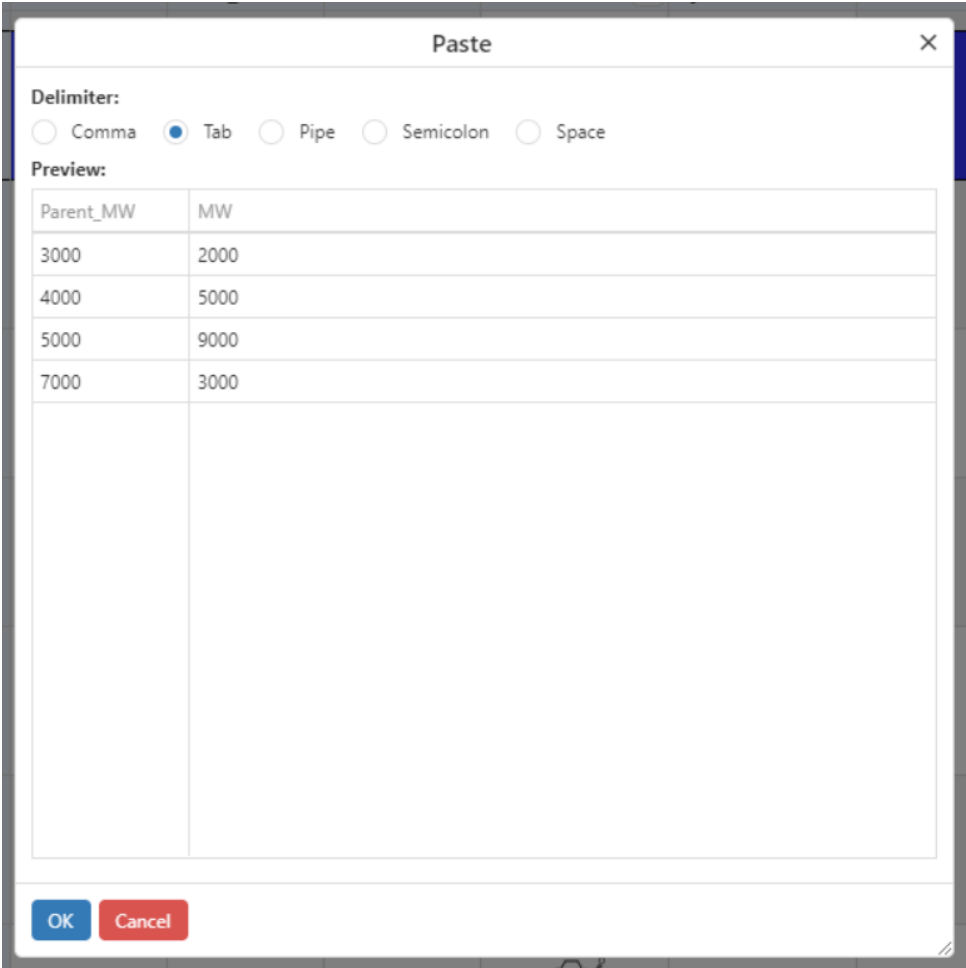


Figure: Continuing from the previous figure, the data from the clipboard has been parsed assuming that it was tab delimited. As can be seen the data will be pasted into the desired columns starting with the row that the user initially right-clicked.

After clicking OK, the data should be pasted into the data table and the table visual will update to reflect the change (see the figure below).

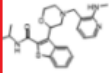
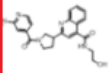
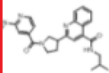
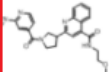
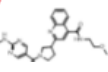
	Code	Parent_MW	MW	Structure	...	My molecule column	Date column	Se
970	MBX026671	3000.00	2000.00					
971	MBX026669	4000.00	5000.00					
972	MBX026670	5000.00	9000.00					
973	MBX026671	7000.00	3000.00					
974	MBX026920	434.50	434.50					

Figure: Table visual after pasting tabular data.

Note that the paste dialog will validate the data that is being pasted into the data table such that if the paste would result in invalid data being pasted into a column, the user is notified. An example of this is shown below where the user is attempting to paste non-numeric data into the numeric Parent_MW and MW columns. In these situations the paste operation for the invalid cells will fail, but the valid cells will succeed.

Paste ✕

Delimiter:

Comma
 Tab
 Pipe
 Semicolon
 Space

Preview:

Parent_MW	MW
3000	2000
4000	word
nope	9000
7000	3000

Figure: Both 'word' and 'nope' cannot be pasted into the Parent_MW and MW columns as they are numeric columns. In this instance these cells will be ignored, but the rest of the cells will be pasted.

Reverting back to original data table

To discard all edits to the data table, right-click and select 'Edit > Discard all edits...'. A dialog will be displayed to confirm. This will discard all the edits to the data table and the table visualization will update to reflect this change.

Venn Diagram

The Venn diagram visualization is used to display the logical relationship between a collection of different sets, and to mark sets and subsets of rows in a data table. Each set is defined using a [Spotfire expression](#) (e.g. [MW] <= 500) and is assigned a name and a color. After sets have been defined, all possible intersections are calculated and the Venn diagram is displayed. The Venn diagram will respond to marking and it is possible to drive the marking by interacting with the Venn diagram. The data displayed in the Venn diagram can be limited by one or more markings from other visualizations (see [Limit by Marking](#)) or by applying one or more of the many possible Spotfire filters. An example Venn diagram visualization is shown below.

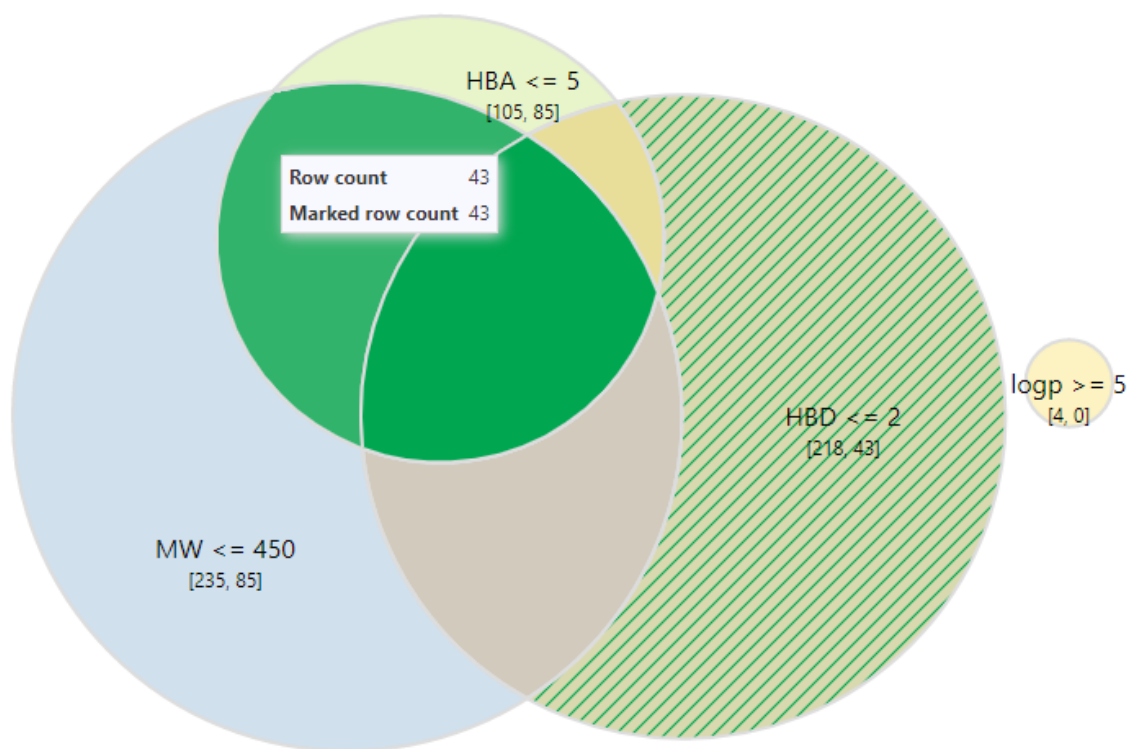


Figure: Lead Discovery ChemCharts Venn diagram visualization.

Here, 4 sets were defined using the following Spotfire expressions: [MW] <= 450, [HBA] <= 5, [HBD] <= 2 and [logp] >= 5. The intersections between the sets are calculated and displayed. In the example above, the Venn diagram is displayed using force directed layout. The relative

diameter of the circles corresponds to the number of members of each set. The overlap area between the circles indicates the magnitude of overlap between the sets.

Each set is labeled with the name of the set as well as the number of items and the number of marked items in the set. For example, the $MW \leq 450$ set has 235 members of which 85 are marked. Hovering over a segment in the Venn diagram will display a tooltip that shows the number of items and the number of marked items in the segment.

If all items in a segment are marked the segments will be colored using the marking color. In the example above, all items (or rows) making up the intersection between $MW \leq 450$ and $HBA \leq 5$ (or $MW \leq 450 \cap HBA \leq 5$) are marked, thus the segments are colored using the marking color. If some, but not all, of the items in a segment are marked, the segment will be drawn with a hatched pattern.

Context menu

Much of configuration for the Venn diagram visualization is accessed through the context menu, which is opened by clicking the right mouse button anywhere in the visual. An example of the context menu is shown in the figure below.

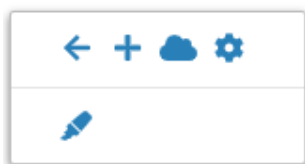







Figure: The Venn diagram visualization context menu.

The table below describes the function of each context menu item:

	Back: returns the user to the visualization 'home' page where the user can select a different visualization or data table to display in the current ChemCharts visualization.
	Add visualization: adds a new ChemCharts visualization to the current page. Used primarily in the web player.
	Web services: opens the web services dialog.
	Properties: opens the Properties dialog.
	Limit by marking: toggles the limit by marking behavior of the visualization

Set configuration

Sets can be added, edited and removed from the Venn diagram in the Venn page of the properties dialog. Open the Properties dialog using the [context menu](#) and navigate to the Venn page. To add a new set, click the 'Add set' button. This will add a new set to the list of sets for the Venn diagram. Users must enter the expression for the set that will dictate whether rows are included in the set. In Spotfire Analyst, the Spotfire expression editor can be used to do this by clicking the pencil icon at the right of the text box. Users can optionally change the color for the set as well as enter a display name for the set. If no name is entered, the expression will be used as the name. Sets can be removed by clicking the remove button next to the expression text box. An example of the Venn page of the properties dialog is shown below.

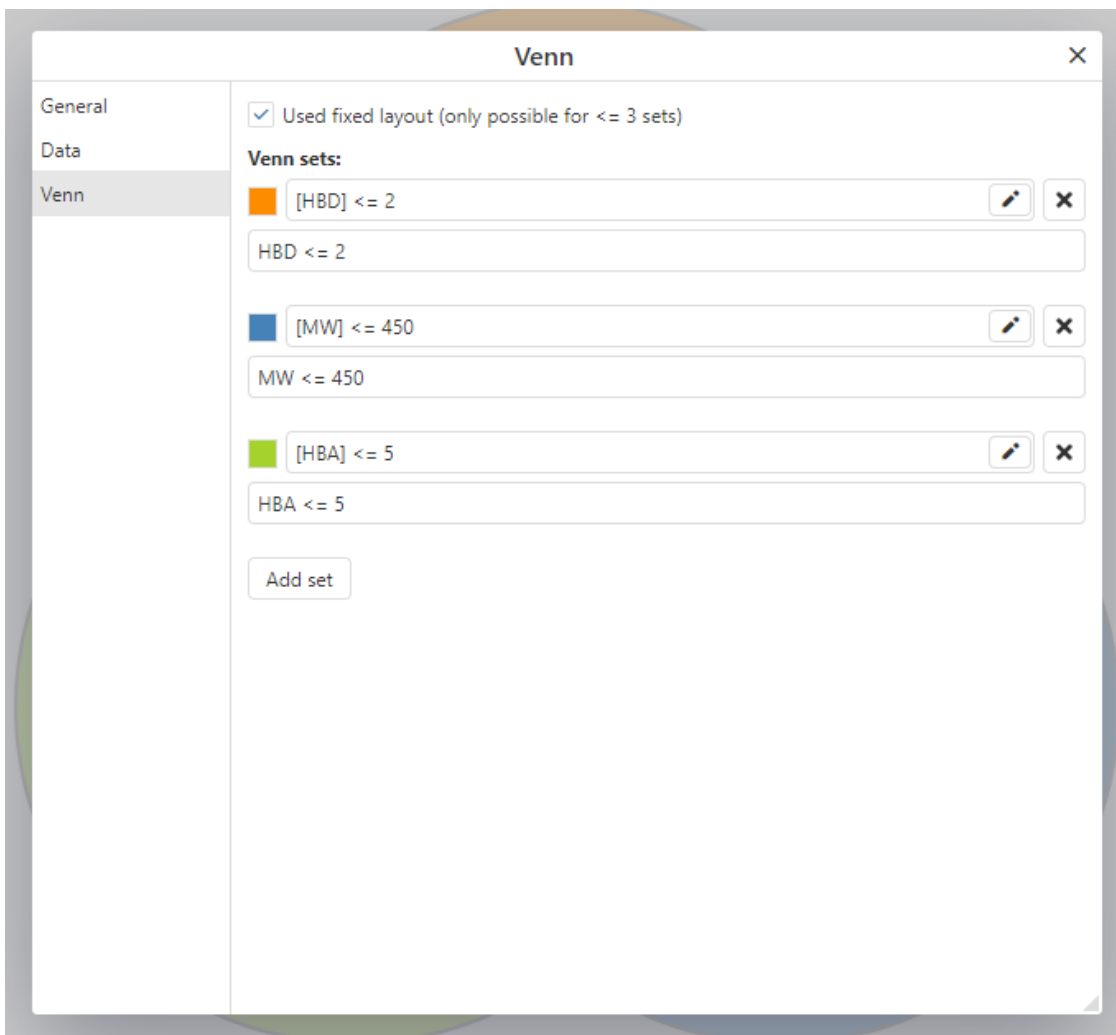


Figure: Venn page of the properties dialog.

