TIBCO® Spotfire® DecisionSite® 9.1.1 for Lead Discovery - User's Manual



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1 Preface

1.1 What is Spotfire DecisionSite?

TIBCO® Spotfire® DecisionSite® is a solution for accessing, analyzing, and reporting on data. It enables you to rapidly identify trends, anomalies, outliers and patterns in your data. Spotfire DecisionSite can access data residing in databases, in a local or networked file system, or on the desktop. It is database independent and extracts data (several hundred thousand records or more, depending on computer performance) from commercial data sources such as Oracle, SQL-Server, Informix, and Sybase.

Spotfire DecisionSite uses the patented Spotfire DecisionSite visualization technology, allowing you to interactively query data and instantly visualize results as scatter plots, bar charts, profile charts and a number of other modes.

Spotfire DecisionSite stores data internally in a proprietary data format, allowing for rapid response times to user interaction. It has a series of built in heuristics and algorithms that helps you find interesting alternative views of data.

Spotfire DecisionSite allows you to share your work. Analyses can be easily presented as structured reports for printing or Internet publishing.

1.2 Third Party Components

1.2.1 SharpZipLib 0.8.4 from IC#Code

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1.2.2 WebFX Menu 4.22 and 4.30 from WebFx

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1.2.3 STLPort 5.1.0

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1.2.4 Numerical Recipes

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1.3 How to Contact Support

If you have any questions about a TIBCO Spotfire® product, please do the following:

- Use the built-in help function.
- Consult the README files which are included with the product.
- Visit the Spotfire web site, http://support.spotfire.com, where you can send questions to our support department.
- Get personal contact from TIBCO Spotfire Support.

TIBCO Spotfire offers a variety of support agreements. Contact TIBCO Spotfire for more information about support, training, consulting agreements, and our Product Subscription Programs.

2 Introduction

2.1 Spotfire DecisionSite Overview

2.1.1 The User Interface

The image below shows the main parts of the TIBCO® Spotfire® DecisionSite® user interface. The entire application window is referred to as Spotfire DecisionSite. It is the core of the Spotfire DecisionSite solution, which encompasses a suite of applications for database access, statistical analysis, data preprocessing and domain-specific tasks.



Visualizations

Visualizations are the key to analyzing data in Spotfire DecisionSite. A variety of visualization types can be used to provide the best view of the data:

Scatter Plots

Bar Charts

Pie Charts

Line Charts

Profile Charts

Heat Maps

Tables

Different types of visualizations can be shown simultaneously. They are linked, and are updated dynamically when the query devices are manipulated (see below).

Visualizations can be made to reflect high-dimensional data by letting values control visual attributes such as size, color, shape, rotation and text labels.

The Query Device window

Query devices are used to filter your data. Query devices appear in several forms, and you can easily select a type of query device that best suits your needs (e.g., check boxes, sliders, etc.). When you manipulate a query device by moving a slider or selecting a check box, all visualizations are immediately updated to reflect the new selection of data.

The Details-on-Demand window

The Details-on-Demand window can be used to show the exact values of a record or group of records. By clicking a record in a visualization, or marking several records by drawing a rectangle around them, you can study their numerical values and textual data in a tabular form.

The Guides pane

The Guides pane is a web browser, fully integrated into the Spotfire DecisionSite environment. This is where you can run Guides, step-by-step instructions for common workflows or tutorials, guiding you through an analysis.

2.1.2 Lead Discovery Features

TIBCO delivers several different Guided Analytical applications. Which tools are present in your DecisionSite depends on which application package you are using and what licenses you have bought. Depending on the nature of the various features, you will find them under the File, Data, Tools or Guides menu.

Tools that are launched in the Guides pane (e.g., Information Builder) or in separate web windows have their own online help files. To access the online help for these applications, you must first start the application by selecting the appropriate link from the menu. Once an application has been launched, the online help is reached via the Help menu in the application window.

2.2 Installation and Setup

2.2.1 Hardware Requirements

Spotfire DecisionSite in itself does not require very high powered computers to run smoothly. However, if your data sets are large they will require both a certain amount of RAM, and will of course benefit from high processor speeds.

Minimal Client Hardware requirements

Processor:	Intel Pentium TM or equivalent, 500 MHz		
RAM:	128 MB (256 MB or greater is recommended)		
Hard Disk:	The installation footprint is approximately 30 MB		
Display:	VGA or better, resolution 800x600 pixels, 256 colors (1024x768 pixels, 16 bit high colors or greater is recommended)		
Others:	Network card or modem Mouse CD-ROM drive (if installation is done from a CD-ROM)		

Graphics cards

When 3D visualizations are used for analyzing, you will find that the graphics card of the computer is an important component. OpenGL support is required and hardware acceleration beneficial to allow the processor to devote its work to other things than presenting the display

with information. Due to the great variety of graphics cards manufacturers, Spotfire DecisionSite has not been tested on all of them. If you experience difficulties or slow performance, check that the most recent drivers for your hardware are installed and that the manufacturer's recommendations are met.

2.2.2 Software Requirements

During the installation process the setup program checks that your computer contains all necessary operating system components. Most components are mandatory, while some may be missing without the installation being aborted. If this is the case you will be warned about the missing system component.

Please visit http://www.spotfire.com/sr for information on which Operating System and other Software versions that are required to run DecisionSite Client.

Web connection

Spotfire DecisionSite requires a Web connection to a Spotfire DecisionSite Analytics Server, either at http://home.spotfire.net or a company specific Spotfire DecisionSite Analytics Server. Microsoft Internet Explorer on the client should be configured to access the Spotfire DecisionSite Analytics Server via the standard Web connection. The security settings in Microsoft Internet Explorer for accessing the Spotfire DecisionSite Analytics Server should be set to Medium Security. This includes enabling ActiveScripting, enabling cookies and enabling the download of signed ActiveX components. Downloading signed ActiveX components and scripts from the Spotfire DecisionSite Analytics Server must be allowed through the firewall.

Other requirements

You must have Administrator privileges to install Spotfire DecisionSite.

Microsoft PowerPoint must be installed on the computer in order to use the PowerPoint presentation tool.

Microsoft Word must be installed on the computer in order to use the Word presentation tool.

2.3 Getting Started

2.3.1 Logging In

Logging In

When you start Spotfire DecisionSite a login dialog appears. First select which DecisionSite Analytics Server you want to log into by clicking on the **Server** drop-down list. Usually you will only have one server so there might not be a need to choose. You can also add a new server if you need to, by clicking on the **Server** drop-down list, selecting **Add new...** and typing in the location and name of the new server.

Then type your **User ID** and **Password**, and click on the **Login** button to start Spotfire DecisionSite.

Logging into Spotfire DecisionSite will give you access to the Guides and Tools that are specific for your profile. Pressing **Cancel** will start Spotfire DecisionSite but will not provide access to these Guides and Tools. See also **Working Offline** below.

Depending on the configuration of your DecisionSite Analytics Server, some of the following options may be available in the login dialog:

Remember me

If you select this check box when you log in, you will not be prompted to log in when you start Spotfire DecisionSite the next time. Your User ID and Password will be saved on your computer and will be used automatically each time you start Spotfire DecisionSite.

Register a new user

If you are not a registered user of Spotfire DecisionSite click on the Register a new user link.

This will display a new window in which you can register. You will then be able to access the specific features of Spotfire DecisionSite that you have a license for.

Working Offline

If you have no network connection to the DecisionSite Analytics Server you can still use most features of Spotfire DecisionSite. Start DecisionSite as usual and log in when prompted. Even though you are working offline without any connection to the Spotfire DecisionSite Analytics Server or the internet, you will still be able to use most of the Guides and Tools if these were cached locally on your computer the last time you were connected to the server. The exceptions are those Guides and Tools that need to connect to databases, etc., which obviously cannot do so while working offline.

Note: Working offline requires at least one previous successful login to the Spotfire DecisionSite Analytics Server. Each time you log into the server it checks to see which Guides and Tools that should be available to you, and if there are any new updates. Spotfire DecisionSite automatically downloads these to your computer so that they are available the next time you log in, whether you are connected to the server or not.

Unsupported Software

If your computer does not have the proper software installed (for example an Internet Explorer version that is too old) a dialog will appear. This dialog will state exactly what is wrong, and also ask you to contact your Administrator for further help.

2.3.2 Welcome to Spotfire DecisionSite

When you have logged in to Spotfire DecisionSite, you will be presented with a Welcome screen.



This will help you get started with the application by providing some useful options: **Get an introduction** – This option gives you a five minute tour of Spotfire DecisionSite and of how to use its features. It is the perfect way to get the basic knowledge of how to get started with the application. **Open a sample file** – This option presents a number of example data sets, and describes the content of each data set. You can easily open any of these data sets in DecisionSite and explore the visualizations on your own.

Open data – This option provides a quick way for you to access your own data. It gives you the choice to open a file, paste data from your clipboard or open data from an information link to a database.

Switch to another DecisionSite – Different DecisionSites have a different set of Tools and Guides. If you are missing a certain Tool or Guide that you believe should be available, you may need to switch to another DecisionSite. This option explains how to do this.

Click on Close this window to close the welcome screen and start using DecisionSite.

If you also select the **Don't show this window at startup** check box, the welcome screen will not appear when you start the application in the future. However, if you wish to display it again it is always available from the **View** menu, by selecting **Getting Started**.

2.3.3 Loading Data

The Periodic table data set

As an example of simple, yet interesting information, the periodic table of the elements will be used. The data set holds 75 records with 9 fields each. The columns are: the name of the element, six of its properties, and finally the coordinates of each element when the periodic table is printed in the familiar layout first suggested by Dimitri Mendeleev. The text file contains the column names, column types (integer or string) and the data itself.

```
Element, Atomic Number, Atomic Mass, Atomic Radius, Ionic Radius,
Ionization Energy, Electronegativity,*P1,*P2
STRING,INT,INT,INT,INT,INT,INT,INT,INT
Ac,89,227,200,126,51,11,140,0
Ag,47,107,144,129,75,18,630,80
Al,13,27,143,67,60,16,750,160
.....
```

This data is stored in one of the data formats recognized by Spotfire DecisionSite. This particular example can be found in the directory named **Data/General/Periodic Table** in the Spotfire DecisionSite distribution as *periodic.csv*.

Loading a data set

To load a data set into Spotfire DecisionSite:

- Start Spotfire DecisionSite by selecting Spotfire DecisionSite from Programs in the Windows Start menu, or by double-clicking the Spotfire DecisionSite icon on the desktop.
- 2. Select **File > Open** in the Spotfire DecisionSite main window. The **File** open dialog will appear.
- 3. The folder *Data* will be shown in the *DecisionSite* directory.
- 4. Browse to the folder General/Periodic/Periodic Table.
- 5. Select the file *periodic.csv* and click the **Open** button.

Spotfire DecisionSite will automatically set up an initial visualization where each record is represented by a marker, along with a number of query devices for manipulating the visualization.

Tip: An alternative way of loading the data is to open the file periodic.sfs. This may be preferable since sfs-files contain Spotfire-specific information on how the visualizations will be initially set up.

2.3.4 Changing Visualization Axes

To change the column to be mapped to each axis, click on an axis selector, and select a column name. For example, to see the Mendeleevian layout of the peroidic.csv example data set, select P1 for the X-axis and P2 for the Y-axis.



Note: You can also select which column to use as an X, Y or Z-axis by right-clicking on the Query Device representing that column, and selecting **Set Property > Axis** from the pop-up menu.

2.3.5 Setting Visualization Properties

To make a visualization more informative, activate the Properties dialog by selecting **Edit** > **Properties**. This dialog contains many settings which can be used to modify the visualization. The keyboard shortcut is [Alt+Enter] or [Ctrl+Enter].

► To adjust the appearance of a visualization:

- 1. Select the Markers tab.
- 2. Move the Size slider towards Max to make the markers larger.
- 3. Set the **Color** control to *Continuous*, and the **By** control to *Electronegativity*. This will cause the markers to be colored according to their electronegative potential. The elements with the lowest values will be red and the highest blue. You may alter these colors with a dialog box that opens under **Customize**.

Pronerties: Scatter Plot			×
Continous coloring mode	│Trellis │Axe ┌─Size	s 3D	Markers
By: Age	Min —	hel	Max
Customize Show deselected	-Drawing big		Size slider
Shape © Fixed Customize	By: (No	ne)	
Click here to	None	This co determ marker	lumn ines how s are colored
C Marked records	By: [No	ne)	
O All records, max 20 🚍 labels By: Dead/live 🔽	Eine connec	ne)	
Color:		ne) Indicating dire	ction

2.3.6 Querying the Data Set

To select a subset of markers to display in the visualizations, change the settings of the query device sliders found in the area to the right. For example, using the Periodic Table data set, move the left drag box of the *Ionization Energy* slider, as shown in the image below, to select only those elements with high ionization energies. We can now see that the elements with high ionization energy are more or less the same as those with high Electronegativity since there are few markers with color representing low electronegative potential in the visualization.



2.3.7 Creating a New Visualization

To create a new visualization:

- 1. Select a visualization type from the **Visualization** menu. For this example, select **New 3D Scatter Plot**.
- 2. Reassign the X-axis to *Electronegativity* the Y-axis to *Ionization Energy* and the Z-axis (along the top of the visualization) to *Ionic Radius*
- 3. View the plot from different angles by pressing Shift and/or Ctrl + dragging with the right mouse button.



The 3D plot created in this example will cover the 2D plot but you can show both plots by selecting Window > Auto Tile.