Fixed Layout

A fixed layout for the Venn diagram can be used instead of the force directed layout. This is only possible when there are 3 sets or fewer. In this case, the size of the circles representing the sets and the degree of overlap of the circles do not reflect the size of the sets or the size of the intersections. To display the Venn diagram using a fixed layout, open the Properties dialog using the [context menu](#), navigate to the Venn page and check the 'Used fixed layout' checkbox. An example of a fixed layout Venn diagram is shown below.

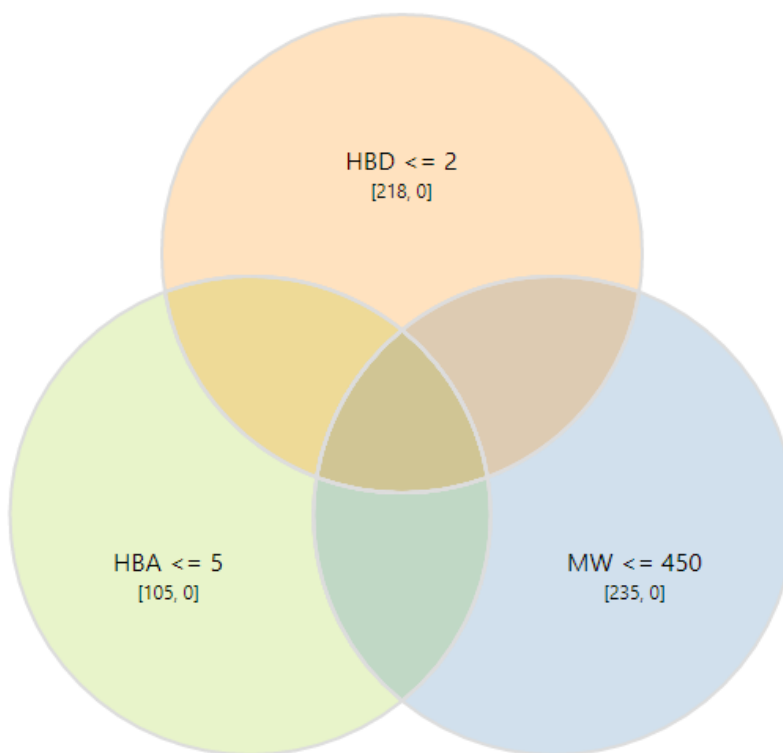


Figure: Fixed layout venn diagram.

Marking

The Venn diagram visualization can be used to mark rows. Clicking on any of the segments in the Venn diagram will mark the corresponding rows. Multiple segments can be marked using mouse clicks in conjunction with the Ctrl key. An entire set (or circle) can be marked by clicking on the set name.

Web Services Visualization

*** Web services are now deprecated in favor of data functions and may be removed in a future version of Lead Discovery ChemCharts. Please see the Data Function User Guide for more details.**

The Lead Discovery ChemCharts Web Services visualization allows users to submit web service requests, monitor the status of running tasks, and load the results from web service tasks into a document. The Web Services visualization will only be included in the list of Charts on the Lead Discovery ChemCharts homepage if the preferences are configured to provide access to a Lead Discovery Web Services server. See [Web Services](#) in the [Configuration](#) section for more information.

The default view of the Web Services visualization is the list of available web services. An example is provided in the following figure.

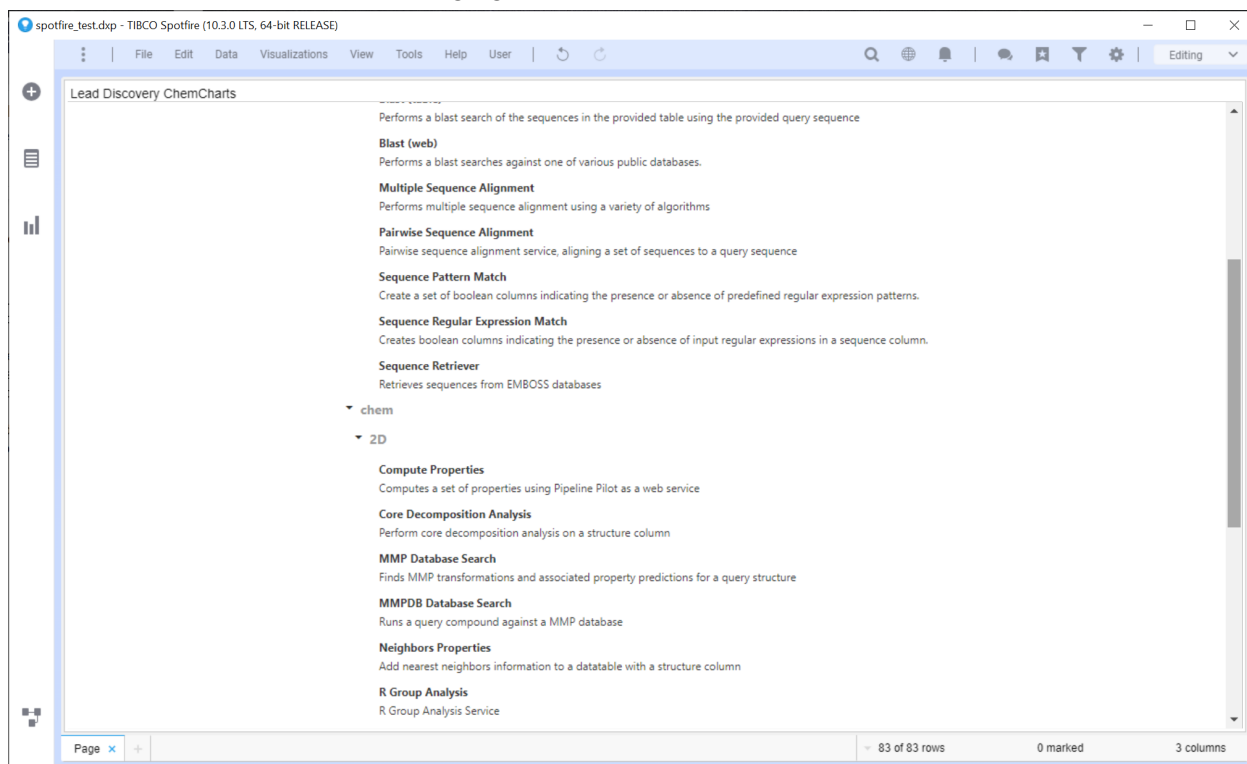


Figure: The Web Services visualization.




Context menu

The Web Services visualization requires little configuration other than the data table from which a subset of data may be submitted to web services. The context menu, accessed by clicking the right mouse button anywhere in the visualization, is spartan.



Figure: The Web Services visualization context menu.

The following table describes the function of each item in the context menu:

	Back: returns the user to the visualization 'home' page where the user can select a different visualization or data table to display in the current ChemCharts visualization.
	Add visualization: adds a new ChemCharts visualization to the current page. Used primarily in the web player.
	Properties: opens the <i>Properties</i> dialog.

The following sections describe the use of the Web Services visualization.

Configuring a data table

The Web Services visualization is configured with a single data table just like other Spotfire visualizations. Data from any data table may be submitted to web services provided that all rows are to be submitted to a service. To send a subset of data from a data table, such as filtered or marked rows, the configured data table must be changed prior to task submission. To send a subset of data from an alternative data table not currently configured, open the Properties dialog from the context menu, navigate to the *Data* page and use the *Data table* dropdown menu to select the desired data table.

Submitting a web service task

Web services are selected by mousing over the desired entry in the list of web services. A green icon will appear on the right of the service name and description. Click the left mouse button to select the service and open the service's *Submission* dialog.

Blast (local) text query

Performs a BLAST search of user selected databases using a query entered as text

Blast (table)

Performs a blast search of the sequences in the provided table using the provided query sequence

Blast (web)

Performs a blast searches against one of various public databases.

Figure: Selecting a web service.

Web Service *Submission* dialogs are unique to each service, and allow the user select options, enter queries, and submit data. See the Lead Discovery Web Services User Guide for additional information. An example Submission dialog is provided in the next figure.

Blast (table)

Performs a blast search of the sequences in the provided table using the provided query sequence

Data source for new task

Data table Previous task

spotfire_test ▾

Select sequence column

Select... ▾

Query sequence

Submit data from

All data
 Data after filters
 Marked data

Task name

Enter name for task

Figure: An example submission dialog.

Web services that require input data from a data table will have a *Submit data from* radio group allowing the user to submit all data, marked data, or data after filters. The *Task name* text entry field allows users to provide a unique name for facile identification of results from the *Tasks* list.

Key columns

Services that operate on data submitted from a data table may offer the option of merging results back into the original data table. Merging data in Spotfire requires row matching on at least one column of data. Providing a key column in the web service Submission dialog, when the option is available, has two positive benefits. First, provided the key column is unique,

results can be guaranteed to merge correctly even if the original data table has changed. Data tables with information link data sources may change in the interval between task submission and results merge. Key column backed data will still merge correctly in this case. Additionally, providing a key column will limit the data submitted to the web service to the minimal amount required to execute a web service request. In the absence of a key column, data from all columns from the original data table are transmitted to a web service, and are subsequently used to merge results back into the data table. The amount of data transmitted may be significantly higher with no key column specified, negatively impacting performance.

Retrieving results

Upon web service task completion, a copy of the results will automatically be downloaded locally. The user will be informed by a message in the visualization from which a task was submitted that the results are available and may be added to the current document, provided the visualization is still visible on the current page. The message alerting the user to the results availability includes a button to initiate loading the results. Completed tasks may also be loaded by selecting the *Tasks* radio button in the upper right hand corner of the Web Services visualization. Clicking the Tasks radio button will display a list of tasks and their current status: *created, running, complete or failed*.

Name	ID	Service	Status	Completed
Neighbors Properties	1468	Neighbors Properties	complete	12 days ago
Neighbors Properties	1467	Neighbors Properties	complete	12 days ago
Neighbors Properties	1466	Neighbors Properties	complete	12 days ago
Neighbors Properties	1465	Neighbors Properties	complete	12 days ago
Neighbors Properties	1464	Neighbors Properties	complete	12 days ago
Neighbors Properties	1463	Neighbors Properties	complete	12 days ago
R Group Analysis	1422	R Group Analysis	complete	21 days ago
R Group Analysis	1421	R Group Analysis	complete	21 days ago
R Group Analysis	1420	R Group Analysis	complete	21 days ago
Similarity Search	1419	Similarity Search	complete	22 days ago
Similarity Search	1418	Similarity Search	complete	22 days ago
Similarity Search	1417	Similarity Search	complete	22 days ago
Similarity Search	1416	Similarity Search	complete	22 days ago
Similarity Search	1415	Similarity Search	complete	22 days ago
Similarity Search	1414	Similarity Search	complete	22 days ago
Similarity Search	1413	Similarity Search	complete	22 days ago

Page x + 83 of 83 rows 0 marked 3 columns

Figure: The list of submitted web service tasks.

Tasks marked complete in the *Status* column are available for loading into a document. Clicking on the task name, which appears as a hyperlink, initiates loading results of the task into the

document. Log files from failed tasks may be downloaded for inspection by clicking the caret on the left hand side of each task name, revealing a list of files that may be downloaded locally.

Configuring Visualizations

Properties dialog

In Lead Discovery ChemCharts versions prior to 2.0, the Properties dialog was written to mimic equivalent visualization Properties dialogs in the Spotfire Professional client. The Properties dialog in Lead Discovery ChemCharts 2.0 has been written to work identically in the Spotfire Professional client and Business Author. The current web browser compatible versions of the Properties dialog also include specific configuration options for some visualizations.

Documentation for visualization specific pages may be found in [Visualizations](#).

General

The title of a visualization may be edited using the *Title* text area in the *General* property page. The *Show title bar* checkbox displays or hides the top title bar in visualizations, depending on the checked state of the control.



Figure: The *General* properties page.

Data

The *Data* property page allows for configuration of essential features of visualizations. The data table from which visualizations draw data may be selected using the *Data table* dropdown menu. Marking may be configured or disabled with the *Marking* dropdown menu (note that users can also switch between markings in ChemCharts visuals using the keyboard shortcut Ctrl+Alt+M). To disable marking, select None. A new marking can be added by clicking the 'Add' button to the right of the marking dropdown and entering a name and color for the marking. Checking the *Limit by* checkbox will limit the visualization to only display data from rows marked

in another visualization. The *Limit data by expression* text area may be used to enter a “where clause” expression used to limit the data displayed in a visualization. The Edit button on the right hand side of the text area opens the Spotfire *Expression Editor* dialog. The dialog is only available for use in the Spotfire Professional client.

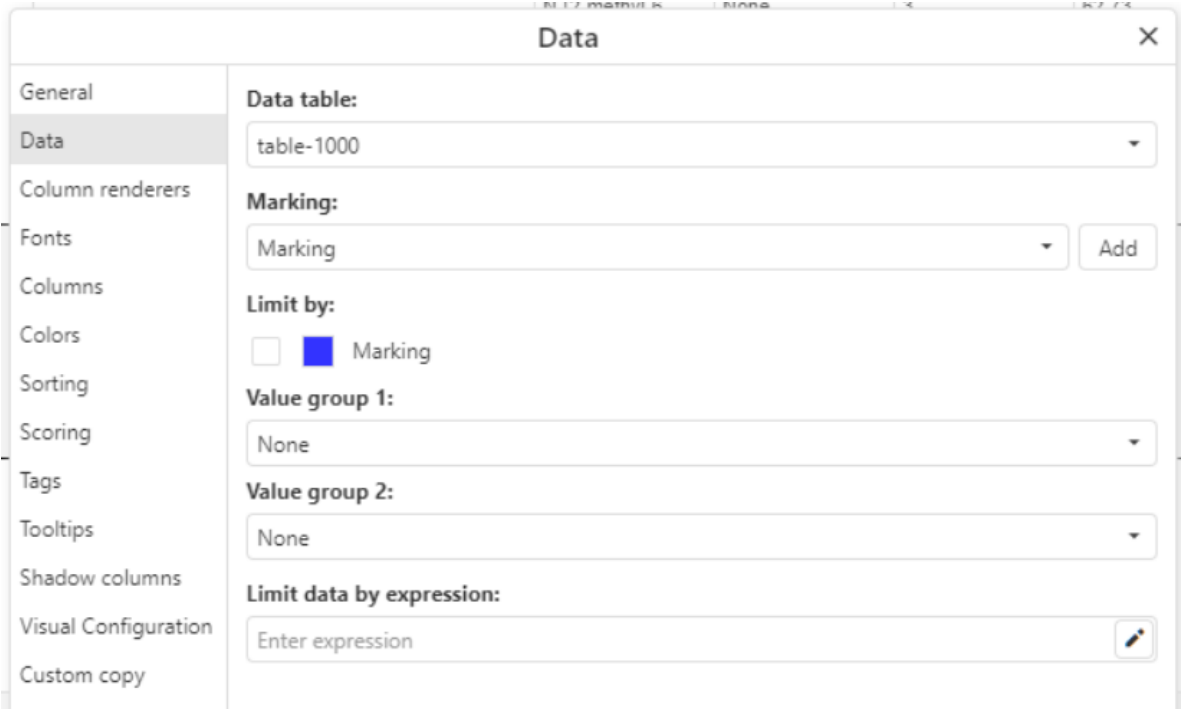


Figure: The Data properties page.

Columns

The *Columns* property page allows the user to configure columns for display in a visualization. The *Columns control* consists of a list of available columns on the left hand side, and configured columns on the right hand side. Use the arrows between the two lists to move checked items from one list to another. The text box filters above each column list facilitate finding columns by pattern or name. Columns may be reordered in the configured list by checking the checkbox next to the column name, and using the buttons on the right hand side of the control to move the checked items one place up or down in the list, to the beginning of the list, or to the end.

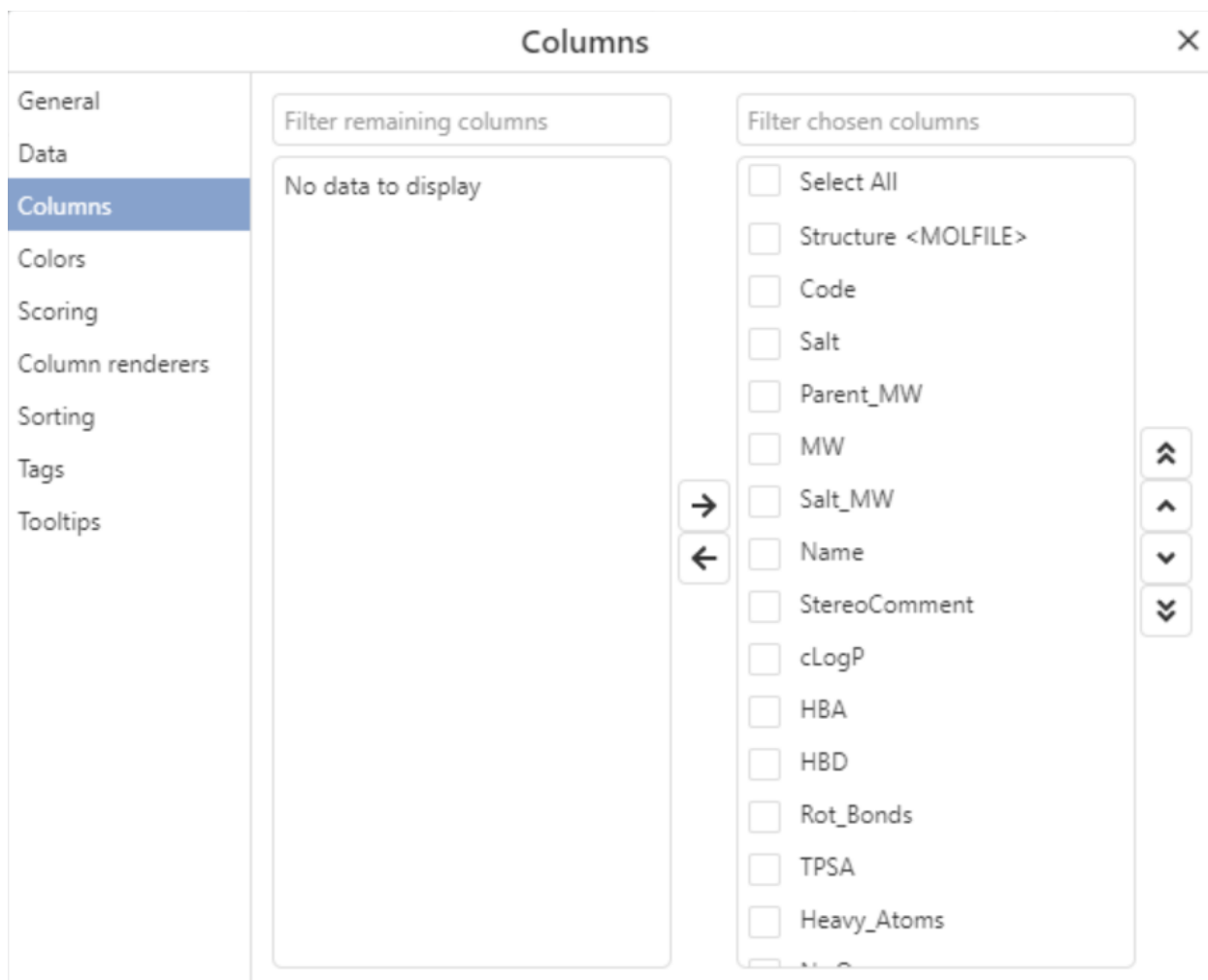



Figure: The Columns property page.

Column renderers

Spotfire visualizations expose configuration of column renderers through the *Columns* property page. The Lead Discovery ChemCharts *Column renderers* property page exposes the same functionality using a different interface. The column for which a renderer is to be configured is selected using the *Columns* dropdown menu. Once selected, the current renderer and alternate possible selections will appear in the *Renderers* dropdown menu. Renderers with settings dialogs that are only available in the Spotfire Professional client may be opened using the *Settings*  button. The *Settings* button will only be enabled if the selected renderer has an associated *Settings* dialog. Renderers that are part of Lead Discovery ChemCharts, such as the *Text* or *Sequence* renderers, will display their settings options on the Column renderers property page below the *Renderers* menu. Settings controls will appear on the page after a Lead Discovery ChemCharts renderer is selected from the *Renderers* menu.

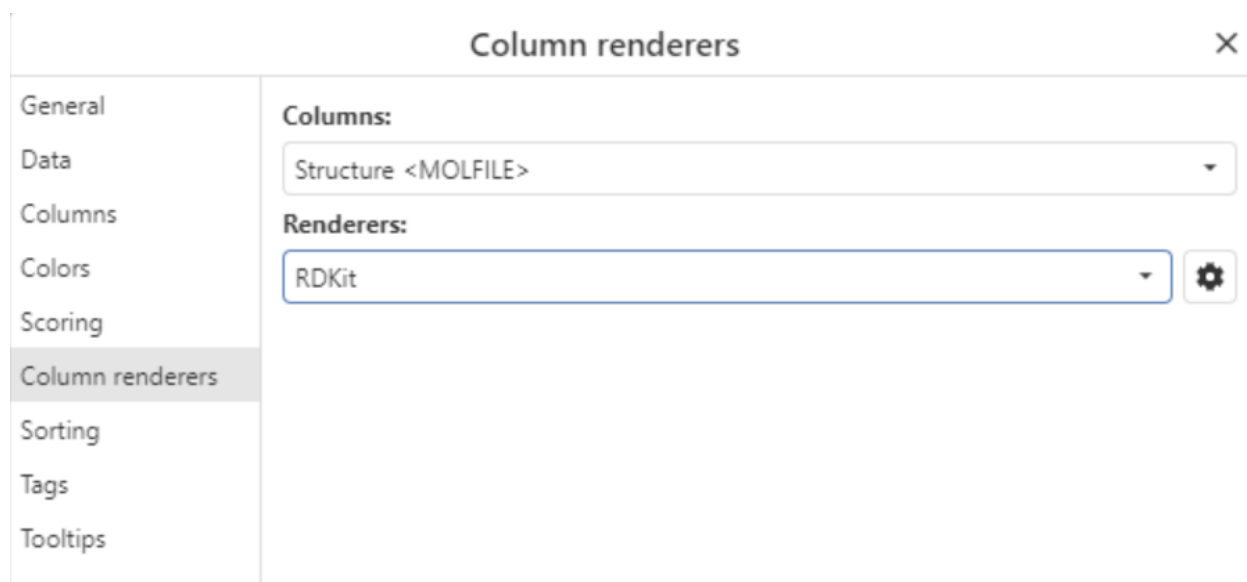


Figure: The Column Renderers property page.

Colors

The *Colors* property page in Lead Discovery ChemCharts provides similar functionality to its equivalent property page in native Spotfire visualizations. Configuration controls work slightly differently due to the constraints inherent in a browser compatible dialog. The same color rule types and groupings may be configured in the Lead Discovery ChemCharts *Colors* property page, but the steps required to define a rule differ. Breakpoints used in gradient and segment color rules are notably different in that they cannot be adjusted by dragging the breakpoint thumb position to alter values. Breakpoint values are entered using the textbox associated with the breakpoint.

Once a set of color rules is defined, it may be saved to an external file or applied directly to other Lead Discovery ChemCharts visualizations in a document. Color rules defined in either an external file or other visualizations in a document may be applied to the visualization currently being configured. These options for transferring sets of color rules between visualizations are found in the *More* dropdown menu on the right hand side of the *Colors* property page.

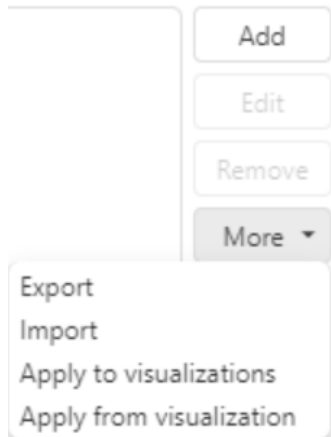


Figure: Options for transferring color rules.