If you move your mouse pointer over one of the markers in the 2D plot, the corresponding marker will also be highlighted in the 3D view. If you activate one element in the 2D plot (by clicking on it) you can move the circle indicating the active element using the arrow keys.

2.3.8 Checklist for Exploring New Data

The following steps are typically helpful when exploring a new data set, especially if its content is unknown.

► To explore a new data set:

- 1. Start off by selecting different combinations of visualization axes to reveal patterns, trends, and anomalies. Use View Tip to browse through different combinations of axes. The anomalies should be scrutinized to determine if they are due to erroneous data.
- 2. Write down particularly interesting combinations of axes, or save the settings so that you can retrieve interesting visualizations later.
- 3. Color the visualization objects, first by category. Again, write down or save variables that produce interesting groupings and/or patterns.
- 4. Color visualization objects by continuous variables, to reveal areas where interesting features such as consistently high or low values occur.
- 5. Go through the range sliders to reveal markers with values occurring in a certain range and observe if they are grouped in some kind of cluster.
- 6. When interesting clusters are identified, these may be either zoomed in on or marked, followed by changing to another view to reveal whether the markers are clustered for a particular reason.

2.4 Lead Discovery Troubleshooting

This topic lists some known trouble situations when working with Spotfire DecisionSite for Lead Discovery and explains how to solve or work around the problems.

The interaction with visualizations is very slow

Problem: Sometimes the interaction between some Lead Discovery tools and the visualizations is very slow.

Explanation: All records in the object that you interact with are marked by default in the visualizations. When you work with a large data set in Spotfire DecisionSite, it takes a long time for the application to mark all records.

Solution: You can switch off the auto-mark function for the Structure Viewer in the Structure Viewer Properties dialog when working with large data sets. You can also switch off the auto-mark function for the Portfolio in the Portfolio: Options dialog by clearing the **Mark on browse** check box.

Columns are not added to the data set

Problem: When I try to add a column from Structure Viewer to the data set, no column is added. A message appears: "The columns were not added correctly".

Explanation: This is a problem caused by the column identification in Spotfire DecisionSite. You may have previously added a column from the same tool and then changed the name of that column in Spotfire DecisionSite.

When you try to add another column, Spotfire DecisionSite thinks the column already exists and therefore no new column is added.

Solution: Do not rename the columns that are added from Structure Viewer. If you have already renamed columns, you need to remove these to be able to add new columns from Structure Viewer.

Added column contains empty values

Problem: When I add a column to the data set from a Lead Discovery tool, the new column contains empty values for some of the records.

Explanation: If you add a column from any of the Lead Discovery tools, the column will only contain values for those compounds that were included in the calculation. If you chose to work on selected compounds, only the compounds that were selected via the query devices and zoom bars will be included in the calculation. All other records in the data set will have empty values in the new column.

Solution: The only solution is to include all records in the calculations. Make sure you set **Work on:** to **All records** in the options dialog of the tool.

If you want to work on selected compounds, there will always be empty values for those compounds that are not included in the calculation.

Structures are not shown in Structure Viewer

Problem: No structures are shown when I interact with records in a visualization, dendrogram or Portfolio list.

Explanation:

The ID field of the database in the structure connection must contain the same type of information as the Spotfire ID column or Portfolio list, or else no structures will be shown. If a compound in the visualization or Portfolio list is not found in the ISIS database, no structure can be shown.

Solution: Make sure you have selected the correct ID fields/columns using the Structure Connection tool.

I cannot mark a list (or a record) in the Portfolio

Problem: When I click on a list (or a compound) in the Portfolio nothing happens with the Structure Viewer tool, nor with the visualizations.

Explanation: The list (or compound) was probably marked before and when you click on it again, the application does not notice any change.

Solution: Click on another object in the Portfolio and then click on the list (or compound) you want to mark again.

If nothing happens in the visualizations when you click in the Portfolio, the interaction concerning marked records has probably been switched off. In the Portfolio:Options dialog, make sure **Mark on browse** check box is selected.

I cannot mark records in the ID list

Problem: When I click on a record in the ID list, nothing happens in the visualizations.

Explanation: There may be a number of reasons why nothing happens in the visualizations. See below.

Solution: You need to make sure the following is OK.

The ID field of the database and the Spotfire ID column in the structure connection must contain the same type of information, or else there will be no interaction with the records in the visualizations.

The compound must be part of the current data set in Spotfire DecisionSite.

No structure keys are added when using Add ISIS Keys

Problem: No structure keys are added to the data set, or structure keys are only imported for some of the records.

Explanation: Structure keys are only imported for records that are included both in the ID list and in the current data set in Spotfire DecisionSite.

Solution: You need to make sure the following is OK.

The ID field of the database and the Spotfire ID column in the structure connection must contain the same type of information, or else there will be no interaction with the records in the visualizations.

To import structure keys for a compound in Spotfire DecisionSite, the compound must be present both in the current data set and in the ID list.

Edit Structure in Structure Search does not seem to work

Problem: When I click on the Edit Structure button in the Structure Search tool, nothing happens.

Explanation: If you have never opened ISIS/Draw on your computer, Spotfire DecisionSite does not find the program.

Solution: Start ISIS/Draw once as a stand alone application (e.g., from the Start menu).

The Structure Analytics tools always use MDL Draw even though I have selected ISIS/Draw as my editor/renderer.

Problem: I have added preferences to always use ISIS/Draw as my structure editor/renderer, but it is always MDL Draw that turns up. This also has the effect that the R-group Search tool cannot be used, since it requires use of ISIS/Draw.

Explanation: This problem occurs when MDL Draw has been installed as the drawing editor to associate with the MDL file extensions and to use in MS Office applications:

MDL Draw - InstallShield Wizard			×
File Association			X
Select the drawing editor to associate with the MI use to edit sketch objects embedded in MS Office	DL file extensions: applications:	ons (.mol, .rxn, .sk	c) and to
MDL Draw			
O ISIS/Draw			
InstallShield	< Back	Next >	Cancel

Since DecisionSite uses the same settings as the Office applications, this will unfortunately make it impossible to use ISIS/Draw, even though it is installed on your computer.

Solution:

Reinstall MDL Draw and select ISIS/Draw as the default drawing editor. Explicitly configure DecisionSite to use MDL Draw for structure editing, where desired.

I cannot send edited structures back from MDL Draw

Problem: I use MDL Draw 2.1 as structure editor. When I edit a structure in MDL Draw and

click on the Transfer button to send the structure back to the DecisionSite Structure Search dialog, an error message is shown: "Unable to update clipboard because the MDLDrawObject component is missing", and no structure is returned.

Explanation: This problem occurs when MDL Draw has been installed as the drawing editor to associate with the MDL file extensions and to use in MS Office applications. See above.

Solution:

Reinstall MDL Draw and select ISIS/Draw as the default drawing editor. Explicitly configure DecisionSite to use MDL Draw for structure editing, where desired.

3 Loading Data

3.1 Loading Data

The Periodic table data set

This data is stored in one of the data formats recognized by Spotfire DecisionSite. This particular example can be found in the directory named **Data/General/Periodic Table** in the Spotfire DecisionSite distribution as *periodic.csv*.

Loading a data set

► To load a data set into Spotfire DecisionSite:

- 1. Start Spotfire DecisionSite by selecting **Spotfire DecisionSite** from **Programs** in the Windows **Start** menu, or by double-clicking the Spotfire DecisionSite icon on the desktop.
- 2. Select **File > Open** in the Spotfire DecisionSite main window. The **File** open dialog will appear.
- 3. The folder *Data* will be shown in the *DecisionSite* directory.
- 4. Browse to the folder General/Periodic/Periodic Table.
- 5. Select the file *periodic.csv* and click the **Open** button.

Spotfire DecisionSite will automatically set up an initial visualization where each record is represented by a marker, along with a number of query devices for manipulating the visualization.

Tip: An alternative way of loading the data is to open the file periodic.sfs. This may be preferable since sfs-files contain Spotfire-specific information on how the visualizations will be initially set up.

3.2 DecisionSite Library

3.2.1 What is DecisionSite Library?

DecisionSite Library provides publishing capabilities for of all your analysis materials, so you can share the data with your colleagues. Using the Library, you can organize your analysis material and collaborate with others in a distributed environment. The Library can be used directly from DecisionSite Client by anyone who has at least read privileges.

The DecisionSite Library is divided into Library Sections which contain all material published to the Library and where access permissions are set. With write access you can open and

publish any type of analysis material; Analyses, Guides, or Posters. If you have read access you can open any material in the Library Section.

For more information, see the Library Help in the DecisionSite Library tool. **Note:** The license for DecisionSite Library must be enabled if you intend to use the Library. **Note:** You must have a license for DecisionSite Posters to use DecisionSite Posters. Please contact your DecisionSite Administrator for information about licenses.



3.2.2 Open from Library

This dialog lets you select and open an item in the Library. Each item type, Analysis, Guide, or Poster, opens in different ways:

- Analysis: opens in the DecisionSite Client as a regular Analysis stored in a Spotfire Analysis File. The Analysis consists of your data, visualizations, annotations and everything else you use to explore your data.
- Guide: opens in the Guides pane where the Guide is run. Guides are captured analyzes made by you or your colleagues for repetitive analysis flows.
- Poster: opens in a separate Microsoft[®] Internet Explorer where the Poster is displayed. Posters are web based snap-shots of your Analysis, designed for easy sharing and collaboration.

To locate the item, either look in a Library Section's content on the **Library** tab, or search for it on the **Search** tab. Navigate in the Library by using double-click on Library Sections and folders.

Open from Library					
Library Search					
Home 3	 DecisionSite for Functional Genomics 				
Туре	Title *	Description			
1					
2	Advanced microarray Guide	Example: This Guide uses a number			
EW	Microarray analysis results	Example: This Poster displays some			
2	Microarray Guide	Example: This Guide shows how visu			
٢	Microarray of yeast	Example: Yeast microarray data. Use			
۲	Principal component analysis	Example: Do a principal component a			
Items of type: All items					
<u>H</u> elp <u>O</u> pen Cancel					

Library tab options	Description
Library tab	All Library Sections, items, and folders are listed in the Library View under the Library tab. Each item is displayed with type, title and description. To open an item, select it by clicking on it and click Open . You can view your position with the flight view. The flight view is seen between the Library tab and the item table. Note: Only the Library Sections that you have access to are listed.
Items of type:	Select the item type you want to view. This filter allows you to see only the options you are interested in. There are four alternatives: All items Analyses Guides Posters
Open	Select the item you want and click Open to open it. See the top of the page about the various responses.
Search tab options	Description
Search tab	Use Search to search for the item you want to open.
Search for:	Enter the search string in the Search for: field and click Search . See Searching in the Library for information about search strings. If you click a folder in the Search result, you will be redirected to the Library View under the Library tab.
Look in:	Select which Library Section you want to perform your search in. Either all Library Sections or one can be searched. Only

	Library sections you have access to are listed.
Items of type:	Select which type of Library item you want to perform your search on. There are four alternatives:
	All items
	Analyses
	Guides
	Posters

Library Sections you have access to are listed.

To reach the Open from Library dialog:

Click File > Open from Library....

3.2.3 Searching in the Library

Search

Searches are performed on title, description, and keywords for a precise result. Searching works according to the following criteria:

- The search is either performed on all Library Sections or one at a time.
- The search is either performed on all Library items or on only one type at a time. (If the Open from Library dialog is reached via the Guides pane or the Guides menu, Guides are always the only items found in the search.)
- The search words are matched according to title, keywords, or description. Note that folders are also included in the search.
- The search words are separated by space.
- All words used in the search must be present in the item properties.
- To find a phrase, use quotation marks (") around it.
- The search is case sensitive.
- Wild cards, asterisks (*), can be used inside words to find variations on that word.

Example

Suppose that there is a Guide in the Library whose properties include:

- Title: "Wafer anomalies Guide"
- Description: "This Guide captures how we find anomalies in our wafer production data. Look closely at Temperature vs Time!"
- Keywords: "Plant A"; "Wafer"; "CODE1A".

Examples of a few search strings which can be used to find the Guide:

- Wafer Finds the title and keyword.
- **anomalies** Finds the title and description.
- wafer Finds the description since "wafer" is lower case.
- "wafer production" Finds the phrase part in the description.
- "wafer production" CODE*A Finds the description and keyword.

Note: The search will only be performed on items that you have read access to.

3.3 Import Data

3.3.1 Importing Data

Spotfire DecisionSite can access data from a variety of sources:

- Spotfire Analysis File (SFS)
- Text files (TXT, CSV, SKV)
- Microsoft Excel Workbooks (XLS)
- MDL SDFiles (SDF)
- Databases (OLE DB or ODBC)
- The Windows clipboard

SFS files, text files and SDFiles can be opened directly using the **Open** option on the **File** menu. This is the quickest way to access unambiguously formatted data from a file. **Note:** You can also enter a URL in the File name field, and access data from a web server. Similarly, properly formatted data on the clipboard can be pasted directly into Spotfire

DecisionSite.

However, if your data resides in a database, or if it needs some kind of preprocessing before being visualized in Spotfire DecisionSite, then use **Import Data**. This dialog is designed to help you access your data, whatever the source and whatever preprocessing you require.

► To import data:

Select File > Import > Import Data....

- 1. Select a data source, such as a file or database.
- 2. Select methods for data conditioning, such as pivoting, aggregation, or normalization. You can also choose to normalize the character case, so the data is imported non-case sensitively.
- 3. Optionally, save all settings for data source and/or data conditioning as a favorite. This will allow you to reuse the same data without having to configure data source and data conditioning each time.