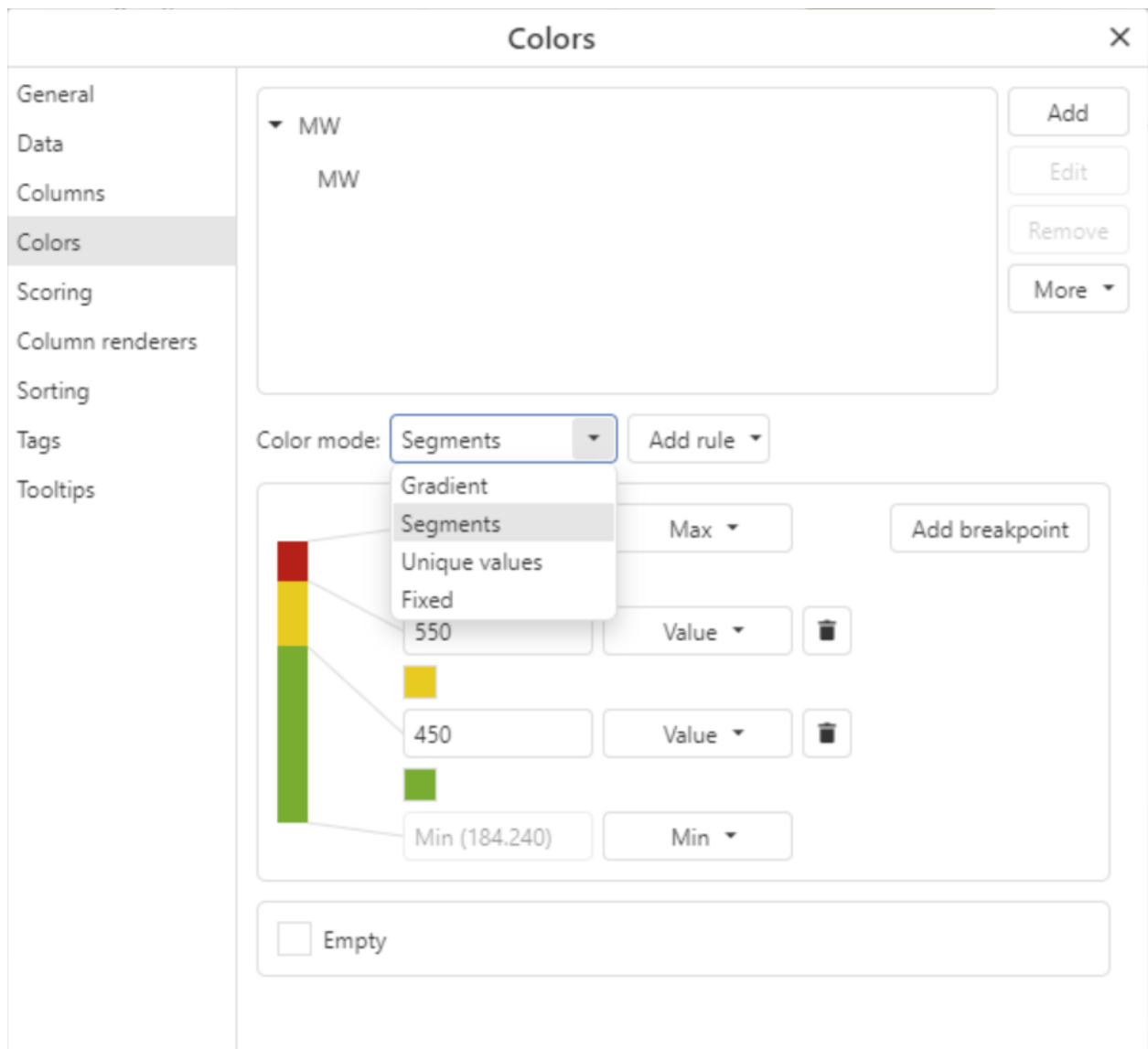


Figure: The Colors property page.

Lead Discovery ChemCharts has a unique feature for applying color rules defined for a column to other columns, even if the target column is a different data type. See the [Applying Color Rules to Different Columns](#) section for additional information.

Scoring

The *Scoring* property page provides the ability to create ranking functions by combining and scaling data in the data table. This feature is commonly used with the [MPO visualization](#), although the Scoring property page is available from multiple visualizations.

To create a new score column, open the *Properties* dialog and navigate to the *Scoring* page. See the *Creating a new score column* figure. If score columns have been created previously, they will be listed in the *Score column/scheme* dropdown menu. To create a new score column, click the *Add score column* button and name the column in the *Enter score column name* text field.

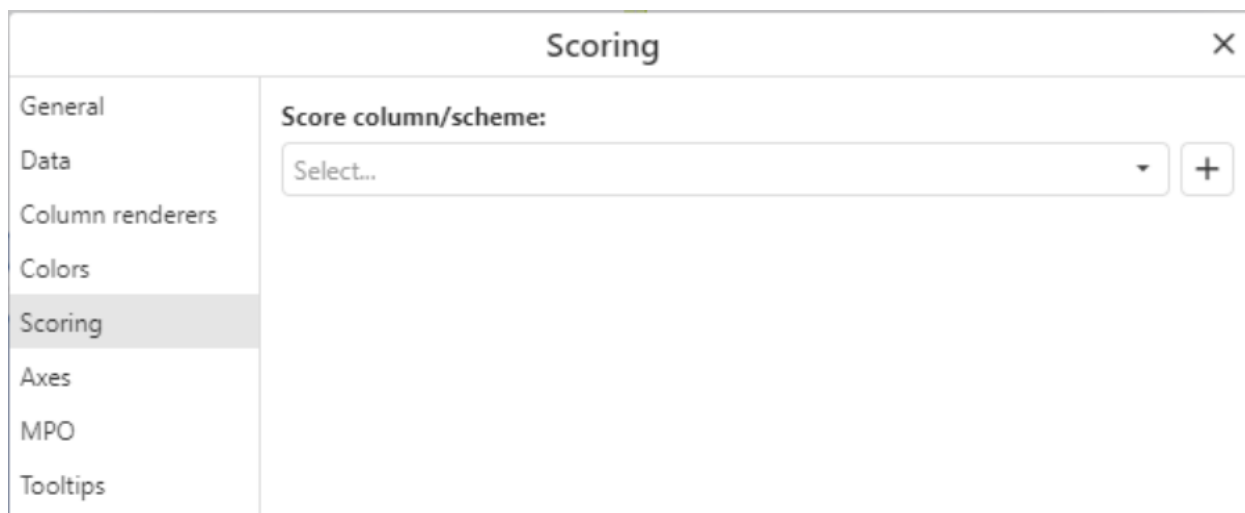


Figure: Creating a new score column.

After a score column has been created, each data column's contribution to the score may be configured. Select a column from the *Column* dropdown menu, then select from the *Score rule type* dropdown menu. See the figure below for an example.

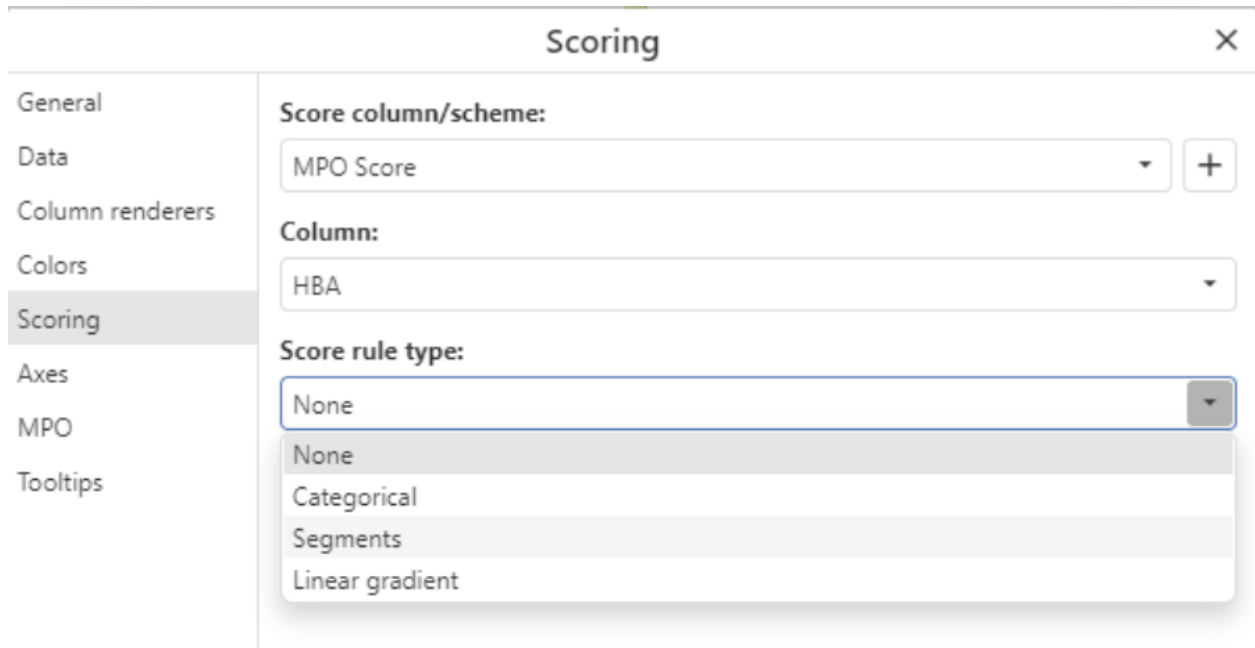


Figure: Configuring a rule type.

Score rule types are analogous to color rule types. The score rule types that may be added for a column depend on the column's data type. Contributions to the score for *Categorical* rules may be applied on a per-category basis. The *Segments* score rule is used to apply a score contribution for a range of values. *Linear gradient* score rules are used to add interpolated contributions to the score based on configured endpoint score values and each data value's relative position within a configured range. A configured segments rule is shown in the next figure.

Scoring ×

- General
- Data
- Column renderers
- Colors
- Scoring
- Axes
- MPO
- Tooltips

Score column/scheme:
 +

Column:

Score rule type:

to 0

🗑

to 10

🗑

to 0

Add breakpoint

Empty value score:

Calculate scores

Figure: A segments score rule.

The HBA, or hydrogen-bond acceptor column has a data type of integer. Lower bounds of each segment are inclusive (\geq), while upper bounds are exclusive ($<$) of values that are equal to the breakpoint value. The configured rule would therefore add a value of 10 to the score for every row that has $0 \leq \text{row value} < 6$. Restated more simply, ten will be added to the combined score for rows with zero to five hydrogen bond acceptors.

Sorting

Lead Discovery ChemCharts visualizations can perform multi-column sorting with up to 5 columns. Multi-column sorting behavior is configured in the *Sorting* property page. Select the first column from the *Sort by* dropdown menu, and set the sort order using the *Ascending* and *Descending* radio buttons. Configuring the *Sort by* column will cause a new *Then by* control to appear. Additional columns are configured using *Then by* controls until the maximum number of

sort columns has been reached. To remove a configured sort column, select None from the dropdown menu.

The image shows a 'Sorting' dialog box with a sidebar on the left containing menu items: General, Data, Columns, Colors, Scoring, Column renderers, Sorting (highlighted), Tags, and Tooltips. The main area is titled 'Sorting' and contains four 'Then By' sections. Each section has a dropdown menu and two radio buttons for 'Ascending' and 'Descending'. The first section is 'Sort by:' with 'cLogP' selected and 'Ascending' selected. The second section is 'Then By' with 'HBA' selected and 'Ascending' selected. The third section is 'Then By' with 'Heavy_Atoms' selected and 'Ascending' selected. The fourth section is 'Then By' with 'None' selected and 'Ascending' selected.

Tags

Spotfire tags are useful when creating hit lists and adding categorized metadata to rows. When the number of entries to be decorated with tags is large, Spotfire tags can be cumbersome to configure and apply. Lead Discovery ChemCharts tags simplify configuration and application of tags to a data table.

Prior to defining a tag group, the Tag property page will appear as follows:

The image shows a 'Tags' dialog box with a sidebar on the left containing menu items: General, Data, Columns, and Colors. The main area is titled 'Tags' and contains the text 'Select the active tag column:' followed by a radio button labeled 'None' which is selected. Below this is a blue link that says 'Create a new tag column.'.

Figure: The Tags property page with tags group defined.

Click the *Create* link to define a new tags group. The *Tags* property page will switch to the tag group definition dialog. The column name in which tags will be stored may be entered in the *Tag column name* text box. The *Tag set* dropdown menu contains a list of predefined tags groups complete with color rules. If none of the predefined tag sets match the desired tags, click the checkboxes next to the *Tags* for the set and click the *Remove tags* button, then click

the *Add tag* button to define new tags. The colors displayed in the color pickers to the left of each tag are used to automatically define color rules if the *Enable color rules* control is checked. Click OK when the tag set definition is complete.

Tags

General

Data

Columns

Colors

Scoring

Column renderers

Sorting

Tags

Tooltips

Create tag column

Tag column name:

Tag Column

Tag set:

Yes/No

Tags:

Yes

No

Enable color rules Add tag Remove tags

Key columns:

If data is not embedded it maybe necessary to set key columns for the tags to persist. Click [here](#) to set key columns.


OK Cancel

Figure: Defining a new tag set and color rules.

The Tags property page will then display a radio button group consisting of the *None* option and all defined tag groups. Select the radio button next to the desired tag group to activate it. Close the *Properties* dialog. When a tag group is active in a Lead Discovery ChemCharts visualization, hitting the spacebar will apply the first tag to all marked rows. Hitting the spacebar again will remove the existing tag and apply the second tag to all marked rows. The space bar can be used to cycle through all tags in the group until no tag is applied, at which point the cycle of tags restarts. In the Spotfire Professional client, tags are applied to the active row if no rows are marked. This facilitates application of tags just by moving the cursor and pressing the spacebar, without having to mark rows.