The details of each of these steps vary depending on which type of data source or data conditioning method is chosen. A sequence of dialogs will guide you through the required interaction in each case. For example, accessing a database involves setting parameters that are not required when working with a text file. The following sections will deal with each of the three steps above, describing in detail the different cases that may arise.

3.3.2 Data Sources

3.3.2.1 Selecting a Data Source

The first step in the Import Data dialog to specify a data source. A data source can be one of the following:

- A file
- The clipboard
- A database
- The Spotfire Text Data Format
- A data source defined in a previous data import session, a so called Favorite.

To select a data source:

1. Select File > Import > Import Data....

<mark>🗖</mark> Import Data - Select Da	ta Source	×
	Select a data source: Common File O tabase via ODBC Clipboard Advanced Advanced Database via OLEDB My personal files Text Spotfire Text Data Format SDFile	
0	Organize Favorites	
< Back	Next > Finish Cancel Help	

2. Double-click a data source, or select an item and click Next >.

3.3.2.2 Importing from a File

To import data:

Select File > Import > Import Data... and:

► To import an SFS file:

- 1. In the Select Data Source dialog, select File.
- 2. Click Next >.
- 3. In the **Open** dialog, select the file containing the data. Click **Open**.
- 4. Unless any conditioning is needed, click **Finish**.

► To import a text file:

- 1. In the Select Data Source dialog, select File.
- 2. In the **Open** dialog, select the file containing the data. Click **Open**.
- 3. In the Specify Delimiter dialog, select a column delimiter. Click Next >.
- 4. In the **Specify Data Types** dialog, click on a data type in the table head to change the type. Click **Finish**.
- 5. Unless any conditioning is needed, click Finish.

► To import an Excel file:

- 1. In the Select Data Source dialog, select File.
- 2. In the **Open** dialog, select the file containing the data. Click **Open**.
- 3. In the MS JET OLE DB dialog, click **OK**.
- 4. In the Database dialog specify which Excel worksheets and which columns to include. (An Excel file is treated as a database).
- 5. Click OK.

► To import an SDFile file:

- 1. In the Select Data Source dialog, select SDFile.
- 2. Click Next >.
- 3. In the **Open** dialog, select the file containing the data. Click **Open**.
- 4. Unless any conditioning is needed, click **Finish**.

3.3.2.3 Importing from the Clipboard

► To import data from the Windows clipboard:

- 1. Mark a number of cells in a text window, a spreadsheet program or another program providing a tabular presentation of data, such as Statistica, Microsoft Excel, Word, etc.
- 2. Select **Edit** > **Copy** or hit [Ctrl+C] to copy them to the clipboard.
- 3. In Spotfire DecisionSite, select File > Import > Import Data....
- 4. From the Common folder, select Clipboard.
- 5. Click Next >. This triggers the same dialog as when importing text files.

Tip: If your clipboard data is formatted using a standard column delimiter, and if no preprocessing is required, you can paste it directly into Spotfire DecisionSite. Press [Ctrl+V].

3.3.2.4 Importing from a Database

By default, Spotfire DecisionSite connects to external sources of data by means of ODBC (Open Database Connectivity). This allows you to import data from virtually any kind of database commercially available.

To learn how to set up an ODBC data source, please refer to the database vendor's documentation and the Windows documentation on ODBC. It might be necessary to install ODBC driver software particular to the database used before being able to utilize the ODBC option.

► To import from a Database:

- 1. Select File > Import > Import Data....
- 2. Select **Database** from the list of data sources.
- 3. Click Next >.
- 4. In the Select Data Source dialog, go to the Machine Data Source tab.

5ele	ect Data Source			? ×
Fi	le Data Source Machine Data	Source		
	Data Source Name	Туре	Description	
	dBASE Files dBase Files - Word	User User		
	ECDCMusic Excel Files	User System User	Personal music CD titles	
	HoxPro Files - Word MS Access Database Visual FoxPro Database	User User User		
	Visual FoxPro Tables	User		
			New.	·
	A Machine Data Source is spe "User" data sources are spec sources can be used by all us	ecific to thi ific to a us ers on this	s machine, and cannot be shared. er on this machine. "System" data machine, or by a system-wide service	
			OK Cancel H	elp

- 5. Select the source from which data should be loaded.
- 6. Click OK.
- 7. Enter login name and password to log on to the database.

Database - Specify Tables and Columns			
Tables, views and columns:		Edit SQL statement:	
🗆 🛄 name	String		
- 🗆 🛄 smal	Double		
- 🗆 🛄 medium	Double		
🗆 🛄 big	Double		
- 🗌 🛄 2 legs	Double		
- 🗌 🛄 4 legs	Double		
- 🗆 🛄 hair	Double		
hooves	Double		
- 🗌 🛄 mane	Double		
- 🗌 🛄 feathers	Double		
- 🗌 🛄 hunt	Double		
🗆 📰 run	Double	-	
🗆 🛄 fly	Double 🚽		
- 🗆 🛄 swin	Double		
- 🗆 🖬 X	Double	✓ Use automatic "WHEBE" clause	
	Double 🔳		
OK Cancel	Hide SQL<<<	Clear SQL Load SQL Save SQL	

- 8. Determine which database fields to import by selecting the corresponding check boxes.
- 9. Edit the SQL statement manually if required. This may be necessary for example when joining tables.

10. Click OK.

3.3.2.5 Importing a Spotfire Text Data File

The Spotfire Text Data format uses a method which enables quick opening of text files. The file is saved as Unicode which makes it possible to read all alphabets. This format is useful when you have data that can be imported wrongly, e.g., if you have strings that contain semicolons or tabs which would otherwise cause the imported file to be split up into the wrong number of columns.

► To import a Spotfire Text Data File:

- 1. Select File > Import > Import Data....
- 2. Select Advanced > Spotfire Text Data Format from the list of data sources.
- 3. In the **Spotfire Text Data Format** dialog, select the file containing the data. Click **Open**.
- 4. In the Data Conditioning dialog, select a conditioning method if desired.
- 5. Click **Next** > to save this as a Favorite, or simply click **Finish**.

3.3.2.6 Importing Using a Favorite

Using a Favorite requires that you have defined a data source and preprocessing methods in a previous session and have saved these settings (see Creating Favorites).

To use a Favorite:

- 1. Select File > Import > Import Data....
- 2. Select a favorite from the list of data sources.
- 3. Click **Finish** to load the data set, or **Next** > to edit data conditioning before loading.

3.3.3 Data Conditioning

3.3.3.1 Data Conditioning

Once you have specified a data source, it is possible to manipulate the data in various ways. Standard methods include the "Tall/Skinny => Short/Wide" conversion (described in What is Tall/Skinny-Short/Wide Conversion?) as well as the Depivot (Short/Wide => Tall/Skinny) conversion, but custom methods designed by Professional Services or a third party may also be available.

You can also select the **Normalize case** filter. This will cause the data to be imported non-case sensitively. This means "Chrome", "chrome" and "CHROME" will be interpreted as the same string. The default when importing is to import case sensitively, thus the examples above would be interpreted as three different strings.

Note: When importing strings, duplicates are removed. In Spotfire DecisionSite version 7.0 and older, comparison ignored differences in case. Version 7.1 and later treats two strings as different if they contain the same sequence of characters but not the same case. Selecting the Normalize case filter will mimic the old behavior.

► To apply a conditioning method:

- 1. Select a data source.
- 2. Click Next >.
- 3. Select a method from the drop-down list.
- 4. Make the required settings.
- 5. Click OK.

3.3.3.2 Applying Multiple Conditioning Methods

When applying several transformations on top of each other, it is important to decide in which order the methods should be applied. Once one conversion has been applied, the next conversion will apply to the output from the previous one, and so on.

► To apply multiple conditioning methods:

- 1. Select a method from the drop-down list.
- 2. Configure the method and click **OK**.
- 3. Repeat from step 1 as many times as required.

3.3.3.3 Tall/Skinny-Short/Wide Conversion

3.3.3.3.1 Tall/Skinny to Short/Wide Conversion

Tall/Skinny to Short/Wide conversion is a method for modifying the format of a data table during import. It can be used for pivoting and aggregating data.

Note: You can also reach this dialog via **Data > Pivot Data...** if you want to apply pivoting to an already opened data set. See Pivot Data for more examples.

To apply Tall/Skinny to Short/Wide conversion to your original data:

- 1. Select File > Import > Import Data....
- 2. Select a data source, and click Next >.
- 3. Select Tall/Skinny -> Short/Wide from the drop-down list.
- 4. Click Configure...
- 5. In the **Identity** list, select one or more columns. Comment: Each unique value in the chosen column produces a row in the generated table. You can choose more than one column. Doing so means that the new table will have a separate row for each unique combination of values in the chosen columns.
- 6. In the **Category** list, select one or more columns. Comment: Each unique value in the chosen column produces a new column in the generated table. Selecting more than one column means that the new table will have a separate column for each unique combination of values in the chosen columns.
- 7. In the Values list, select one or more columns. Comment: The column selected under Values is the column from which the data is pulled. It is possible to select more than one Value column. The values in the generated table are always computed as the average of values in the original table, unless the original values are strings. If so, values in the generated table will consist of concatenated strings. To change the way the values are calculated, right-click on the Method and select a different method from the list, or use Ctrl+click to select multiple methods.
- 8. In the **Other Columns** list, select one or more columns.
- Comment: This option allows you to include an overall average of a particular measurement, for each row in the generated table. For each column selected here, one new column will be created in the new table. To change the way the measurements are calculated, right-click on the Method and select a different method from the list, or use Ctrl+click to select multiple methods.
- 9. Click OK.

Option	Description
Identity	Each unique value in the chosen column produces a row in the generated table.
	You can choose more than one column. Doing so means that

	the new table will have a separate row for <i>each unique combination</i> of values in the chosen columns.
Category	Each unique value in the chosen column produces a new column in the generated table. Selecting more than one column means that the new table will have a separate column for <i>each unique combination</i> of values in the chosen columns.
Values	The column selected under Values is the column from which the data is pulled. It is possible to select more than one Value column.
	The values in the generated table are always computed as the average of values in the original table, unless the original values are strings. If so, values in the generated table will consist of concatenated strings. To change the way the values are calculated, right-click on the Method and select a different method from the list, or use Ctrl+click to select multiple methods.
Other Columns	This option allows you to include an overall average of a particular measurement, for each row in the generated table. For each column selected here, one new column will be created in the new table. To change the way the measurements are calculated, right-click on the Method and select a different method from the list, or use Ctrl+click to select multiple methods.

Method Selection List

Right-click on the Method to change the method of calculation for your column. Ctrl+click to select multiple methods.



For examples of how Tall/Skinny to Short/Wide conversion can be used, see Pivoting and Pivoting and Aggregation.

3.3.3.3.2 Pivoting

Pivoting, in its simplest form, means rotating a table. Mostly, though, it also includes performing some form of aggregation, so that the new table is more compact than the original. Pivoting a data set means changing it from a tall/skinny format to a short/wide format. Consider the following tall/skinny table, based on a series of temperature measurements:

City	Month	Temp
London	February	4
New York	February	6
London	May	16
New York	May	19
London	August	28
New York	August	26
London	November	13
New York	November	11

As we add more observations, the table grows taller, but remains three columns wide. While useful during data collection, this format may not be appropriate for certain types of calculations or visualizations. For example, the entities that interest us are the different cities, so

calculations or visualizations. For example, the entities that interest us are the different cities, so we may want a representation with a single record for each city.

Tall/Skinny=>Short/Wide conversion lets us pivot this table, producing the following (note that avg(Temp) is the average of a single cell):

City	avg(Temp) for August	avg(Temp) for February	avg(Temp) for May	avg(Temp) for November
London	28	4	16	13
New York	26	6	19	11

Each city is now represented by a single record, which makes this format very suitable for Spotfire DecisionSite profile charts. This example demonstrates three steps:

- Creating a row for each unique value in City.
- Creating a column for each unique value in Month.
- Entering a value from Temp for each cell in the resulting grid.

In the Tall/Skinny => Short/Wide dialog, the following settings would be made: Identity: City

Category: Month

Values: Temp

3.3.3.3.3 Pivoting and Aggregation

Note: To understand this example, it is recommended to read Pivoting first. Apart from changing format from tall/skinny to short/wide, pivoting can be used to create a more compact table. Consider the following table, based on a series of temperature measurements:

City	Month	Day	Тетр
London	February	1	5
London	February	15	8
London	May	1	15
London	May	15	22
New York	February	1	9
New York	February	15	7
New York	May	1	18
New York	May	15	24

Tall/Skinny=>Short/Wide conversion lets us pivot and aggregate this table, producing the following:

City	avg(Temp) for February	avg(Temp) for May
London	6.5	18.5
New York	8	21

A smaller table has been created, summarizing the original table. In the Tall/Skinny => Short/Wide dialog, the following settings would be made: Identity: City Category: Month

Values: Temp

3.3.4 Favorites

3.3.4.1 Creating Favorites

Favorites are combinations of data sources and data conditioning methods. A favorite stores all settings made during a session with the Import Data dialogs. A favorite may, for example, specify a database, all the information required to log on, and a data conditioning method. Favorites can also specify just a data source, or just a preprocessing method.

► To create a favorite:

- 1. Define a data source as described in Selecting a Data Source.
- 2. Define a data conditioning method as described in Data Conditioning.
- 3. In Save Session dialog, specify a name for your favorite, e.g., "Average temperature 1961-1991". You can also add a description.
- 4. Under Favorite options, select both Include reference to data source and Include reference to data conditioning methods

🗗 Import Data - Save Ses	sion	×
	Do you want to save this session as a favorite? To continue without saving, leave the text box empty. Name: Average Temperature 1966-1998	
	Average remperature rootrists Description: Data Aggregated from the oceanography data set. Select or write a group name to place your favorite in: Favorites Favorite options © Save complete session © Save complete session	
< Back	Next > Finish Cancel Help	

5. Click Finish.

Note: Your choice of Favorite options affects how the favorite can be used. If a data source is included, then the favorite can be opened directly from the Select Data Source dialog. If only the method is saved, then you must first select a data source, and then in the second step apply the favorite as a data conditioning method.