Tooltips

Tooltips are enabled by default in Lead Discovery ChemCharts visualizations. To disable tooltips, uncheck the box next to the Tooltips enabled control in the *Tooltips* property page. In addition to the default tooltips, form-based tooltips may be defined for Lead Discovery ChemCharts visualizations. Check the box next to the *Use form-based tooltips* control. Click

the *Edit local form-based tooltips* link to open the [form editor](#). To activate the new form as a tooltip, click the radio button next to the form name. To make the form available to other Lead Discovery ChemCharts visualizations, click the  button to promote the local form to one that is available to all Lead Discovery ChemCharts visualizations in the document.

Tooltips ×

General

Data

Columns

Colors

Scoring

Column renderers

Sorting


Tags

Tooltips

Tooltips enabled

Use form-based tooltips

Select active form-based tooltip:

 Default [local]

* Local form-based tooltips are available to all charts in the current visualization. Global form-based tooltips are available to all visualizations in the document. Global tooltips cannot be edited.

[Edit local form-based tooltips](#)

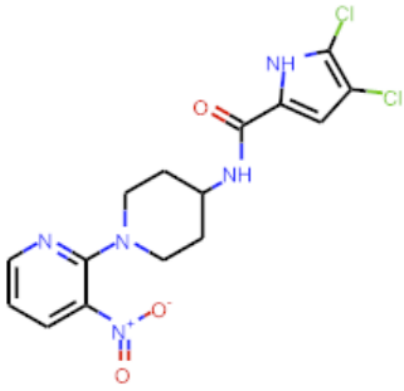
Form Editor

The [Details](#) and [Gallery](#) visualizations, and form-based tooltips may be configured using the Form Editor. To edit form-based tooltips, see the [Tooltips](#) section. To enter the editor from a visualization, click the right mouse button to open the context menu and select *Edit form*. The visualization will switch to the form editor, displaying example data in the current form configuration. An example is shown in the next figure.

AZ1001

Form

Control



Forms: ☰

Size:

Spacing:


Save And Return
Save
Discard changes


LogP	PSA	MW	HBA	HBD
3.36	108.54	384.22	5	2

Figure: The form editor.

Working with multiple forms

The form to be edited may be selected from the *Forms* dropdown menu, which contains the forms currently defined for a visualization. A new form may be created by opening the form

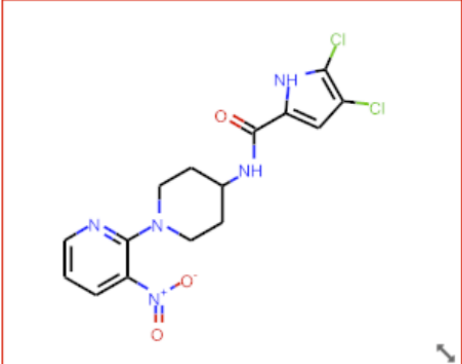
menu button  at the top right of the editor and selecting *New* from the dropdown menu. A dialog will appear allowing the user to name the new form, and specify a layout. The current

form may be deleted by clicking the form menu button  at the top right of the form editor and selecting *Delete* from the dropdown menu. Forms become part of the document once defined. To transfer a form to a new document, click the form menu button and select *Download* to save the form to a file, then import the saved file to another visualization by clicking the form menu button and selecting *Upload* in the form editor of another Gallery or Details visualization.

Editing forms

If multiple forms have been defined for a visualization, the form to be edited may be selected from the *Forms* dropdown menu at the top right of the editor. Once the form to be edited has been selected, controls within the form may be re-ordered by clicking and dragging the controls to another position within the form. The figure below shows the structure display control repositioned at the bottom of the form by left mouse click + drag operation relative to the position shown in the previous figure.

AZ1001				
LogP	PSA	MW	HBA	HBD
3.36	108.54	384.22	5	2



The chemical structure of AZ1001 is shown within a red-bordered control. It features a pyridine ring substituted with a nitro group and a piperidine ring, which is further substituted with a 2,4-dichlorophenylamino group.

Form Control

+ Add X Remove

Columns:
[Structure <MOLFILE>](#)

Save And Return Save Discard changes

Figure: Repositioned structure display control.

Note that controls may also be resized by mousing over a control and left mouse click + dragging the resize button at the bottom right of the control. When attempting to rearrange controls horizontally by dragging, it is important there be space to the right or left of the control for another control to be placed adjacent. Shrinking a control to less than the width of the form will allow another control to be placed horizontally adjacent to another control.

Configuring controls

New controls may be added by clicking the *Control* tab at the top right of the form editor, then selecting a control type from the *Add Control* dropdown menu.

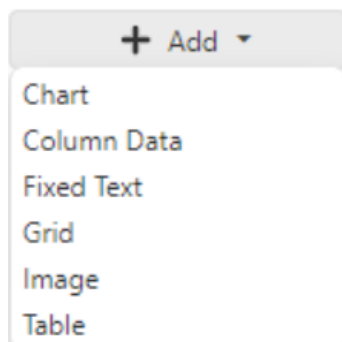


Figure: The Add Control menu.

This will add a new control to the bottom of the form. The newly added control may be repositioned within the form by dragging it to the desired position. The supported control types are:

Chart	Displays a chart generated from configured column data.
Column Data	Displays values for configured columns in a table.
Fixed Text	Static text display of user input. May also be used as a spacer when configured with no text.
Grid	A grid control that facilitates multi-column selection and layout.
Image	Displays an image from configured column data. May be used to display chemical structures.
Table	Displays a table of data from a Related data table or a web service. Table Relations may be configured using the Spotfire <i>Data Table Properties</i> dialog in the Relations tab.

After adding a new control or selecting an existing control, the options for configuring the control appear on the right hand side of the form editor. The following sections describe the configuration of the various control types.

Column Data

The column data control allows the user to display data from configured columns in a table. By default, data from each column is added to a two row table where the column names are the header and the values are displayed in the second row. The next figure shows an example of a simple column data control in a form.

AZ1001

LogP	PSA	MW	HBA	HBD
3.36	108.54	384.22	5	2

Form
Control

+ Add
✕ Remove

Columns:
[LogP, PSA, MW, HBA, HBD](#)

Display mode:

Value
 Header
 Header and value

Horizontal alignment:

Left
 Center
 Right

Gridlines
 Wrap headers
 Wrap values

Layout:

Horizontal
 Vertical

Vertical alignment:

Top
 Middle
 Bottom

Fonts

Header	Edit
Value	Edit

Save And Return
Save
Discard changes

Figure: Configuring a column data control (highlighted in red).

The columns that are added to the column data control can be added or removed using the *Columns* tag box. There are three display modes: Header + Value, Value only and Header only. Selecting one of these options will result in a table that displays one of the following: the column header and the value from the data table row, only the column headers or only the values from the data table row. The horizontal and vertical alignment of the text in the cells can be set using the *Horizontal alignment* and/or *Vertical alignment* radio groups. The table can be displayed in a horizontal or vertical layout, which can be configured using the *Layout* radio group. The figure below shows the difference in horizontal and vertical table layout.

LogP	PSA	MW	HBA	HBD
3.36	108.54	384.22	5	2

LogP	3.36
PSA	108.54
MW	384.22
HBA	5
HBD	2

Figure: Horizontal (top) and vertical (bottom) table layouts in the column data control.

Grid lines can be enabled or disabled using the *Gridlines* checkbox. The columns in the column data control can be resized by dragging the mouse (note that the control has to be selected in order to do this). The fonts used in the column data control may be configured in the *Fonts* section in the lower right hand corner of the forms editor.

Grid

The *Grid* control is similar to the Column Data control in that it displays columnar data, but it differs in that the *Grid* control integrates fixed text fields and makes it easy to configure a grid layout of more than one column or row of data. The Grid control is especially useful when displaying multiple categorized assays.

The grid control may be configured by clicking the *Edit Grid* button in the form editor. The *Grid editor* dialog is shown in Figure 5.

	Column 1	Column 2
Row 1	HBA	*molname
Row 2	HBD	First Sample Reg. Date

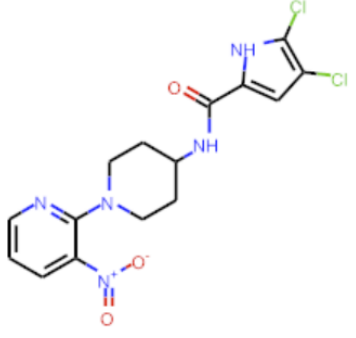
Number of columns: 2 Number of rows: 2

OK Cancel

Figure: The Grid Editor dialog.

The cells on the far left are text entry fields for which the Grid control will display fixed text. The same is true for the cells on the top row. The dropdown menus in the middle of the grid are used to select columns from which data will be displayed. The dimensions of the grid may be altered using the *Number of columns* and *Number of rows* text entries at the bottom of the dialog. An example of the Grid control display is shown in the next figure.

AZ1001



Molecule Properties

	Column 1	Column 2
Row 1	5	AZ1001
Row 2	2	6/10/2002

Form Control

+ Add - Remove

Edit Grid

Horizontal alignment: Vertical alignment:

Left
 Center
 Right

Top
 Middle
 Bottom

Gridlines
 Wrap headers
 Wrap values

Save And Return Save Discard changes

Figure: Grid control in a form (highlighted in red).

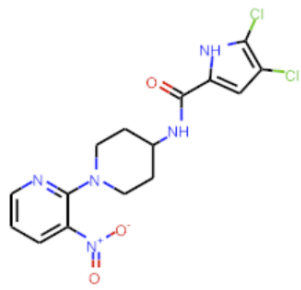
Image

The image control is a simple control that displays an image from a URL, or depictions of molecules in the configured column. The only option here is to select the column from which the molecule is taken using the *Columns* selector.

Fixed Text

The fixed text control allows users to add a header or label to a form. The next figure shows an example of fixed text control in a form. The text displayed in the control can be entered using the Text text box. The horizontal and vertical alignment of the text within the control can be configured using the Horizontal alignment and Vertical alignment radio groups. The fonts used in the fixed data control can be configured in the *Fonts* configuration found in the lower right hand corner of the forms editor.

AZ1001



The chemical structure of AZ1001 consists of a pyridine ring substituted with a nitro group (-NO₂) at the 3-position and a piperidine ring at the 2-position. The piperidine ring is further substituted with an amide group (-NH-C(=O)-) at the 4-position, which is connected to a 2,4-dichlorophenyl ring.

Molecule Properties	
LogP	3.36
PSA	108.54
MW	384.22
HBA	5
HBD	2

Form Control

+ Add - Remove

Text:

Molecule Properties

Horizontal alignment: Vertical alignment:

Left
 Center
 Right

Top
 Middle
 Bottom

Fonts

Fixed [Edit](#)

Save And Return Save Discard changes

Figure: Fixed text control in a form (highlighted in red).

Chart

The chart control displays charts in the form using data from the configured columns in the data table. At present the only chart available is a bar chart. The figure below shows an example of a chart control in a form.

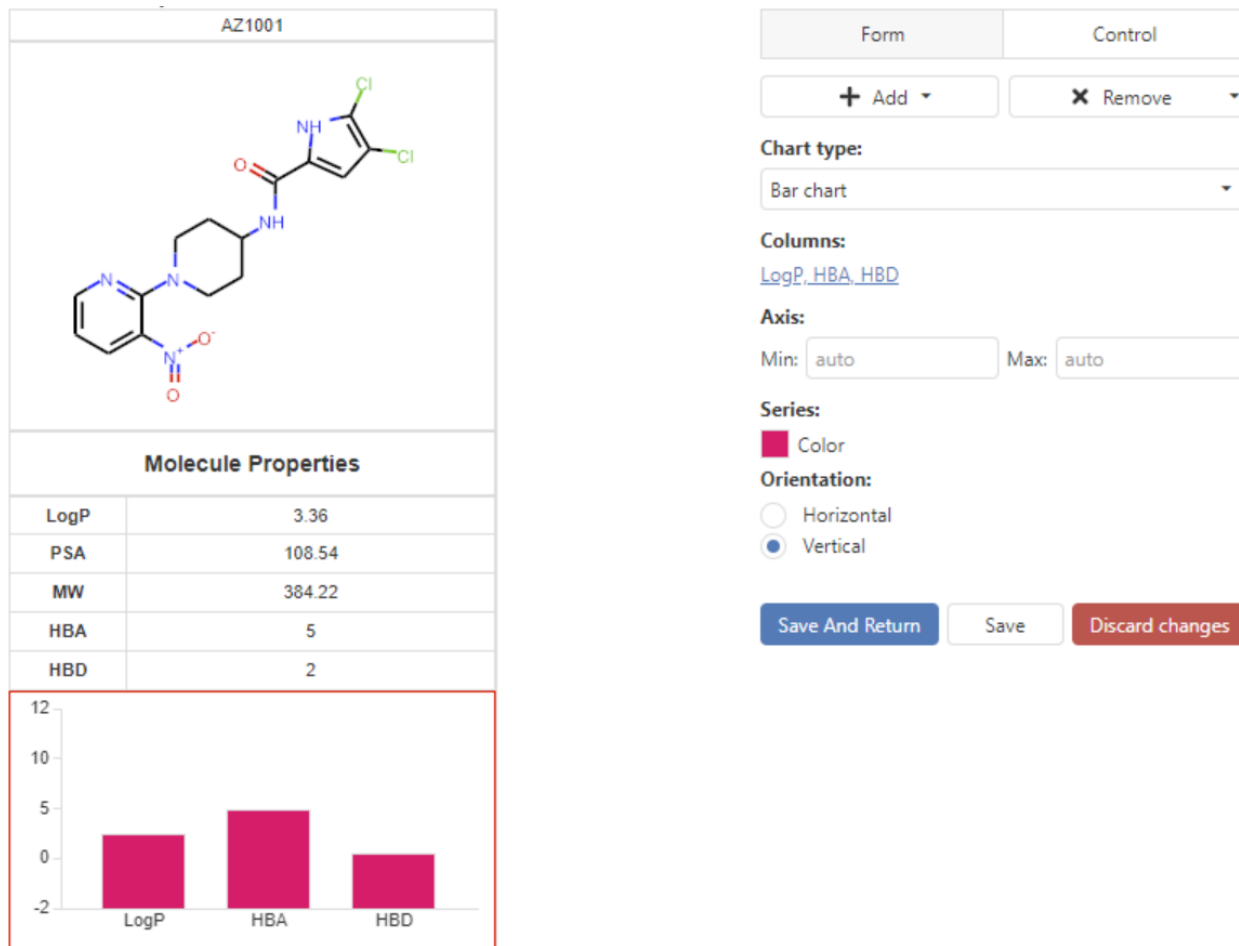


Figure 8: Chart control in form (highlighted in red).