3.3.4.2 Organizing Favorites

Favorites are organized in folders. Click Organize Favorites in the Select Data Source dialog.

.

Organize Favorites	×
Favorites:	
E- Gavorites L	Delete Change Group
Data sources Conditioning methods	OK Cancel

The **Data source** tab contains favorites that are linked to data. These can be loaded directly from the **Select Data Source** dialog.
The **Conditioning methods** tab contains favorites that are not linked to a data source. These can only be applied from the **Data Conditioning** dialog (i.e., you must specify a data source before using them).

► To move a favorite to a different folder:

- 1. Highlight a favorite.
- 2. Click Change Group.
- 3. Select a group from the list, or enter a new group name.

► To remove a favorite:

- 1. Highlight a favorite.
- 2. Click Delete.

3.3.5 Text File Formatting

3.3.5.1 General Text File Specifications

A data set imported into Spotfire DecisionSite consists of the following:

One line containing the name of each column (optional)

One declaration line describing the type of data in each column (optional)

The first two single lines make up the header. If the original data set has no header (i.e., it consists of raw data) Spotfire DecisionSite will name the columns Column1, Column2, ... One line per data record

[Carriage return] followed by [Line feed] end each row

Note:

- The type declaration is case insensitive.
- Data sets must contain at least 3 rows to be valid. Add an empty row if you need to import a data set with 2 rows.
- The number of columns present in the first row determines the number of columns used in the entire data set. Additional columns in subsequent rows will be ignored. Therefore, make sure the first row contains the correct number of columns.
- The first row of a data set must never be empty, i.e., it should only contain a row break or similar.

The following are examples of well-formatted text files:

```
City,Month,Day,Temp
String,String,Integer,Integer
London,May,5,14
New York,May,5,23
London,May,10,16
New York,May,10,27
London,May,15,20
New York,May,15,24
London,November,5,7
New York,November,5,12
```

Location;Day;Temp London;5;14 New York;5;23 London;10;16 New York;10;27 London;15;11 New York;15;29 London;20;13 New York;20;20

3.3.5.2 Spotfire Text Data Format Specifications

A Spotfire Text Data file imported into Spotfire DecisionSite consists of the following: One line containing information about the format. Two lines which explain how the file was generated. One line containing the name of each column. One declaration line describing the type of data in each column. One line per data record. [Carriage return] followed by [Line feed] end each row; each column ends with a semicolon.

Note: The type declarations and the column names are case sensitive.

The following is an example of a well-formatted text file:

```
\! filetype=Spotfire.DataFormat.Text; version=1.0;
City;Month;Day;Temp;
String;String;Integer;Integer;
London;May;5;14;
New York;May;5;23;
London;May;10;16;
New York;May;10;27;
London;May;15;20;
New York;May;15;24;
London;November;5;7;
New York;November;5;12;
```

3.3.5.3 Supported Formats

The following standardized text file formats are supported:

CSV – values are separated by the default list separator. (This is a Regional Setting property of your system. Comma is used in the US.)

TXT - values are separated by tabs

SKV - values are separated by semicolons

All these file formats are simple and text based – they do not contain any formatting or product specific information. The CSV and SKV formats can be exported from many spreadsheet and database programs. Many research tools produce output in these formats as well.

Note: Spotfire Text Data Format is also available see Spotfire Text Data Format Specifications for more information.

3.3.5.4 Column Separators

Individual fields (column names, type strings, and values) are delimited by column separators usually commas, semicolons or tabs, but the | (pipe) symbol is also recognized.

Spotfire DecisionSite automatically decides which character is interpreted as separator. To do this, Spotfire DecisionSite checks the first line in the database for the following characters:

Separator	Name	ASCII code
[tab]	Horizontal tab (invisible on screen)	9
,	Comma	44
;	Semicolon	59
	Pipe	124

The most common character of the ones above is selected as separator (characters enclosed in quotation marks are not considered). All following lines are assumed to use this most common character as column separator.

Note:

• To load text data that uses a column separator different from those mentioned above, use the Import Data option. This will allow you to specify manually which character to interpret as separator.

Dialog Box Controls for the Specify Delimiter dialog:

Delimiter – Select one of the four common delimiter symbols, or enter a character of your choice.

Column names – Check the box if you know that the first row contains column names and not data.

Data preview – The table shows how the file will be interpreted, given the specified delimiter

• Values in a Spotfire DecisionSite data set may contain any character (including white space) except the column separator. If enclosed in double quotation marks, columns may also contain separator characters. Column headers are allowed to contain separators if double quoted and the first double quotation mark is preceded by a backslash.

3.3.5.5 Name and Type Strings

The first one or two lines in a text file or file may be interpreted as name and type information according to the following rules:

If the second line appears to be type information, i.e., containing columns with strings like INT, STRING, DATE etc., it is used as type information. The first line is then expected to contain name information. For example, a small database with personal data and both name and type information looks like the table below. Here, the second line is interpreted as type information and the first as name information.

Data	Spotfire DecisionSite Interpretation
Name,Age	name info
STRING,INT	type info
Peter,26	data
John,35	data

If the first line contains only type information, Spotfire DecisionSite will use that line for type information. The column names are automatically generated as "Column1", "Column2", etc. **Note:** The type determined by the type declaration line has the highest priority when determining the type of each individual data line. If a value cannot be converted into the relevant type, it will be set to empty. For example, a string appearing in a column defined as integer cannot be converted and will therefore be set to empty.

Data	Spotfire DecisionSite Interpretation
STRING,INT	type info
Peter,26	data
Susan, 19	data
John,35	data

Spotfire DecisionSite tries to find type information in lines one and two. If it cannot, line one is used as name information, and the program makes a qualified guess of the types contained by analyzing the type of the following first non-empty 100 values in each column.

If more than 80% of the values can be interpreted as one and the same type other than String, the column will be set to that type. Any values not corresponding to that type will be set to null. If there are the same numbers of records for two different types among the 100 analyzed values, then the type guessing will be done according to this priority list:

- 1. Integer
- 2. Decimal
- 3. Date
- 4. Time
- 5. TimeStamp

If more than 80% of the values cannot be interpreted as a type other than String, then all values in the column will be set to String.

Note: Date format is determined in a similar way. Please see Date for more information. The following is a small database with personal data, but no type information. Here, the first line is interpreted as name information, and the types are set to STRING and INT.

Spotfire DecisionSite Interpretation
Type guess: STRING, STRING
Type guess: STRING, INT
Type guess: STRING, INT
Type guess: STRING, INT

If 1,2 and 3 fail, the column names are automatically generated as "Column1", "Column2", etc. The program then makes a qualified guess of the types just as in section 3 above.

For example, for a small database with personal data with no type or name information, the type information is set to STRING and INT, and the names are set to Column1 and Column2:

Data	Spotfire DecisionSite Interpretation
Peter,26	Type guess: STRING, INT
Susan, 19	Type guess: STRING, INT
John,35	Type guess: STRING, INT

Note: If a column is declared as being of one type, but some values in the column are of a different type, then the incongruous values will be set to null.

3.3.6 Data Types

3.3.6.1 General Specifications for Data Types

White spaces and ASCII control characters (i.e., all code characters less than 32) are always ignored at the start of a string. Type strings (strings that declare the data type) are not case sensitive.

In the descriptions of data types, the following abbreviations are used:

[] (i.e., square brackets)	For any item, this indicates optional items or groups of correlated items.
YY	Year as two digits.
YY[YY]	Year as two or four digits.
MM	Month as one or two digits.
DD	Day as one or two digits.
HH	Hours as one or two digits
Mm	Minutes as one or two digits.
SS	Seconds as one or two digits.
fff	Fractions of a second, as many digits as there are.
MonthString	In English only. This may also be the abbreviated version of the month, e.g., Jan stands for January.

If you are uncertain about whether or not Spotfire DecisionSite supports a data type, or how it must be formatted to be recognized during import, use a text editor to write a short file with sample data using the types that you want to test. Copy and paste the text directly into Spotfire DecisionSite, and use Details-on-Demand to verify the results.

The following tab-separated file can be used as a template for such a file:

int_col	time_col	date_col	str_col
int	sfTime	date	string
1	11:01:32 PM	990807	"hello"
2	110132.6	08/07/99	hello
3	11:01 AM	99-08-07	""Hello!", I said"

Fields

HH:Mm[:SS[.fff]][AM|PM]

HH.Mm[.SS[.fff]][AM|PM]

HHMm[SS[.fff]][AM|PM]

3.3.6.2 Time

Format

Description

Colon as field separator Dot as field separator No field separator

Type strings

time, sfTime

Remarks

The format requires that hour and minute be specified. Optionally seconds and fractions of seconds can be included. The fractions must be in the range of real values, and must begin with a period or the decimal separator defined by the regional settings in Windows.

In addition to a colon separator (as above), it is also possible to use a decimal point or no character at all.

AM or PM can optionally be specified at the end of a time string.

Time must be within legal values. For example, **13:00** AM is not supported. Negative times are not supported.

Examples

Accepted	Not accepted
14:05:32.6	14:05:32:6
14.05	25.05
140532	140532,6
2.05.32 PM	14.05.32 PM
2.05.32 AM	14.05.32 AM
2.5.2	

The display format of a Time column can be changed in the Time Format dialog.

3.3.6.3 Date

Please see the Remarks section following the formats table for more information on priority formats and other important details of the formats.

It is recommended that you use Long ISO formats, since there is no ambiguity in these. When type guessing a text file that is being imported, DecisionSite makes a qualified guess of any dates contained by analyzing the format of the following first non-empty 100 values in each column.

DecisionSite checks to see how many matches each of the following format receives, and then chooses the one with the most matches. If several formats should receive the same amount of matches, then DecisionSite will choose the date format according to the Interpretation Priority as seen in the table below.

Dates not matching the selected format will be discarded as conversion errors.

Formats

Fields	Interpretation Priority
YY[YY]-MM-DD	Highest
<ms setting="" windows=""></ms>	
DD-MM-YY[YY]	
MM/DD/YY[YY]	
DD/MM/YY[YY]	
YY[YY]/MM/DD	
YYYYMMDD	
YYMMDD	
DD.MM.YY[YY]	
	Fields YY[YY]-MM-DD <ms setting="" windows=""> DD-MM-YY[YY] MM/DD/YY[YY] DD/MM/YY[YY] YY[YY]/MM/DD YYYYMMDD YYMMDD DD.MM.YY[YY]</ms>

Long ISO format:	DD MonthName YY[YY]	
Long ISO Internet:	DD-MonthName-YY[YY]	
Long USA & UK format:	MonthName DD, YY[YY]	Lowest

Type strings

date, sfDate

Remarks

The year, YY, can always be specified in two or four digits, e.g., **89** or **1989**. If only two digits are given for the year, the date is assumed to belong to the 20th century if the number representing the years is higher than the dividing year, and to the 21st century if equal to the dividing year or below. Microsoft Windows settings provide the dividing year. Windows default dividing year is 31. If alterations have been made there, they will be reflected in the way Spotfire DecisionSite calculates dates.

Months can be written using the initial three letters. If spelled out, names should be in U.S. English. Month names are not case sensitive.

Spotfire DecisionSite performs a leap year control when importing data of type *Date*. Once date data is loaded into Spotfire DecisionSite it will be presented in localized format (set in the Regional Properties of your system).

Years may range from 100 to 9999.

The display format of a Date column can be changed in the Date Format dialog.

3.3.6.4 DateTime

DateTimes are also known as TimeStamps.

Formats

DATE TIME DATE/TIME Where DATE is any date as described above, and TIME is any time as described above. Note that there must be at least one of the following between both main groups: a single Space a single Slash Multiple Spaces are allowed and ignored, but multiple Slashes are illegal.

Type strings

datetime, timedate, timestamp, sfTimeStamp

Remarks

The DateTime format is used to combine date and time in a single data column. In previous documentation it has been referred to as TimeStamp.

A value is accepted as DateTime even if it lacks the Time component.

Examples

DateTime	Interpreted as
99-08-07 11:01:32.6	August 7, 1999, 11:
99-08-07 11.01.32	August 7, 1999, 11:
08/07/99 11:01	August 7, 1999, 11:

1:01:32.600

1:01:32 1:01:00

08/07/99 11.01.32.6 PM	August 7, 1999, 23:01:32.600
99/08/07 11:01	August 7, 1999, 11:01:00
990807 11:01:32.6	August 7, 1999, 11:01:32.600
990807 110132 AM	August 7, 1999, 11:01:32
07 aug 99 11:01	August 7, 1999, 11:01:00

The display format of a DateTime column can be changed in the Date and Time Format dialog.

3.3.6.5 String

Format

Any string of characters, with or without quotation marks

Type strings

string, text, str, sfString

Remarks

Matching pairs of quotation marks at the beginning and end of the string are removed. Column separators appearing within outermost quotes are not interpreted as separators (see the last example below).

Columns beginning or ending with empty noise (control characters except the separator currently being used) will be stripped of that noise.

Strings are by default case sensitive, e.g., a12 is treated as different to A12.

Sorting

Spotfire DecisionSite handles Strings case-sensitively. Strings are sorted based on ASCII (see also Unicode and Character Encodings) which means that all uppercase characters will be sorted before any lowercase characters (A, B, C, a, b, c).

For example, strings would be sorted as seen below:

1 1005 34 Arizona Beethoven Zebra anaconda bakery

Be mindful of this when using Query Devices, since setting a Range Slider to include everything between Arizona and Zebra, will not include anaconda or bakery.

The reason for handling sorting this way, and not according to the locale setting on the computer, is to insure that a Spotfire DecisionSite file looks exactly the same where ever it is opened. Therefore country-specific characters may be sorted in other ways than according to the locale setting.

String	Interpreted as
Hello	Hello
"Hello"	Hello
""Hello""	Hello
""Hello""	Hello

Examples

"Hello "there""	Hello "there"
"3" 5"	3" 5'
one, two, three	one two three (separate columns)
"one, two, three"	one, two, three (one column)
""Hello", I said"	"Hello", I said

3.3.6.6 Integer

Format

[#|##|###][[|,]###]*[%]

Type strings

int, integer, long, mapstring, sfInt

Remarks

An integer can include a grouping symbol for thousands, millions, etc. Permitted symbols are comma and white-space.

However, every value in the entire column must be a valid integer, or else the entire column will be interpreted as Decimal or even Invalid.

Optionally, the %-character can be appended at the end. The %-character will be removed during import, thus 68% will be interpreted as 68 not 0.68.

Examples

Accepted	Interpreted as
6843	6843
6 843	6843
6,843	6843 (see Remarks above!)
68,432,701	68432701
68%	68
Not Accepted	Interpreted as
68,43	68.43 Decimal
68,432,70	Invalid

3.3.6.7 Decimal (Real, Double)

An 8 byte floating point number.

Format

[#|##|###][[|,]###]*[.#*]][][%]

Type strings

decimal, real, float, real1, real2, real3, real4, real5, dbl, num, dreal, double, dfloat, sfReal, sfDecimal

Remarks

Written as an integer, optionally followed by a decimal part. The decimal separator can be a comma or period, but must be different from the thousands separator.

Optionally, the %-character can be appended at the end. The %-character will be removed during import, thus 0.68% will be interpreted as 0.68.

In Spotfire DecisionSite 6.1 and later versions, all Decimals are treated as Doubles. Older versions differentiate between 4 byte Reals and 8 byte Doubles.

Examples

Accepted	Interpreted as
6,84	6.84
6,843	6.843 (see Integer description!)
6.843	6.843
6 843.27	6843.27
6 843,27	6843.27
6,843.27	6843.27
0.68%	0.68
1E17	1E+017
1d17	1E+017
Not Accepted	Interpreted as
6.843,27	Invalid
6.843.27	Invalid
6,843,27	Invalid

3.3.6.8 Data Type Constraints in Current 32 Bit Operating Systems

Int

Integer 32 bits signed	
Maximum (signed) int value	2147483647
Minimum (signed) int value	-2147483647

Double

64 bits	
Number of decimal digits of precision (That is the total number of digits, not to be confused with number of digits after the decimal point)	15
Smallest such that (1.0+DBL_EPSILON !=1.0) The minimum difference between numbers that are to be calculated as having different values	2.2204460492503131e-016
Number of bits in mantissa	53

Maximum value	1.79769313486231e+308
Maximum decimal exponent	308
Maximum binary exponent	1024
Minimum positive value	2.22507385850720e-307
Minimum decimal exponent	(-307)
Minimum binary exponent	(-1021)
Exponent radix	2
Addition rounding: near	1

Real

In Spotfire DecisionSite 6.1 and later versions, all Real are treated as Double. For older versions see below:

Float 32 bits	
Number of decimal digits of precision (That is the total number of digits, not to be confused with number of digits after the decimal point)	6
Smallest such that (1.0+FLT_EPSILON !=1.0) The minimum difference between numbers that are to be calculated as having different values	1.192092896e-07F
Number of bits in mantissa	24
Maximum value	3.402823466e+38F
Maximum decimal exponent	38
Maximum binary exponent	128
Minimum positive value	1.175494351e-38F
Minimum decimal exponent	(-37)
Minimum binary exponent	(-125)
Exponent radix	2
Addition rounding: near	1

3.3.7 OLE DB

3.3.7.1 Connecting to a Data Source Using OLE DB

An OLE DB data provider allows native access to data, such as a SQL Server or Oracle database. Using an OLE DB provider, Spotfire DecisionSite can retrieve and manipulate data from a wide variety of data sources, not just relational databases. When you create a data link, you specify the OLE DB provider that is designed to work with your data. For example, you could access a flat file system using the **CSV provider** and display the data in Spotfire DecisionSite.

You can create data links for any Microsoft or third party OLE DB provider. The following providers are included with the Microsoft data access components:

Microsoft Jet 3.51 OLE DB Provider

OLE DB Provider for Oracle

OLE DB Provider for SQL Server

OLE DB Provider for ODBC Drivers

Note: For more information about OLE DB providers, see the OLE DB Programmer's Reference. This documentation is available in the Microsoft Data Access SDK.

► To import data using an OLE DB provider:

- 1. Click **Open** on the **File** menu, and select **Full OLE DB Connect** from the **Files of type** drop-down list.
- 2. Use the **Data Link Properties** dialog box to specify initialization properties for your OLE DB provider. Data link properties may vary depending on your OLE DB provider. **Next** navigates to the **Connection** tab for the selected OLE DB provider.

Before you can access data from OLE DB, you must provide specific connection information such as:

- The type of *data* that you want to access
- The *server* on which the data resides
- The *database* in which the data is stored

Use the **Connection** tab to specify how to connect to Oracle data. Enter the server where the database you want to access is located. Click **Test Connection** to attempt a connection to the specified data source. If the connection fails, ensure that the settings are correct. For example, spelling errors and case sensitivity may be the cause of a failed connection. Click **OK** to connect.

For more information about advanced initialization properties, see the documentation provided with your OLE DB provider. Use the **All** tab to view and edit all of the OLE DB initialization properties that are available for your OLE DB provider.

3.3.8 Rearranging the Data by Formatting

If you have a Time, Date or a DateTime (TimeStamp) column in your data set, you can change what you actually filter on with the query devices just by changing the format of the column.

Example 1:

You have a data set containing stock prices for a number of different stocks during a selected time period:

Date	Stock Price	Stock
1/1/2002	100.0000	Barkley Books Ltd.
1/1/2002	150.0000	Cameo Cars Inc.
1/1/2002	60.0000	Flinc Foods Inc.
1/1/2002	180.0000	Machton Machinery Ltd.
2/1/2002	120.0000	Barkley Books Ltd.
2/1/2002	175.0000	Cameo Cars Inc.
2/1/2002	70.0000	Flinc Foods Inc.
2/1/2002	170.0000	Machton Machinery Ltd.
3/1/2002	122.0000	Barkley Books Ltd.
3/1/2002	190.0000	Cameo Cars Inc.
3/1/2002	85.0000	Flinc Foods Inc.
3/1/2002	150.0000	Machton Machinery Ltd.
4/1/2002	110.0000	Barkley Books Ltd.
4/1/2002	160.0000	Cameo Cars Inc.
4/1/2002	90.0000	Flinc Foods Inc.
4/1/2002	180.0000	Machton Machinery Ltd.
5/1/2002	135.0000	Barkley Books Ltd.
5/1/2002	130.0000	Cameo Cars Inc.
5/1/2002	95.0000	Flinc Foods Inc.
5/1/2002	220.0000	Machton Machinery Ltd.
6/1/2002	140.0000	Barkley Books Ltd.
6/1/2002	165.0000	Cameo Cars Inc.
6/1/2002	100.0000	Flinc Foods Inc.
6/1/2002	190.0000	Machton Machinery Ltd.
7/1/2002	145.0000	Barkley Books Ltd.
7/1/2002	175.0000	Cameo Cars Inc.
7/1/2002	110.0000	Flinc Foods Inc.
7/1/2002	210.0000	Machton Machinery Ltd.

Traditionally, you could plot the data in a scatter plot or a profile chart to see how the price of each stock has varied during the time period:



But by changing the way the date column is represented, you can obtain new views of the data. Right-click on the date column in the Query Devices panel and select **Set Property > Format > Date...** to display the Date Format dialog. Here, you can select Day of week, Monday first (day name), to show the different weekdays instead. The language is determined by your current locale.

Date	
•	Monday
V	Tuesday
	Wednesday
V	Friday
	Saturday

This way, you can get a completely different view of the data and spot whether the stock prices tend to be higher or lower on a certain day of the week:



According to this scatter plot, it looks like it would be a good idea to buy new stocks on Tuesdays. (This example does not contain any real data and the advice should therefore not be taken literally.)

Example 2:

Another example of how the data interpretation can be changed via formatting is if you have a time column where hours, minutes and seconds are displayed, and then change the formatting to a HH:MM format.

	Data values:	Represented in a scatter plot:
Original data:	Column 1 Column 2 1 11:59:00 2 11:59:30 3 12:00:00	3 2 1 1 11:59:00 11:59:30 12:00:00
Formatted data:	Column 1 Column 2 1 11:59 2 11:59 3 12:00	3- 2- 1- 11:59 12:00

Hence, the number of unique values is reduced from three to two.

The following formats change the perceived data type of the column from a Date, Time or DateTime into an Integer or String:

Format	Perceived type
Year (YYYY)	Integer
Year, short (YY)	Integer
Day of week, Monday first (day name)	String
Day of week, Sunday first (day name)	String
Day of month (dd)	Integer
Day of year (ddd)	Integer
Week of year (ww)	Integer
Month of year (mm)	Integer
Month of year (short name)	String
Month of year (full name)	String
24 hour time, hour only (HH)	Integer

Resetting the formatting to the original brings back the original data type as well as any temporarily trimmed values.

3.4 Information Links

3.4.1 Introduction to Information Library

Information Library is a tool for accessing data from databases. This is done by opening *information links*. An information link is a preconfigured database query, specifying the columns to be loaded, and any filters needed to reduce the size of the data set prior to visualization in Spotfire DecisionSite.

Information Library is built on top of the *Information Model* (IM). This model resides on your server, and is a representation of one or more databases which may be geographically dispersed. It allows you to execute advanced database queries without any knowledge of the underlying database structures. The model appears as a folder structure (see Information Library Dialog). Information Library is part of a suite of tools called *Information Services* (IS). The other tools are Information Builder and Information Designer. While Information Library is primarily designed to execute predefined queries stored in the IM, Information Builder lets you create such queries from building blocks such as columns and filters. Information Designer is the administrative tool for designing the Information Model, configuring the database connections and assigning user permissions for accessing various parts of the model.

3.4.2 Using Information Library

3.4.2.1 Opening an Information Link

Information Library provides a set of information links (predefined queries), organized into different domains. Which domains are available to you depends on how your permissions have been set by the administrator. The information links are defined in Information Builder.

► To open an information link:

1. Select File > Import > Open Information Link....

Response: The Information Library dialog is shown.

In the Information Links pane, select a link, IL.
 Response: Information about the selected link is displayed in the Information Link details pane.

Comment: Click the + symbols to see the contents of a domain.

3. Click Open.

Comment: To open a link directly, double-click the link icon, 2.

Response: The information link is opened, and the data is shown in DecisionSite. If the information link includes run-time filters, one or more dialogs will now appear. See Filtering Data During Retrieval for details.

3.4.2.2 Filtering Data During Retrieval

An information link can include columns with *run-time filters*. For each such column that is loaded, you are asked to specify the values that you are interested in. Only records with the selected values will then be loaded.

Note: To enable run-time filtering for a column, or to set the type of control used for selecting values, use Information Builder to edit the information link.

► To open an information link with run-time filters.

- 1. Select File > Import > Open Information Link....
 - Response: The Information Library dialog is shown.
- In the Information Links pane, select a link with run-time filters. Response: Information about the selected link is displayed in the Information Link details pane. You will see here whether or not the link includes columns with run-time filters.
- 3. Click Open.

Comment: To open a link directly, double-click the link icon, **E** Response: The first Set Filter for Column dialog appears.

- 4. Specify the values or range of values in which you are interested. Comment: Information links may include more than one run-time filter. In this case each prompt will reduce the data set, such that subsequent prompts may present fewer values. See the Run-time Filter Example for more details.
- 5. Click **Next** > (or **Finish** if this is the last filter).
- 6. Repeat steps 4 and 5 for each column with a run-time filter.

3.4.2.3 Using Current Query Device Settings as a Filter

When opening information links with run-time filters that prompt for values or value range (see Filtering Data During Retrieval) it is possible to use the visual capabilities of Spotfire DecisionSite to set these values.

► To use the current visualization for filter definition:

- 1. Open a suitable data set in DecisionSite.
- 2. Choose a subset of data either by using the query devices, or by marking records. Comment: *Marking* means clicking and dragging a rectangle around a group of markers in a visualization.
- 3. Open the information link.
- 4. When the **Set Filter for Column** dialog for the desired column appears, click **Get Values...** or **Get Range...**.

Response: The Get Values from Data Set dialog is displayed.

5. From the **Matching column** drop-down list, select the column (in the visualized data set) from which you want to get the values or the range.

- 6. Click **Selected records** or **Marked records**, depending on which values you want to use.
- 7. Click OK.
- 8. In the **Set Filter for Column** dialog, click **Next** > (or **Finish** if this is the last prompted column).
- 9. Repeat steps 4 to 8 for each column that has a run-time filter. Response: The data is loaded and displayed in a visualization.

3.4.2.4 Using Structure Search

Users of DecisionSite for Lead Discovery can use structure search in run-time filters. This means using substructure or similarity search to limit the data set to chemical structures of a particular type.