The options for the various chart types will vary. In the case of the bar chart there are controls to set the columns that appear in the chart, a minimum and a maximum for the axis as well as the color.

Table

The table control is used to display a table of data from a related data table. Related tables may be configured using the *Relations* tab in the Spotfire *Data Table Properties* dialog. The table control configuration options are shown in the figure below. The data source for the table control can be selected from the Data source dropdown menu.

Form	Control
------	---------

+ Add ▾	✕ Remove ▾
---------	------------

Data source:

Associated data table ▾


Associated data table:

None ▾

Associated data table columns:

[No columns](#)

Expression to limit data:



Display mode:

Value

Header

Header and value

Horizontal alignment:

Left

Center

Right

Vertical alignment:

Top

Middle

Bottom

Gridlines

Wrap headers

Wrap values

Fill vertical

Figure: Configuration options when the data source is a related (associated) data table.

If the data source is an associated data table, the user must select the associated data table, using the Associated data table drop down. The columns from the associated data table can be selected using the Associated data table columns tag box.

The table control has many of the same styling options as the column data control e.g. display mode, horizontal alignment, vertical alignment, grid lines. See the [Column Data](#) section for more information.

Limit by Marking

It is quite common to use the marking from a visualization in Spotfire to control the display of another visualization. This is often known as 'limit by marking'. For example, a table visualization might be configured to only display the rows that were marked by selecting items in a scatter plot visualization. Items cannot be marked in visualizations that are being limited by marking.

Limit by marking can be enabled or disabled in appropriate Lead Discovery ChemChart visualizations by right-clicking to display the context menu and selecting either 'Enable limit by marking' or 'Disable limit by marking' (the text that appears in the context menu depends on whether limit by marking is enabled or not). If present in the context menu of a visualization, the

limit by marking menu item appears as  when disabled, and  when enabled.

Import/Export visualization configuration

Setting up visualizations can be quite time consuming. As such, ChemCharts allows the export of the configuration from an existing (source) visual to a file and the subsequent import of the configuration from that file to configure a new (destination) visual.

The visual configuration JSON in many cases will contain references to columns from the source visualization. For example, if a user exports the visual configuration for the ChemCharts table visualization, then the exported configuration will contain references to the columns that are displayed in the table. This presents a challenge when importing the visual configuration as there are no guarantees that columns with the same ID/name and data type will exist in the active data table for the destination visual. As such, during the import, ChemCharts will make a best attempt to map the columns from the configuration file (or source columns) to the columns contained in for the active data table for the new visual (or destination columns). Users can manually edit this mapping during [import](#).

Export visualization configuration

To export a visualization configuration, open the property dialog and select the *Visual Configuration* tab. Then click the *Export* link displayed in that page. This will open a file dialog allowing the user to save the configuration file (e.g. visconfig.json).

Import visualization configuration

To import a visualization configuration file, users can:

- Open the property dialog and select the *Visual Configuration* tab. Then click the *Import* link displayed in that page.

- Click the Import visual configuration link on the 'home' page of a new ChemCharts visualization.

In both cases this will open a file dialog where the user must locate the visual configuration JSON file (e.g. visconfig.json) they want to import.

Once the visual configuration is loaded, a table is displayed showing the column mapping between the 'source columns', i.e. the columns in the visual configuration file, and the 'destination columns', i.e. the columns in the active data table for the visual. The initial column mapping is made using column ID/name and data type. Users can alter the mapping, by clicking on entries in the 'Destination column' and selecting a different column.

Clicking OK, completes the import and the ChemChart visualization should be configured.

Manipulating Sequences

*** Sequence Tools formerly found in this section of the documentation have been deprecated in favor of data functions. Please see the Data Function User Guide for descriptions of the data functions that have replaced Sequence Tools.**

Shadow Columns

Lead Discovery ChemCharts allows users to configure shadow columns. A shadow column is defined as a column in a data table that is assigned to a chosen column, thus shadowing the chosen column, after which any coloring displayed for the chosen column will be the coloring defined for the shadow column. Additionally, values from the shadow column can also be used in place of those from the chosen column for sorting purposes.

A common example is assay data that is represented by two columns: one text, the other numeric. Assay data columns may have qualifiers or text values that cannot be represented in a numeric column, so a primary view of the assay values is often stored in a column of text. A parsed copy of numeric assay data may then be stored in a separate column of data type Real (double precision floating point) or Single Real (single precision floating point). Coloring and sorting work is naturally carried out via the numeric representation, while the text representation may contain rich data that captures the assay result (i.e. "NV" for "no value"). Representing assay data in this fashion requires extra display area to view data from two columns instead of just one. The solution to this dilemma in Lead Discovery ChemCharts is to make the numeric column a shadow column of the text column, such that the color rules and sorting behavior of the numeric assay column are applied to the text assay column. The numeric column can then be hidden while retaining the ability to color and sort based on the numeric values.

Configuring Shadow Columns

Shadow columns can be configured via the *Shadow columns* panel in the ChemCharts property dialog. An example is shown in the figure below.

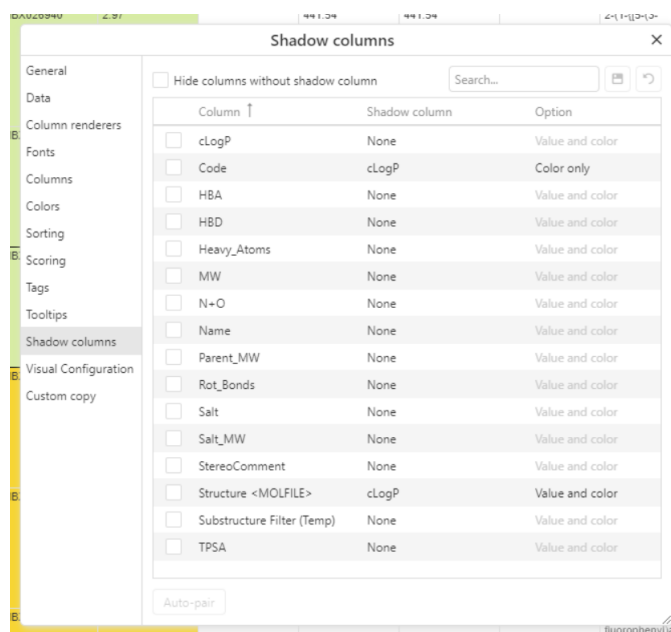


Figure: Configuring shadow columns using the ChemCharts property dialog.

In this example, the *Code* column is being shadowed by the *cLogP* column and has been configured to only apply the coloring from the *cLogP* shadow column to the *Code* column (i.e. the *Code* column will still sort according to the values taken from the *Code* column). The *Structure <MOLFILE>* column is also being shadowed by the *cLogP* column, however, the coloring is taken from the *cLogP* shadow column as well as the value for sorting purposes. The effect of this configuration is shown in the figure below. The *cLogP* column is displayed on the right and has a segmented coloring scheme configured for the column. The *Code* column has the same coloring as the *cLogP* column and the *Structure <MOLFILE>* column has the same coloring as the *cLogP* column (small square in the bottom right of each molecule image). Note that the table is being sorted by the *Structure <MOLFILE>* column, which is using values from the *cLogP* shadow column to determine sort order - hence being sorted by ascending *cLogP* value.

	Structure	Code	cLogP	Salt
728		MBX026940	2.97	
729		MBX014260	2.99	HCl
730		MBX016341	2.99	
731		MBX007256	3.00	
732		MBX009486	3.00	

Figure: Effect of shadow column configuration.

Configuration of the shadows columns is relatively straightforward. Find the column for which a shadow column is to be applied and then choose the shadow column from the drop down list. Users can choose whether the shadow column should only provide coloring to the chosen column (*Color only*) or whether both coloring and values for sorting purposes should be provided to the chosen column (*Value and color*). Once all the shadow columns have been configured users must save the configuration by clicking the save button at the top right of the dialog (see the figure below).

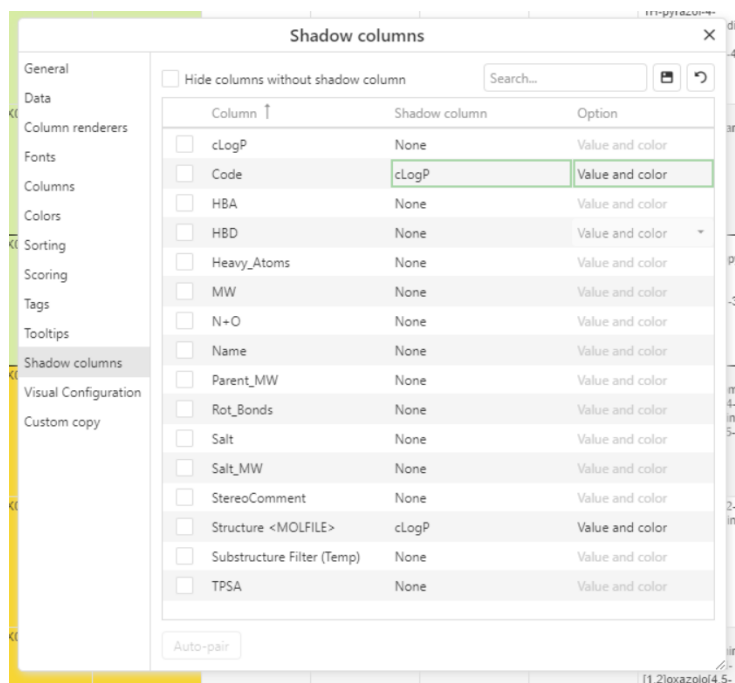


Figure: Shadow column configuration. Here the user has made changes to the shadow column configuration for the Code column (these are highlighted in green in the user interface). The user must now click the save button at the top right to save the configuration.

Custom Copy

Custom copy commands can be created for providing users a shortcut to copying subsets of columns and rows from a table. An good example would be the configuration of a custom copy action that would copy the data from an ID and structure column for a set of marked rows.

Custom copy actions can be configured in the *Custom copy* tab of the ChemCharts *Properties* dialog. First users must select the data table for which the custom copy action is to be applied. To add a new custom copy action click the add button to the right of the Custom copy configuration drop down. The drop down will be replaced by a text box such that the name for the custom copy configuration can be entered. Entering the name and clicking the confirm button will create the new custom copy configuration and add it to the drop down. See the figure below.