► To use a run-time filter with structure search:

- 1. Open an information link that contains columns with structure search run-time filters. Response: The system will begin to retrieve data. For each column with run-time filter the Set Filter for Column Dialog will appear, asking you to specify the filter conditions for this column.
- 2. Select **Substructure** or **Similarity**, depending on the type of search you want to perform.
- 3. Click Edit Structure.

Response: ISIS/Draw is launched.

4. Draw a structure to use as search template.

Comment: See ISIS/Draw documentation for more information on how to edit structures.

- When you are done drawing the structure, click the button in ISIS/Draw. Response: ISIS/Draw is closed and the structure appears in the Set Filter for Column dialog.
- Click Next > (or Finish if this is the last prompted column). Response: The data is retrieved. If this is the last run-time filter, then the data is displayed in a visualization.

3.4.2.5 Run-time Filter Example

Information links may include more than one column with run-time filters (which prompt you for input during retrieval). In this case, each filter will reduce the data set, such that subsequent prompts may present fewer values. Consider the following example:

Name	Salary	Location
Prompt: None	Range	Check Boxes
Miller	1300	New York
King	1400	New York
Clark	700	New York
Ford	1100	Dallas
Adams	900	Dallas
Scott	1300	Dallas

This is the data as it would look if no filters were being applied:

Jones	1200	Dallas
James	800	Chicago
Turner	1000	Chicago

As the information link is opened, Salary will be filtered first (the order is set using Information Builder).

Lower	Upper
1100	- 1300

The user enters the limits 1100 to 1300. After the first filter, the following remains:

Name	Salary	Location
Prompt: None	Range	Check Boxes
Miller	1300	New York
Ford	1100	Dallas
Scott	1300	Dallas
Jones	1200	Dallas

Several rows, including all Chicago employees, have been filtered out. This means that when the Location filter is shown, Chicago will not be presented as an option:

3.4.3 User Interface

3.4.3.1 Information Library Dialog

🚰 Information Library	×
Information Links: ActivityBase_Pivoted_Stored_Information_Links ActivityBase_Stored_Information_Links Contrables UQI UQI UQI UQI_actbase_spotlab UQI_dblink_1	
Element details: No description Columns: Protocol Result Mol weight Filters: Substructure 1	-
Help Open Cancel	

Part	Description
Information Links	Displays the information links to which you have access organized in a folder structure.
Information Link details	Describes the selected information link (click an information link once to select it). The pane will show the data elements that are included and a description if one exists.

► To reach the Information Library dialog:

Select File > Import > Open Information Link....

3.4.3.2 Set Filter for Column Dialog

The Set Filter for Column dialog appears when an information link is being opened, and a column is encountered that has been set up with a run-time filter. The dialog may take various forms depending on the type of prompt selected. Strings containing commas can be included both as values, as well as range limits by escaping the comma with a backslash.

alues			
Set Filter for C	olumn		
Step 1 of 3 : Selec	ct Employe		
Please enter a co	mma separated list of values below:		
Get values from o	current visualization		
Get values from a	a text file Browse		
<u>H</u> elp	< <u>Back</u> <u>N</u> ext > Cancel		
Part	Description		
Fext field	Enter a comma-separated list of column values that you want to use as a constraint. You can also paste values of a column from a Microsoft Excel® sheet. The data will automatically be formatted in the right way.		
	Enter to include a comma as a value. Enter \\ to include a backslash as a value. For Procedures, enter \ NULL to include the null value. Example: apple,pear,\NULL,orange,banana		
Get Values	Use this button to set the column filter by fetching values from the current visualization in DecisionSite. Opens the Get Values from Data Set dialog.		
Browse	Fetch filter values from a text file.		

Range

🧉 Set Filter for	Column X	
Step 1 of 1 : Sel	ect Salary	
Please enter th	e range:	
Lower	Upper	
Get range from	current visualization Get Range	
' <u>H</u> elp	< <u>B</u> ack Finish Cancel	
Part	Description	
Lower	Enter the lower limit for the values of the column.	
Upper	Enter the upper limit for the values of the column.	
Get Range	Use this button to set the column filter by fetching values from the current visualization in DecisionSite. More	

List Box	
• Set Filter for Column	<u> x</u>
Step 1 of 3 : Select Day	
191 192 193 194 195 196 197 198 199 200 201 202 203 204 205 206	
207 208 209 210 211	
Include empty values for this step Help	< <u>Back</u> <u>N</u> ext > Cancel
Part Description	

List box	Select the individual values for the column by clicking the entries in the list. To select consecutive values, click the first item, press and hold down SHIFT, and then click the last item. To select multiple entries that are not consecutive, press and hold down CTRL, and then click each item. To select all the values in the list, press CTRL+A.
Include empty values for this step	Select this check box to also include records that contain no data for this column (consequently not available in the list).

Check Boxes

• Set Filter for	Column XI
Step 3 of 5 : Sele	act Day
51	
L 65	
77	
96	
99	
104	
118	
119	
L 145	
146	
150	_
, — □ Include <u>e</u> mp	ty values for this step
Links [Canada Nauto Canada
Part	Description
Check boxes	Select individual values for the column from the list. To select all the values in the list, press CTRL+A.
Include empty values for this step	Select this check box to also include records that contain no data for this column (consequently not available in the list).

• Set Filter for Column		×
Step 3 of 4 : Select month_year		
C August- 1994		_
C August- 1995		
C August- 1996		
C August- 1997		
C August- 1998		
C August- 1999		
December- 1991		
C December- 1992		
C December- 1993		
C December- 1994		
C December- 1995		
C December- 1996		
C December- 1997		
C December- 1998		-
Include empty values for this step		
Li ala	C Deale News	Concel

Radio Buttons

Part Description

Radio buttons Select a unique value for the column by clicking an entry in the list.

IncludeSelect this check box to also include records that contain no data for thisempty valuescolumn (consequently not available in the list).for this step

Structure Search



3.4.3.3 Get Values from Data Set Dialog

🚰 Get Values from Data Set 🛛 🔀			
Matching column:			
Year			
Get values from:			
C Marked records			
Selected records			
ок (Cancel		

Part	Description
Matching column:	Use the drop-down list to select the column in the current data set from which to get the values.
Get values from:	Select whether to use Marked records or Selected records as filter values (or range limits).

To reach the Get Values from Data Set dialog:

- 1. Open an Information Link with run-time filters.
- 2. When the **Set Filter for Column** dialog for the desired column appears, click **Get Values...** or **Get Range...**.

3.5 Import SAS Data

3.5.1 Importing SAS Data Files

In order to open SAS data files in Spotfire DecisionSite, you will need the SAS OLEDB driver. More information on how to get this can be found at http://www.spotfire.com/sr.

► To import SAS data files:

- 1. File > Import > Import Data....
- 2. In the Select Data Source dialog, select File.
- 3. In the **Open** dialog, select the file containing the SAS data. Click **Open**. Response: The SAS Data Import Column Selection dialog is opened.
- 4. In the **Available SAS columns** list, click to select the columns that you want to import.

Comment: For multiple selection, press **Ctrl** and click on the desired columns in the Available SAS columns list. You can sort the columns in the list alphabetically by clicking on the Column name bar.

Click on the **Add** >> button to send the selected columns to the **Imported columns** field.

Select whether you want to map your data to Spotfire compatible types.

Comment: See SAS Column Formatting for more information on this.

Select whether you want the description to be the column name once imported into Spotfire DecisionSite.

Click Next >.

Response: The Import Data - Data Conditioning dialog is opened.

5. Select a conditioning method if desired and click Finish.

Response: The data from the selected SAS file is imported into Spotfire DecisionSite as a new data set.

3.5.2 SAS Data Import - Column Selection Dialog

SAS Data Import - Column Selection	×
Available SAS columns: Type Column name Description E Enter text here Enter text here Image: Column name String Pct_Female Total Number of Househ String Pct_Female String Pct_Under18 String Pct_Under18 String Pct_Over62 String Pct_NoEnglish String Pct_NoCollege String Pct_Unemployed Decimal Avg_HHSize Decimal Avg_HHInc String Pct_PoorFamilies String Pct_PoorFamilies String Avg_HomeValue String Avg_HomeValue String Avg_HomeValue	Imported columns: Type Column name String USPS ZIP Code3 digit String String Dec Tot_Pop String Per_Capita_Income Dec Mean_PovertyRatio Move Up Move Loom Move Loom Import settings
File: C:\Census Data\Census.sas7bdat	 ✓ Map data to Spotfire compatible types ✓ Use Description as column name (if available)
Help	< <u>B</u> ack <u>N</u> ext > Cancel

Option	Description
Available SAS columns:	The columns in the SAS file available to be imported into Spotfire DecisionSite. Click a column name in the list to select it. To select more than one column, press Ctrl and click the column names in the list. Then click Add >> to send the selected column to the Imported Columns field.
Enter text here 🔽	If you have a data set with many columns, you can right-click on the header of the columns in the Available columns list box and select Show Search Field from the pop-up menu. This will display a search field where you can type a search string and limit the number of items in the list. It is possible to use the wildcard characters * and ? in the search.
Add >>	Moves selected columns from the Available SAS columns field to the Imported columns field.
<< Remove	Removes a column and brings it back to the Available SAS columns field.
Add All	Adds all columns from the Available SAS columns field to the Imported columns field.
Remove All	Removes all columns from the Imported columns field and brings them back to the Available SAS columns field.
Move Up	Moves the selected column up in the list.
Move Down	Moves the selected column down in the list.
File:	The pathname of the SAS data file.

Map data to Spotfire compatible types	Allows you to map the data types to Spotfire compatible ones. If this check box is cleared, the SAS formatting will be unchanged.	
Use Description as	Allows you to specify whether to use the SAS description as the	
column name (if	column name once imported into DecisionSite. If this check box is	
available)	cleared, the current column name will be unchanged after import.	

► To reach the SAS Data Import - Columns Selection dialog:

- 1. Select File > Import > Import Data...
- 2. In the Select Data Source dialog, select File.
- 3. In the Open dialog, select the SAS data file. Click Open.

3.5.3 SAS Column Formatting

Spotfire DecisionSite allows you to import SAS Data files of the format **.sas7bdat** and **.sd2** into DecisionSite. It is also possible to open .sd7 files if they are first renamed to have a .sas7bdat extension. Other file formats are not supported at this time.

If the "Map data to Spotfire compatible types" check box is selected in the SAS Data Import -Column Selection dialog, or if a SAS file is opened without the data import dialog; Spotfire DecisionSite attempts to reproduce the data type that SAS would for the same data. If it is not selected, raw data will be read from the SAS data file and columns will be of the type string or decimal.

The table below shows how the SAS formats are used to map the data to Spotfire DecisionSite specific data types:

SAS Format	Spotfire Type
Date	Date
Dateampm	DateTime
Datetime	DateTime
Day	Integer
Ddmmyy	Date
Downame	String
Dtdate	DateTime
Dtmonyy	DateTime
Dtyear	Integer
Dtyyqc	DateTime
Hour	Integer
Julian	String
Mmddyy	Date
Mmyy	Date
Monname	String

Month	Integer
Monyy	Date
Octal	String
Qtr	Integer
Qtrr	String
Timeampm	String
Tod	Time
Weekdate	Date
Weekdatx	Date
Weekday	Integer
Worddate	Date
Worddatx	Date
Xyymmdd	Date
Year	Integer
Yymm	Date
Yymmdd	Date
Yymmn	Date
Yymon	Date
Yyq	String
Yyqr	String

4 Visualizations

4.1 Scatter Plots

Scatter plots are similar to line graphs in that they use horizontal and vertical axes to plot data points. However, they have a very specific purpose. Scatter plots show how much one variable is affected by another. Each record (or row) in the data set is represented by a marker whose position depends on its values corresponding to the X and Y axes.



The above picture demonstrates how scatter plots can be used. Say, for example, that you want to show whether studying longer hours helps you improve your test grades.

The scatter plot shows that according to this set of data, the longer you study, the better grade you will get on your test.

A third variable can be set to correspond to the color or size of the markers, thus adding yet another dimension to the plot.

Two-dimensional scatter plots are the default visualization of many data sets.

Make a new 2D scatter plot in one of the following ways:

- Press Ctrl+1 on the keyboard.
- Click the **New Scatter Plot** button on the toolbar,
- Select New Scatter Plot from the Visualization menu.

By right-clicking in a visualization a pop-up menu appears. This context menu lets you access many features in a fast and easy way. For example, you can select to show structures in marker labels:



A 3D scatter plot is used to show the relationship between three variables. It shows the data set in three dimensions, using three columns as axes. Each record (or row) in the data set is represented by a marker whose position depends on its values corresponding to the X, Y and Zaxis. A fourth variable can be set to correspond to the color or size of the markers, thus adding yet another dimension to the plot.



3D scatter plots allow a lot of information to be encoded into visualizations. They are especially useful when analyzing data that is not clustered along any of the axes (columns) of the data set.

Make a new 3D scatter plot in one of the following ways:

- Press **Ctrl+2** on the keyboard.
- Click the New 3D Scatter Plot button on the toolbar,
- Select New 3D Scatter Plot from the Visualization menu.

3D visualizations have the Z-axis selector and zoom bar along the top edge of the visualization. The Z-axis initially points towards the viewer, out from the screen.

4.2 Bar Charts

A Bar Chart is a way of summarizing a set of categorical data. It displays the data using a number of bars of the same width, each of which represents a particular category. The length of each bar is proportional to the count, sum or the average of the values in the category it represents, such as age group or geographical location. In DecisionSite it is also possible to color or split each bar into another categorical column in the data, which enables you to see the contribution from different categories to each bar in the bar chart.

anne	5500	Year	City	Revenue	
<u>لَّ</u> 5000-	4000	1999	Boston	3000	
'ㅎ 4000 독 3000		1999	Dallas	2000	
2000-		1999	Seattle	500	
I 1000-		2000	Boston	2000	
-1000-		2000	Dallas	-3000	
-2000		2000	Seattle	-1000	
	2000	2001	Boston	2500	
	1993 2000 2001 2002	2001	Dallas	1000	
- Ju Bar Chart		2001	Seattle	500	
		2002	Boston	3000	
		2002	Dallas	500	
		2002	Seattle	1000	

The above picture demonstrates how bar charts can be used. Say, for example, that you want to show the total yearly revenue of a company with offices in three different cities. The bar chart sums the revenue for the three cities and displays them per year.

Bar charts can also be categorically colored, which means that the partial sums of the bars are colored differently. Expanding the Legend shows the meaning of each color.



When categorical coloring is applied, you have the option to display the categories in four different ways:

- Stacked bars
- Side-by-side bars
- 100% stacked bars
- 100% side-by-side bars

If you want to compare the proportions of different categories for, e.g., different time periods, you can use either of the 100% layout options in the Properties dialog. With 100% stacked bars, all bars will be of equal height (100%), unless some negative values exist in the data.



In the example above, one can see that the Seattle revenue (yellow) has affected the total revenue more during 2002 than in previous years, whereas the Dallas revenue (blue) has decreased in importance. See Bar chart layout details for more information.

If the categories are split to several columns, categorical coloring can also be shown via differently colored bars in multiple columns (see below).

▶ Make a new bar chart in one of the following ways:

- Press **Ctrl+4** on the keyboard.
- Click the New Bar Chart button on the toolbar,
- Select New Bar Chart from the Visualization menu.

Count / Sum / Average

The height of the bars can be set to represent three different aggregation methods: Count, Sum or Average. You select this by clicking on the Axis Selector for the Y-axis.

- Count the height of a bar represents the number of records with a particular value.
- Sum the height of the bar indicates the total sum of the values of all records in that bar.
- Average the height of the bar indicates the average value of all records in that bar.

Multiple Columns

You can display multiple columns as side-by-side bars. This is useful if you want to compare many parameters at the same time, and the categorical data exist in different columns. (When the categorical data is included in a single column, you should instead use one of the side-by-side options in the Layout section of the Bars tab, see Categorical Coloring Layout below.)



► To Display Multiple Columns:

- 1. Click on the Axis Selector for the Y-axis.
- 2. Select Multiple Columns.

Response: The Multiple Columns option will be selected with a check mark the next time you open the list.

- 3. Click on the Axis Selector for the Y-axis.
- 4. Select an additional column to display. Selected columns will be indicated by a colored square.

Note: You can also click on the **Select Columns...** option, which will display the **Bar Chart Columns tab** of the **Properties** dialog. From this dialog you can easily add or remove several columns to the bar chart.

Sorting using Right-Click

By right-clicking in a visualization a pop-up menu appears. This context menu lets you access many features in a fast and easy way. If you are not using Multiple Columns you can sort the bars in ascending or descending order; selecting the Reverse sort order will arrange your bars in the reverse order of the current sort order. This is an instantaneous sorting of the bars; if you filter the data with the query devices so the height of the bars change, their horizontal order will not change until you choose to sort them again.

Note: Ascending and descending sorting is available when you are viewing single columns with fixed coloring or categorical coloring in stacked bar layout. You cannot use sorting when you are using multiple columns or either of the categorical coloring 100% bars layout options.

Tip: If you want to sort multiple column bar charts, first apply the sorting you want to a bar chart with only the sorting column on the Y-axis. Then, select Multiple Columns and add more columns to your visualization.

4.3 Pie Charts

Pie charts are circle graphs divided into pieces, each piece displaying the size of some related piece of information. Pie charts are used to show percentages of a whole.



A pie chart visualization can consist of one or more pies. Multiple pies are used to split the data by different categories in a column. This is accomplished by setting the X-axis and/or Y-axis selectors to represent a categorical column in the data set.



Make a new pie chart in one of the following ways:

- Press **Ctrl+5** on the keyboard.
- Click the New Pie Chart button on the toolbar,
- Select New Pie Chart from the Visualization menu.

By right-clicking in a visualization a pop-up menu appears. This context menu lets you access many features in a fast and easy way.

4.4 Line Charts

A line chart is a way to summarize how two pieces of information are related and how they vary depending on one another. Line charts are useful for visualizing data that behaves like a function with respect to the variable on the X-axis, such as time series data. This visualization type is ideal for showing trends or changes in data over a period of time, at even intervals. Line charts emphasize time flow and rate of change rather than the amount of change.



The above picture demonstrates how line charts can be used. Say, for example, that you want to show how fast a car devaluates the more mileage it gets. The line chart shows that according to this set of data, the longer a car is driven, the more its value decreases.

Make a new line chart in one of the following ways:

- Press Ctrl+6 on the keyboard. •
- Click the **New Line Chart** button on the toolbar. •
- Select New Line Chart from the Visualization menu. •

By right-clicking in a visualization a pop-up menu appears. This context menu lets you access many features in a fast and easy way.

4.5 **Profile Charts**

A profile chart maps each record as a line, or profile. Each attribute of a record is represented by a point on the line. This makes profile charts similar in appearance to line charts, but the way data is translated into a plot is substantially different.

Consider, for example, a data set with three different applicants for a job position. Through tests or interviews, the recruiter may have provided percentage estimates of each candidate in terms of experience, social competence, and creativity. The data may look as follows:

Applicant	Experience	Grades	Creativity
Lisa	85	95	60
Joe	70	75	95
Anne	100	80	80

For each applicant, it is now possible to plot a personality profile. This will give a good (if somewhat simplified) overview of characteristics, and a possibility to visually match an applicant against a "model profile" for the job. The profile chart would look as follows:


► To create a profile chart:

- Press [Ctrl+7], or click the New Profile Chart button on the toolbar, or select Visualization > New Profile Chart.
- 2. Go to the axis selector of the X-axis and uncheck columns that you do not want to include in the chart, such as identifier columns.
- 3. Use the **Properties** dialog to adjust the various properties of the chart.

By right-clicking in a visualization a pop-up menu appears. This context menu lets you access many features in a fast and easy way.

4.6 Heat Maps

Heat Map plots are also known as Intensity plots or Matrix plots. A Heat Map can be likened to a spreadsheet, where the values in the cells are instead represented by colors.

Heat Maps can be used to identify clusters of records with similar values, as these are displayed as "areas" of similar color.

The easiest way to understand a heat map is to think of a table or spreadsheet which contains colors instead of numbers. The default color gradient sets the lowest value in the heat map to bright green, the highest value to a bright red, and mid-range values to black, with a corresponding transition (or gradient) between these extremes.

Test	Time 1	Time 2	Time 3	
Test A	2,02	3,21	5,57	
Test B	2,92	4,37	6,02	
Test C	2,64	5,02	7,19	
Test D	2,37	3,48	8,21	
Test E		2 4 4	5 20	
	Time 1	Time	2 Time 3	

► To create a Heat Map:

- Press [Ctrl+8], or click the New Heat Map button on the toolbar, or select Visualization > New Heat Map.
- 2. Go to the axis selector of the Y-axis and select the columns you wish to order the rows by.
- 3. Use the **Properties** dialog to adjust the various properties of the chart.

Order of rows

By default, the order of the rows in the heat map is set to **None**, meaning that they are in the same order as they were before the data set was imported. However, you may want to sort the rows differently, such as if a certain column was pre-generated to contain a relevant sorting order. The order of the rows is shown numerically in the X-axis selector of the Heat Map.

Click on the vertical axis selector to select which column (or None) to order the rows by.

(leu	Type to search		
<u>z</u>	(None)		Ν.
•	X	Integer	K)
_	Y	Integer	
	Year	Integer	
	Cadmium	Integer	
	Chrome	Integer	
	InChrome	Integer	
	Copper	Integer	
	InCopper	Integer	
	Nickel	Integer	
	Lead	Integer	
	InLead	Integer	
	Vanadin	Integer	
	Zinc	Integer	
		-	

Activating and Marking Records

Making a record active or marking several records in a heat map plot differs somewhat from other plots. In a heat map, one row always equals one record. Consequently you always select or mark one or more entire rows, which equals one or many records.

Making a record Active

When you click on a row, a black triangle appears at both ends of the selected row to indicate that it is active. Information about the row is displayed in the Details-on-Demand window.



Marking Records

By clicking and holding the mouse button while the mouse pointer is on a row and dragging it to cover several rows, these rows all become marked. This is indicated by a small bar shown at the left and right of the rows in question. Details on these records are shown in the Details-on-Demand window.

By right-clicking in a visualization a pop-up menu appears. This context menu lets you access many features in a fast and easy way.



Show/hide deselected records

Records that have been deselected by using the query devices become gray (default color) in the heat map. To hide these records, clear the **Show deselected** check box in the Heat Map tab of the Properties dialog.



Note: If you have had a dendrogram associated to the heat map, this will no longer be valid after hiding the deselected values. In this case, the dendrogram tree will be removed. You can show the dendrogram again by selecting the Show deselected check box.

Row Labels

It is possible to show row labels either to the left or to the right of the heat map. This setting, plus the selection of the column to display as row labels, are set on the Heat Map tab of the Properties dialog.

When row labels have been displayed, it is possible to adjust the space available for the labels by dragging the line between the heat map and the row labels with the mouse pointer. If the height of the rows is so small that it is impossible to see row labels, row labels will not be shown on every row. Instead, the number of row labels that fit into the heat map will be displayed at an equal distance from each, for example only on every fifth row. If rows have been deselected, no row labels will be shown for these rows.

Row labels that are too long to be displayed correctly will be truncated and end with an ellipsis (...). In this case, hovering over the row label with the mouse pointer will display a ToolTip of the entire row label text.

4.7 Tables

The Table visualization presents the data as a table of rows and columns. The Table can handle the same number of rows and columns as any other visualization in DecisionSite.

In the Table, a row represents a record. By clicking on a row, you make that record active, and by holding down the mouse button and dragging the pointer over several rows, you can mark them.

You can sort the rows in the table according to different columns by clicking on the column headers, or filter out unwanted records by using the query devices.

City V Seattle Seattle Seattle Seattle Dallas	Year 1999 2000 2001 2002	Revenue 500 -1000 500	-
Seattle Seattle Seattle Seattle Seattle Seattle Seattle Seattle Dallas	1999 2000 2001 2002	500 -1000 500	
Seattle Seattle Seattle Dallas	2000 2001 2002	-1000 500	
Seattle Seattle Dallas	2001 2002	500	
Seattle Dallas	2002	1000	
Dallas		1000	
	1999	-2000	
Dallas	2000	-3000	
Dallas	2001	1000	
Dallas	2002	500	
Boston	1999	3000	
Boston	2000	2000	
Boston	2001	2500	
Boston	2002	3000	
			•

► To create a Table:

- Press [Ctrl+9], or click the New Table button on the toolbar, or select Visualization > New Table.
- 2. Click on the header of the column you wish to sort the rows by, or rearrange the order of the columns by dragging and dropping the column headers horizontally.
- 3. Use the **Properties** dialog to further adjust the various properties of the chart.

By right-clicking in a visualization a pop-up menu appears. This context menu lets you access many features in a fast and easy way.

You can sort the vertical order of the rows in the table. This can be done in several steps, for example: first sort according to the values in column 1, then by the values in column 5, then by the values in column 3, etc.

► To sort the data:

- 1. Click on the header of the first column you wish to sort the data by.
- 2. Press Shift and click on another column header to make a subsequent sort according to the values in that column.
- 3. Repeat step 2 on other columns as many times as you like.

A small digit will appear in the column headers indicating the sorting order. **Note:** Click an additional time on a column header to toggle between Ascending and Descending row order.

Note: For more information on how strings are sorted in a Table see the topic String.

► To change the column order:

- 1. Click on a column header and hold the mouse button down.
- 2. You can now drag and drop that column horizontally. Move the header to the position you want it to be placed.
- 3. Release the mouse button when you wish to insert the column.

Note: You can move a column to the first or last position by right-clicking in the column header and selecting **Move First** or **Move Last** from the menu that appears.

► To resize the column width:

Place the mouse pointer to the right of the column header you want to resize (just between it and the next column header). The cursor changes into a cross with arrows.

By double-clicking, the column width will automatically expand so that all the items in the column can be displayed without being truncated.

If you want to rescale the column width by hand, you can instead hold down the mouse button and move the mouse horizontally, which will adjust the width. Release the mouse button when you are satisfied.

Note: You can also set the width of a column by right-clicking in the column heading, and selecting **Column Width** from the menu that appears. Enter the width in number of characters and press **OK**.

In a table with many columns you often need to scroll horizontally. However, sometimes you may want certain columns to always be displayed regardless of scrolling. This is achieved by freezing one or more columns.

► To freeze columns when scrolling horizontally:

- 1. Place the columns you want to freeze to the far left, using drag and drop.
- 2. Select **Edit > Properties** and choose the **Table** tab.
- 3. Select the number of **Frozen columns** from the drop-down list box.
- 4. Close the Properties dialog.
- 5. The leftmost column(s) you specified will be displayed at all times, when you are scrolling horizontally.

Activating and Marking Records

Moving the mouse over a record will highlight it with a thin black rectangle.

To make a record Active simply click on it. The Active record is indicated by a thick black rectangle around it. You can use the arrow keys to move the active record indicator up or down, thus making another record active instead.