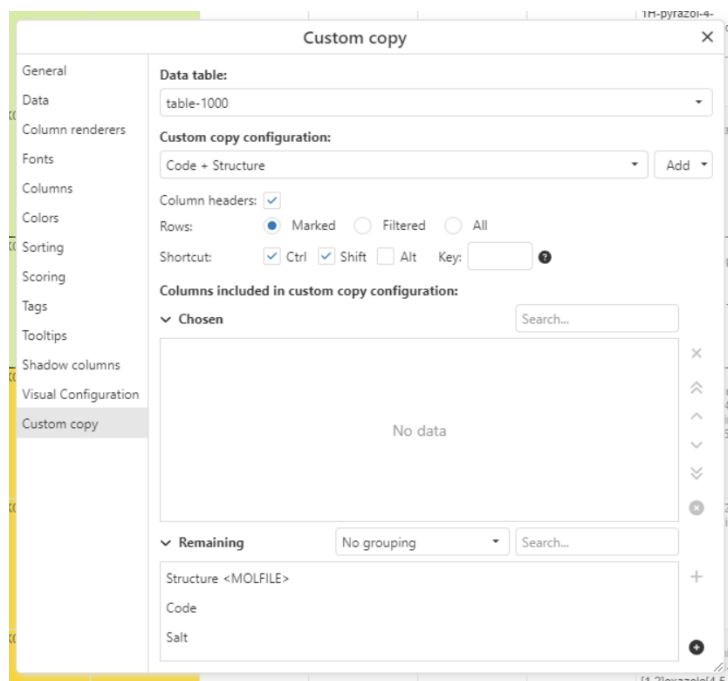


Figure: Newly created custom copy configuration named 'Code + Structure'

After the configuration has been created, users can select whether:

- Whether column headers should be copied
- Which rows are copied - marked, filtered or all
- The keyboard shortcut for the copy action
- Which columns are copied

Once the configuration is complete, the custom copy action should be available to all ChemCharts visualizations provided the active data table is the data table for which the custom copy action is configured. Users can either access the custom copy action via the keyboard shortcut or via the copy menu accessed by right clicking to display the context menu and clicking the copy icon (see the figure below).

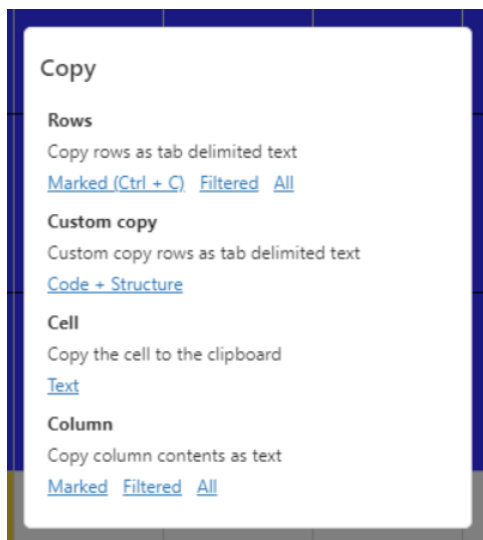


Figure: Custom copy actions appear in the copy menu - if there are any custom copy configurations defined for the active data table

Column Aliases

The column names displayed in Lead Discovery ChemCharts visualizations may be altered without renaming columns by virtue of a column alias property. The column alias property is stored for each column in its column properties. As such, the column aliases will be used in preference to the real column names in all Lead Discovery ChemCharts visualizations.

To configure column aliases open the ChemCharts *Property* dialog and navigate to the *Column aliases* tab - this is shown in the figure below.

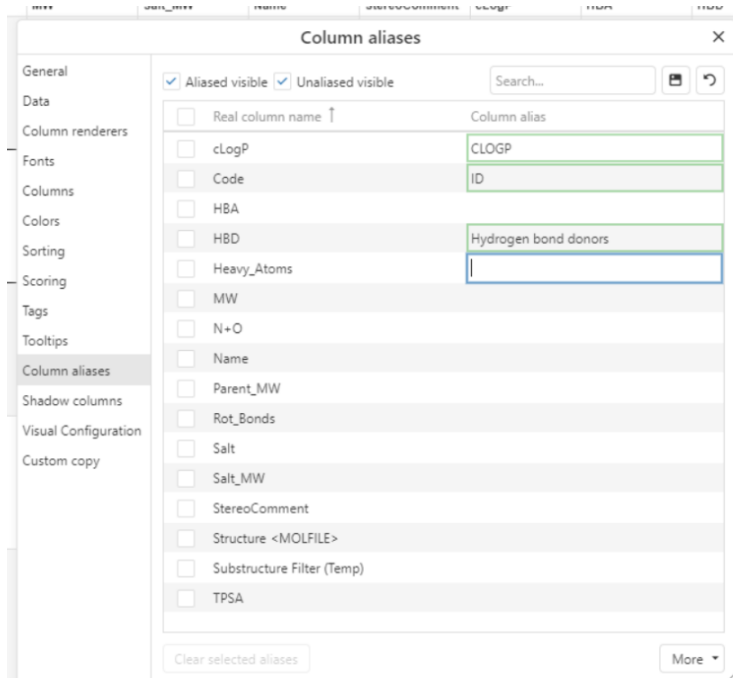


Figure: The column alias property dialog panel

As can be seen, the column alias panel displays a list of all the columns in the data table. To set a column alias for a column, simply type in the desired name for the alias in the *Column alias* column next to the *Real column name*. In the example above the aliases *CLOGP*, *ID* and *Hydrogen bond donors* have been entered for the *cLogP*, *Code* and *HBD* columns respectively. Once the aliases have been set, users must save the configuration by clicking the save button at the top right of the *Column aliases* panel. Unsaved changes are displayed in the UI with green borders.

It is possible to export the currently configured set of column aliases to a JSON file by clicking the *More* button and selecting *Export*. The JSON file can be imported into a different document via the *More* button and selecting *Import*. The column aliases will be applied to any matching columns in the active data table.

Release Notes

Version 4.3.0.0

New Features

- Added support for CheckBox marking to table plot (CHARTS-447)
- Added optional column grouping to table plot (CHARTS-511)
- Limitby per-column in data functions (CHARTS-547)
- Added confirm submit modal for data functions (CHARTS-548)
- Copy visible nodes in Neighbor Properties visualization (CHARTS-546)

- Added context menu option to mark multiple nodes in Neighbor Properties visualization (CHARTS-545)
- Added support for list box filter and item filter in column header menus in table plot (CHARTS-403, CHARTS-425)
- Added 'Find' to the Gallery visualization (CHARTS-367)
- Increased maximum number of core structures supported in SAR map visualization (CHARTS-307)
- Corrected 'display all when nothing marked' in Details visualization (CHARTS-250)
- Data function visual enabled by default without ScriptSync configuration by embedding data functions and related Python libraries
- Improved performance of column grouping when working with wide tables
- Enabled tautomer enumeration in search of cores in R-group decomposition
- Enabled data function execution from user-defined path
- Custom copy actions (CHARTS-502)

Bug Fixes

- Molecule viewer now updates when underlying data is modified (CHARTS-538)
- Fixed depiction size in Distribution visualization (CHARTS-533)
- Corrected Venn diagram behavior when nothing is selected (CHARTS-419)
- Properties modal contents are always visible regardless of screen size (CHARTS-517)
- Corrected inability to rearrange the layout of Details and Gallery visualizations (CHARTS-619)
- Fixed wide bond highlights in the RDKit renderer
- Fixed associated data table control in tooltips and form cells

Version 4.2.0.0

New Features

- Updated to Vue 3 (CHARTS-426, CHARTS-428, CHARTS-431, CHARTS-443)
- Editable tables (CHARTS-430)
- Export table to Excel (CHARTS-467, CHARTS-493)
- Improved link rendering in the table and form-based visualizations (CHARTS-474, CHARTS-475)
- V3000 format molecules supported in 3D viewer
- Structure search tag columns (CHARTS-459)
- Add a new marking via the Data Panel in the properties dialog. Switch between markings using Ctrl+Alt+M - the ChemChart visual must have keyboard focus. (CHARTS-526)
- Ctrl + M (filter to marked) is now implemented in ChemCharts visuals (CHARTS-37)
- Find in gallery visual (CHARTS-367)
- Tagging in gallery visual (CHARTS-19)
- Table visualization now has a gutter at the bottom and right edges allowing for easier column/row resizing at the limits of the table

- If a column in the table visualization is being dragged to reorder and it is outside the bounds of the scrollable area of the table, the table will scroll
- Optional line style for grid-lines in forms (CHARTS-484)
- Editor for the grid control in forms now has the capability for adding a row or column between existing rows/columns (CHARTS-485)
- Input fields in ChemCharts data function definitions can be grouped, with optional surrounding collapsible (CHARTS-489)
- Added the following property calculations using RDKit in the Chemistry visual (CHARTS-477)
 - Lipinski property violation count
 - Rule of 3 pass/fail
 - Rule of 3 violation count
 - Heavy Atom count
 - Atom Count
 - Halogen Count
 - Positively charged atom count
 - Negatively charged atom count
 - Aromatic ring count
 - Ring Atoms
 - Ring Bonds
- Data tables other than the active data table can be used in ChemCharts data functions (CHARTS-488)
- R-Group bioisosteric replacement ChemCharts data function (CHARTS-379)
- Create regions in sequence viewer based on regex of annotation name (CHARTS-472)
- Reorder form configurations by dragging and dropping the tabs in the gallery and details visualizations. Can also reorder in the form editor. (CHARTS-40)
- Where a list of columns appears in a filterable environment, users can now search using disconnected strings e.g. typing 'c p' would now match 'clogP' and 'substructure filter (temp)'. (CHARTS-454)

Bug Fixes

- Export of ChemCharts visuals to Image and PDF fixed (CHARTS-513, CHARTS-515)
- Modal contents always accessible regardless of screen size/resolution (CHARTS-517)
- Fixed neighbor properties visual: molecule images appear then disappear (CHARTS-492)
- Fixed gallery scrolling issues. Switched forms in view mode such that they are rendered using a canvas rather than the hybrid approach used previously. (CHARTS-479)
- Fixed issue with multi-line find highlighting in both table and gallery visualizations (CHARTS-466)
- Fixed empty cell layout issue with the grid control in form-based visualizations (CHARTS-462)
- Spottfire image renderer is supported in table and form-based visualizations. Publisher/ChemCharts image renderer was removed (CHARTS-516)

- Fixed keyboard shortcut Ctrl+A to mark 'filtered', not 'all' in visuals that support the shortcut.
- Re-enabled RDKit render options other than the default ACS 1996 settings.
- RDKit depictions enabled when exporting visuals to an image or PDF.

Version 4.0.1.0

Bug Fixes

- Fixed value group comparison of MOL and MOLV3000 R groups
- Fixed R group decomposition in cases where query hydrogens on the core should not be suppressed
- Fixed ScriptSync failures
- Fixed failures when performing Scheduled Updates
- Fixed name assignment for Data Functions that create multiple tables
- Fixed R group rendering for non-standard smiles representations
- Fixed R group decomposition failures when DataFxn not configured
- Fixed R group decomposition crash for compounds with double bond stereochemistry on input structures

Version 4.0.0.0

New Features

- Added Data functions visualization.
- Column/row header menus.
- Column filter indicator.
- Find in table.
- Column finder popup.
- Ability to alter filter types from the column header menu.
- Import/export visual configuration.
- Dark theme support.
- SAR Map copy structure and rows.
- SMILES molecule rendering in distribution visual group-by.
- Order columns/axes in radar, MPO and distribution plots.
- Color area on radar and MPO chart.
- Distribution axis can optionally take min and max after filtering.
- Better active visualization support.
- RDKit molecule renderer settings.
- Improved performance through the use of serving static files.
- Added ability to create form cells in table plot.
- Increased number of sort columns to 20.
- Structure searches in Chemistry visual may now be reordered.
- Added a git client called ScriptSync to manage DataFxn and associated Python and IronPython libraries.

Bug Fixes

- Disabled keyboard events for non-active ChemCharts visualizations.
- Fixed an issue where the table visualization was not correctly returning to the stored scroll position on a refresh.
- Fixed an issue where the core column in the SAR map property dialog was not reflecting the selected core column.

Version 3.0.1.10

New Features

- Added option to Venn diagram to handle empty values.

Bug Fixes

- Fixed bug in Venn diagram coloring.

Version 3.0.1.9

Bug Fixes

- Fixed bug in internal 'limit-by-marking' mode that would return one fewer than the correct number of rows in some circumstances.

Version 3.0.1.8

Bug Fixes

- Suppressed console warnings when making rapid sequential changes from the SAR Analysis App.

Version 3.0.1.7

Bug Fixes

- Calls to 'AddRange' skipped if DataColumnReferenceCollection is a Snapshot.

Version 3.0.1.6

Bug Fixes

- Fixed issue where column names failed to appear in Columns configuration tab of Properties dialog due to renamed column collisions
- Fixed failure to display Core columns in SAR Map when a structure column in the table is stored as 'string'

Version 3.0.1.5

Bug Fixes

- Fixed display of Core columns in SAR Map
- Fixed incorrect sorting when multiple columns were selected and first column had empty values where subsequent columns had valid values
- Fixed column reference issue that prevented opening ChemCharts visuals

Version 3.0.1

Bug Fixes

- SAR Map made to work with MOL files
- Enabled depiction templates in some cases for invalid molecules
- Alignment/highlighting from substructure searches are now only applied to target column (previously, the changes were applied to all structure columns in document)
- Fixed issue with renamed columns in Gallery and Details visuals
- Corrected copying structure to clipboard in Business Author with MOL files stored as strings
- Neighbor Properties visual made to work with chemistry toolkits other than RDKit

Version 3.0.0

New Features

- Added Venn diagram visualization
- Added Chemistry visualization
- Removed eowp.exe requirement
- Moved near neighbor calculation for Neighbor Properties visual from web service to client (Analyst/WebPlayer)

Bug Fixes

Version 2.1.0

New Features

- Performance improvements to support very wide data tables in all visualizations.
- Redesigned column selection widgets.
- Added font configuration on a per document and per ChemChart visualization basis.
- Added a property page to configure shadow columns.

- Opening the property modal will maximize the visualization to ensure that the property modal is always fully visible. The visualization will be restored when the property modal is closed.
- Opening the form editor in a form-based visualizations (e.g. details, gallery) or when editing form-based tooltips will maximize the visualization. The visualization will be restored when the editing is complete.
- Capabilities that alter the data contained in a data table are disabled in the WebPlayer when in 'Viewing' mode e.g. Tagging, Shadow column configuration, switching data tables etc. To enable these features users must switch to 'Editing' mode.
- Neighbor properties and structure network visuals now have a configurable short-list of active columns.
- Radar charts can now be configured to hide/show item labels, axis titles and axis range.
- Limit-by-marking added to the Dendrogram visualization context menu.
- Added font settings to table control in form-based visualizations (used for displaying data from associated data tables).
- Number formatting should be respected where it makes sense to do so.
- MPO chart display range filter bounds on mouse over slider controls or, optionally, all the time.
- FE bundled JS is around 20% smaller.

Bug Fixes

- It is impossible to open a download dialog from JavaScript in the WebPlayer due to security issues with sandboxed iframes. Therefore, in the WebPlayer, wherever there is an option to download or export to file the content will be copied to clipboard instead. This assumes that the amount copied is not so large that it can still be copied to the clipboard.
- When structures are copied to the clipboard ChemCharts should attempt to copy as the native format and where possible add a text version of the molecule to the clipboard as well.
- Horizontal bar chart bars in form-based visuals are now ordered top to bottom, rather than bottom to top.
- Updated 'Configure column as' capabilities to include genbank, sequence, sequence pair and smart cell content-types.
- Replaced missing top-left corner core renderer in the SAR Map.
- Style changes to tabs used in UI. Selected tab should now be blue.
- Active tag column is now saved.

Version 2.0.0

New Features

- Added Neighbor Properties visualization.
- Added Structure Network visualization.
- Added “Smart Cells” to Table visualization.
- Charts properties dialogs are now written in JavaScript, enabling identical configuration abilities in the pro client and WebPlayer.
- Web services can be accessed and run in the WebPlayer.
- A new grid control in the forms view allowing the placement of values from data table columns into cells arranged in a grid.
- Copying structures and images to the clipboard is enabled in the WebPlayer.
- Rows copied to the clipboard from the table plot will reflect the current ‘standard’ or ‘transposed’ view state of the table plot.
- Structures are automatically converted to SMILES when rows are copied to the clipboard as tab-delimited text.
- Axis control in the radar chart has been improved (min, max, invert and log).
- Distribution plots no longer require grouping, making it easier to plot columnar data.
- Distribution axis controls have been improved (set min, max, invert and log). Axes can be configured such that there is one axis per column or a single axis for all columns.
- Distribution plot is more responsive for large data sets.
- Coloring/sorting behavior of a column can be made to reflect a different numeric column by setting the NumericShadow property of a column to the name of the numeric column.
- The Alias property may be used to alter display names of columns in ChemCharts without renaming the column.
- Text alignment may be altered on a per-column basis in the table plot by changing the text renderer settings. Text wrapping can also be configured and is enabled by default.
- Column header heights in the table plot are adjustable.
- Columns (as well as rows) can be fixed in the table visualization.
- New color-picker that has a basic and advanced mode.
- Web services are now displayed in a filterable tree view.
- Associated tables should be configured using the Spotfire ‘Related Tables’ dialog available from Table Properties.
- The Sequence view is more responsive for large data sets.
- Form-based visualizations (like Gallery and Details) now display a tab-panel if there is more than one form configured for the visualization, allowing for easy switching between layouts.
- The MPO visualization has been improved by changing the chart type from parallel line to distributions.

- Creating an MPO score has been moved from the MPO chart to the chart properties page. MPO scores may be created from multiple chart types.
- Built-in ChemDrawJS. Serving ChemDrawJS from a web server for use with Lead Discovery Web Services is no longer required.

Version 1.4.4.0

Bug Fixes

- Fixed auto-configure for Details view with wide tables.
- Added protections against memory allocation failure.
- Corrected color range and color rules for values equal to breakpoints.
- Added eowp.exe to distribution to correct an issue caused by a suspect update of Windows 10.

Version 1.4.2.0

Bug Fixes

- Set a maximum for an auto-configured columns control in the Details panel to avoid a crash due to excessive memory consumption.

Version 1.4.1.0

New Features

- Added custom annotation styles to Genbank renderer settings.
- Improved web services task submission speed. Enabled key columns to limit data sent to most services.
- Added progress dialogs when sending and receiving data from web services.
- Updated form based gallery and details with ability to set up to a maximum of 36 columns.
- Molfiles represented as strings are now submitted to web services as base64 encoded gzipped strings.
- Added comparative character scheme (dots) to denote identity relative to a reference (fixed) sequence.

Bug Fixes

- Corrected behavior of property pages when resizing parent dialog.
- Improved responsiveness of Colors and Columns property pages when working with wide tables.
- Fixed issue preventing data returned from web services from being merged back into the original table.
- Corrected where clause expression dialog for Spotfire ≥ 10 .

Version 1.4.0.0

New Features

- Context menus have been redesigned to offer a more compact layout.
- Form-based tooltips can be created and used instead of the default tooltips for the following table, sequence viewer, MPO and SAR-Map visualizations. The form editor (used to layout forms in the gallery and details visualizations) is used to create the form that is then used as the tooltip for the aforementioned visualizations.
- A sequence control has been added to the form editor. This allows the display of a sequence (and annotations) in the form-based visualizations (details and gallery visualizations).
- Column selection in the form editor is carried out using the column selector dialog. Columns can be added, removed, filtered and reordered. Column order is now respected in the column data controls.
- Images can be copied from the gallery and details visualizations.
- Copying data from visualizations is now carried out using a copy menu. Where it makes sense, marked data can be copied using Ctrl+C and images can be copied using Ctrl+Shift+C (gallery and details visualization).
- Copy column is now available for the table visualization. This copies the data for the column the mouse is currently over as text. The user can select whether they want all the data, filtered data or just the marked data.
- Distribution chart can now be sorted by any of the statistics generated by the grouping of the data by clicking on the row headers. The columns for each of the groups can be resized using mouse drag. If the sum of the column widths is larger than the viewport, a horizontal scrollbar will appear.
- Sequence motifs can be highlighted in both the sequence and table visualizations. The motif and coloring can be configured in the column renderer settings.
- Sequence motifs can be searched for and highlighted in the sequence visualization (Ctrl+F). This should work exactly like a find dialog in a web browser.
- Simplified tagging has been added to the table visualization. A tag column can be added to the table with a dictionary of values and associated colors. This column can be nominated as the active tag column. When a tag column is active, pressing the space bar will cycle through the dictionary of tags replacing the tag in the tag column for the marked or active rows (if no rows are marked).
- Annotations can be displayed in every row of the sequence visualization (where they are available). Resize the row to display the annotations if they are present.
- Sequences can be translated in the table visualization (DNA to protein).
- Partial sequences can be copied from a sequence column in the table and sequence visualizations.
- The ability to add and edit color rules for groups of columns has been improved.
- Small molecule renderers in Lead Discovery may now be used with Lead Discovery ChemCharts visualizations.

Bug Fixes

- Several issues with color rule creation have been resolved.
- Fixed copying CDX records to the clipboard.

Version 1.3.2.0

New Features

- Changed default comparison color scheme to 'Simple' from none for Sequence viewers.
- Enabled CDX files represented as strings in ChemDraw renderer.
- Added support and preference fields for ChemDraw JS.
- Added additional control in preferences to disable specific visuals.
- Added ability to copy partial sequences to the clipboard.
- Hide/show sequence and annotation display in table and sequence viewer for Genbank columns.

Bug Fixes

- ChemDraw render workers would not stop when Spotfire was closed in some cases.
- Fixed RDKit renderer failures.

Version 1.3.1.0

New Features

- MPO and Sequence visualizations will now only select data up to the first 20 configured columns. Columns should be ordered appropriately for their data to be available to the visualizations.
- Distribution visualization performance improved by only fetching columns required to generate the distributions.
- Improvements to the Distribution visualization and distributions in the Sequence visualization, including:
 - Optionally exclude empty distributions.
 - Tooltips for the values in the statistics table.
 - Bug fixes for text fitting and axis number formatting.
 - Users can now choose the column used for the labels in the Dendrogram visualization.

Bug Fixes

- Fixed limit by value group bug for Table and Gallery visualizations.
- ImageFetcher now guards against null response from publisher when rendering images.
- Added "MarvinSuite" to the classpath for the ChemAxon molecule renderer.
- Resolved log4net.dll version collision in the WebPlayer.

Version 1.3.0.0

New Features

- Added Biomolecule Viewer visualization.
- Added MPO visualization
- Added Distributions visualization
- Pan and zoom in dendrogram visualization.
- Collapse nodes in dendrogram visualization to make display clearer.
- Columns can be resized in table-like controls in form-based visualizations (i.e. Details and Gallery).
- Identity regions in sequence viewer can be based on all sequences, marked sequence or visible sequences.
- Added ability to invert regions in sequence viewer.
- Sequences containing amino acids can be displayed using three-letter codes in all visualizations.
- Active residue highlighting in the sequence viewer.
- Associated tables allowing a join to be configured between the active data table and another data table in the document.
- Added display of data from associated tables in form based visualization via the Table control.
- Web services can be run from the context menu in suitable visualizations.
- Configure/enable/disable protein cartoons/ribbons in the 3D viewers.
- Copy data from visualizations in Spotfire Professional client on to the clipboard. Copy text, images and structures depending on the data and visualization.
- Log scale in all distribution plots (i.e. the one in the sequence visualization as well as the distribution visualization).
- Min and max can be set on the bar chart in form-based visualizations.
- Spinner is displayed during loading of molecules from URL in 3D viewers.
- Added capability to coerce columns to different content types (SMILES, sequence, 3D molecule) in the Table visualization via Configure column as in the context menu.
- Enabled printing and PDF creation of visualizations.

Bug Fixes

- Fixed hard crash issue for very small ranges in the distribution plots.
- Fixed max JSON return size issue in the WebPlayer.
- Fixed gallery keyboard event bug.

Version 1.2.3.0

New Features

- Added Dendrogram visualization for viewing the results from multiple sequence alignment. Dendrogram may be viewed horizontally, vertically, or radially.
- Added Sequence Viewer visualization for exploring structure-activity relationships among a set of sequences.
- Improved performance of adding a new visual.
- Added comparison color scheme selection for sequence renderers.
- Added IronPython script execution to configure visuals upon loading results from Web Services.
- Added ChemDraw Direct support in web services forms.
- Blosum comparative color scheme added for sequences in both the sequence and table visualizations.
- Added plain (no-color) scheme for sequences.
- Removed maximum row limit on Details visualization.
- Scrolling in the Gallery visual changed to scroll by row (or column) instead of snaking through gallery items.
- Tooltips added for column data controls.
- Improved table plot scrolling behavior -- data is updated continuously while scrolling.
- Tooltips added for text cells in the table plot.
- Added core display to top left corner of SAR map.
- Color rules can be displayed when using the text cell renderer in the SAR map.
- Axes in the radar chart can be configured to display a log scale.

Bug Fixes

- Structure renderers are now assigned for columns that have been configured automatically.
- Improved compatibility with Internet Explorer 11 and above.

Version 1.1.0.0

New Features

- Biovia renderer. Note that BioviaDraw must already be installed on target machines to enable. On 64 bit machines, the 64 bit version of BioviaDraw must be enabled for the renderer to work.
- Support for Internet Explorer 11 when viewing documents in Spotfire Consumer (WebPlayer).
- Tooltips are enabled on Table visualization by default.
- Backported to Spotfire version 6.5 (available upon request).
- Enable v3000 Molfile handling in all renderers that support the format.

- Fonts in Details and Gallery visualizations are now configurable.

Bug Fixes

- Renderers on Windows Server 2012. Corrected by inclusion of system libraries missing on default install of Windows Server 2012.
- 3D viewer controls persist until closed by the user.
- Enabled Publisher charts in Spotfire Consumer served by a remote server.
- Fixed renderer settings dialogs to stay on top of all windows while modifying settings.

Version 1.0.0.0

New Features

- Table visualization. View data as a set of columns and rows.
- Gallery visualization. View data using a set of gallery items or cards that can be configured to display the data as the user chooses.
- SAR Map visualization. View the results of an R-Group decomposition as a grid (or matrix).
- Details visualization. View the details of an active row or page through marked rows.
- Radar visualization. Simultaneous comparison of numeric values/properties in multiple marked rows.
- The following software for molecule rendering is supported: Lead Optimization, ChemDraw, RDKit.