There are several ways to help you mark a set of records in the Table, as explained in the table below. Marked records are by default indicated by a dark green background.

The following instructions explain how to mark one or more records in the Table:

► To mark one single record:

Mouse:

Drag the mouse over the record while holding down the left mouse button. A dotted rectangle will indicate the drag operation.

Keyboard + mouse:

Click on the record you want to mark. Then click on it again, while holding down the Shift key. **Keyboard:**

Press the Spacebar to mark the currently active record (only in table visualizations).

► To mark a range of records:

Mouse:

Drag the mouse over the records you want to mark. A dotted rectangle will indicate the drag operation.

Keyboard + mouse:

Click on the first record in the range. Hold down the Shift key and click on the last record in the range. The records in the range will be marked.

Keyboard only:

Move the active record to the first record in the range using the up and down arrow keys. Press the Spacebar to mark this record and to start a new "marking session". Hold down the Shift key while pressing the up/down arrow keys. The records will be marked one after another.

► To mark multiple records:

Keyboard + mouse:

Drag the mouse over the records in the first range. Hold down the Ctrl key and drag over another range. The records will be added to the set of marked records.

Alternative: Hold down the Ctrl key while clicking on individual records. This will include the clicked records in the set of marked records.

Keyboard only:

Mark a range of records as described above. Continue to move the active record with the arrow keys. Hold down the Ctrl key and press the Space key to add the currently active record to the set of marked records.

4.8 **Properties Dialog**

4.8.1 Annotations Tab

4.8.1.1 Annotations Tab

Edit > Properties > Annotations tab

Properties: Resear	ch 2004-03			×
Trellis Annotations	Axes Data and Backgroun	3D d Columns	Markers Details Columns	
Visualization title:	Visualization title: Research 2004-03			
Annotation:	Append axes names	to visualization title		
This is the resear	ch done on the samples t	aken in 2004-03.	A	
			V	

You can give any visualization a title and an annotation. The title will appear as the caption of the window. It can also appear in the heading of printouts. The annotation will appear as a ToolTip when you place the mouse pointer over the paper clip at the bottom-left corner of the visualization.



► To set title and annotation:

- 1. Go to the **Annotations** tab of the **Properties** dialog.
- 2. Type a title and/or an annotation.
- 3. Select the check box **Append axes names to visualization title** if you want the current axes to be appended to the title.

You can type in a lot of text in the **Annotation** field, as well as cut and paste to and from other Windows applications; this can only be done with text, however. This is a good place for adding information about the purpose and methods used in the visualization, features to look for and other helpful information concerning the data. The annotation can be printed together with the visualization, by selecting the Include annotation option available in the Print Layout Wizard on the **File** menu.

4.8.2 Data and Background Tab

4.8.2.1 Data and Background Tab

Edit > Properties > Data and Background tab

Properties: Pie Chart	×
Annotations Data and Background Columns Details Columns	Pies
Axes	[
Labels: 🔽 X axis Grid: 🔽 X grid lines	Data Range
🔽 Y axis 🔽 Y grid lines	
🗖 Z axis 🗖 Z grid lines	Labels
Background image	
File: Browse	Position
HTML Details-on-Demand	
Template: Pie	Edit
Limit maximum number of records shown: 20	
Statistical measures	
Average +-2.0 standard deviations for X axis, using selected r	A <u>d</u> d ▼
Vertical Error Bars	Edit
\square Curve: $y(x) = x$	
	Remove

Option	Description
Axes	The Axes section allows you to control axis labels, data range and grid lines for bar charts, pie charts, line charts and heat maps. This section does not appear for scatter plots since these have a separate Tab for more advanced settings, see Axes for Scatter Plots.
Background image	Background image lets you select a file to use as background. You can also specify how the background image is positioned.
HTML Details-on- Demand	Details-on-Demand lets you choose templates for formatting the HTML display of record details.
Statistical measures	Statistical measures offers control over the standard deviation marking lines, error bars, and different types of curves and curve fits. Available for 2D scatter plots and pie charts only. In bar charts, you can select to add a vertical reference line from the

Add menu under Statistical measures.

4.8.2.2 Axes

Edit > Properties > Data and Background tab

The Axes section of the Data and Background dialog appears in all plots except for Scatter Plots. Scatter Plots can handle more advanced axis labels and have a separate properties tab for this, see Axes tab for Scatter Plots. For all other plots please continue below.

The **Axes** section of the **Data and Background** tab lets you define attributes for labels, axes and grids. The check boxes allow you to control which labels and grid lines to display.

Data Range

In the **Data Range** dialog, the minimum and maximum values of the axes can be set. This allows you to get more space around the data whose range is otherwise set to the range of the records of the data set.

D	ata Range 🛛 🔀
	Data range
	Z Low: -1 Z High: 1
	Y High: 2521.5
	Y Low: -61.5 Low High X
	X Low: 0.215909(X High: 24.78409(
	Default OK Cancel

Labels

If you click the **Labels...** button you can set the label orientation, the label spacing and the maximum number of labels for each of the axes.

Labels	×
Label Orientation	Tick spacing
X Axis: © Horizontal	X Axis: At Even Values 💌
YAxis: O Horizontal Vertical	Y Axis: At Even Values 💌 Z Axis: At Even Values 💌
Max no. of ticks X Axis: 11 Y Axis: 11 Z Axis: 11 T	The actual number of displayed ticks might be considerably lower and will not always change when the max number of ticks is changed.
Reset	OK Cancel

Option	Description
Label Orientation	Specifies whether the labels should be oriented horizontally or vertically on the X-axis and on the Y-axis.
Tick spacing	 For spacing you can select to show axis ticks in four ways: Even Distribution will attempt to distribute ticks evenly between the highest and lowest value . At Values will not place a tick where there is no value. At All Values will place ticks at all values (within density constraint). At Even Values will attempt to place ticks at evenly spaced whole numbers.
Max no. of ticks	Specifies the maximum number of allowed ticks. However, the actual number of displayed ticks might be less than this number depending on which option you have selected under Tick spacing above.
Reset	Resets all settings in this dialog to its default value.

4.8.2.3 Background Images

4.8.2.3.1 Image Files and Background Maps



Background maps, images, and figures may be displayed along with visualization markers in a Spotfire DecisionSite visualization. Such images can ease the interpretation of the data by providing a context in which it can be interpreted. For example, some aspects of the environmental database described earlier can be examined more easily if data is seen together with a map of Sweden. Another example where an image provides context to the data is the metabolic pathway for yeast genes used in the microarray sample file included in the Spotfire DecisionSite distribution.

Background images can be added to 2D scatter plots, line charts, profile charts, bar charts and pie charts.

Formats of background images and maps

Supported background image formats:

- Windows bitmap images (*.bmp)
- JPEG images (*.jpg, *.jpeg)
- PNG bitmap images (*.png)
- TGA files (*.tga)
- PCX files (*.pcx)

Supported background map formats:

- MapInfo Interchange Format files (*.mif). These are typically tagged with for example with zip codes, which Spotfire DecisionSite can use to position visualization markers.
- Spotfire mapping files (*.sfm)

4.8.2.3.2 Adding a Background Image

Edit > Properties > Data and Background tab

To add a background image to the current visualization:

- 1. In the Properties dialog, open the **Data and Background** tab.
- Enter the path and name of the image file to use in the file box.
 Tip: The Browse... button can be used to search the file system for appropriate files.
 You can also enter an URL to an image available on a server.
- 3. Click **Position...** in the **Background Image** section to adjust the positioning of the image relative to the markers.

Tip: If desired, adjust the **Data Range...** in the Axes section to increase the visible area of your visualization. This might be necessary if you want the picture area to be larger than the area covered by markers.

4.8.2.3.3 Position a Background Image

Edit > Properties > Data and Background tab > Position...

On the Data and Background tab of the Properties dialog, click the **Position...** button. The dialog that appears allows you to specify how the background image is positioned, by giving the coordinates for two opposing corners. These coordinates refer to the current X and Y-axes. This means that the corners are "pinned" to values in the data range. Zooming and panning will cause the image to stretch and scroll with the data.

Position Background In	nage	×
Position-		
Y High: 8.8	Y A High	
Y Low: 0	Low High X	
X Low:	0 × High: 1	
Default	OK Cancel	

Option	Description
Y High	Specifies the top position of the background image.
Y Low	Specifies the bottom position of the background image.
X Low	Specifies the left edge of the background image.
X High	Specifies the right edge of the background image.
Default	Reverts to the default coordinates.

4.8.2.3.4 Adding MapInfo Background Files

MapInfo is a leading geographic information system software package. MapInfo Interchange Format (MIF) is an ASCII format developed by Mapping Information Systems Corporation (http://www.mapinfo.com/) to facilitate the transfer of data from other geographical information system packages to MapInfo.

Spotfire DecisionSite can import MIF files to use as background maps. This allows you to position visualization markers in two dimensions based on a single column such as zip code, area code, or area name.

Suppose, for example, that you have a data file with information about various countries, such as name, population, language, etc. However, the data set includes no information about geographical coordinates. By using a MIF file as background, you get not only a background map, but also two new columns of data. Each record is given map coordinates depending on which country it represents.

► To use a MIF file as background:

- 1. Create a scatter plot visualization.
- 2. Activate the **Properties** dialog and select the **Data and Background** tab.
- 3. Click the **Browse...** button by the **Background Image** field and select **MapInfo Interchange Files**, then browse to the file you want as a background.
- Click Open. The Match Data and Background dialog is displayed, where it is possible to match a database column with a tag in the MIF file.
- 5. In the left field, select the column in your data set that identifies geographical position, in this case **Country**.
- 6. In the right field, select the MapInfo tag in the MIF file that relates to the same information, in this case **Country**. (The names are not necessarily the same.)
- 7. In the two text fields, enter names for the new columns that will be added to your data set, specifying X and Y position.
- 8. Make sure **Use current axes** is cleared. If you select this option, then no new coordinates will be extracted from the MIF file. You will then only get a background image.
- 9. If you want to add *all* the information in the MIF file (i.e., not just the coordinates) to your data set, then select **Make new columns for background columns**.
- 10. Click **OK**.

(with variables in italics):

Comment: Spotfire DecisionSite will try to match data and background. The background image is shown, and the axes changed to the new coordinate columns.

4.8.2.3.5 Spotfire DecisionSite Mapping Files (SFM Files)

The Spotfire DecisionSite mapping file (*.sfm) format first establishes a coordinate system, which relates the data set's coordinate system to that of the polygon set being defined. After that, a number of polygons are defined. A polygon is defined by a fill color, an origin point, a border color, the number of points and the X, Y, and Z coordinates of the points. The Z coordinates are ignored, but they must be included. The format of the file as follows

COORDSYS xmin xmax ymin ymax zmin zmax ADD POLY fillcolor xorigin yorigin zorigin !yes numberofpoints x1 y1 z1 x2 y2 z2

A sample file could look as follows:

```
COORDSYS 0.0 1.0 0.0 1.0 0.0 1.0
ADD
POLY LimeGreen 0.0 0.0 -0.02 0.0
!yes
5
0.677419 0.976261 0.0
0.680645 0.977745 0.0
0.680645 0.983680 0.0
0.677419 0.985163 0.0
0.677419 0.988131 0.0
```

The *env.sfm* file in the Spotfire DecisionSite distribution serves as an example of this background map format.

To map a data file to a Spotfire mapping file:

In your visualization, select the two axes from the data that serve as coordinates. In the **Data and Background** tab in the **Properties** dialog, select an SFM file which has a coordinate system matching the coordinates in the axes file.

4.8.2.4 HTML Details-on-Demand

Edit > Properties > Data and Background tab

The information of each record can be displayed in an external or internal HTML browser.

2
ies
Data Range Labels
Position
Edit
Add

HTML Details-on-Demand templates are accessed through the Data and Background tab.

4.8.2.5 Statistical Measures

4.8.2.5.1 Statistical Measures

Edit > Properties > Data and Background tab

Some statistics and curves can be visualized directly in 2D scatter plots. This section of the **Edit > Properties > Data and Background** dialog offers control of several kinds of statistical measures:

Average and Standard Deviation – X-axis and Y-axis average and standard deviation marking lines. The standard deviation is an indication of how dispersed the probability distribution is about its center.

Error Bars – Error bars are used to indicate the estimated error in a measurement. Errors bars indicate the uncertainty in the x and/or y values.

Orthogonal Straight Line Fit – This is suitable when it is reasonable to assume randomness for both the X-axis values and the Y-axis values.

Curve – This option lets you enter a custom expression using the full power of the SXL language, which is drawn as a curve overlaying the visualization.

Curve Fit – This adds a best fit curve to the graph using one of several different models. Curve fit should be used when there is no randomness for the markers along the X-axis.

Note: If you designate X and Y axes for a Pie Chart, you can add some statistical measures to that visualization as well.

► To add a measure or a curve to a visualization:

- 1. Open the **Properties** dialog and select the **Data and Background** tab.
- 2. Click on the **Add** button.
- 3. Choose a measure from the drop-down list.
- 4. Make the appropriate settings in the dialog that appears.
- 5. Click OK.

► To edit a statistical measure:

- 1. Select a measure from the list by clicking on it.
- 2. Click on the **Edit** button.

or

• Double-click on the statistical measure in the list.

To remove a statistical measure:

- 1. Select a statistical measure from the list by clicking on it.
- 2. Click on the **Remove** button, or press **Delete** on your keyboard.

You can show or hide a statistical measure without removing it permanently from the list.

► To show/hide a statistical measure:

- Select the check box beside a statistical measure to show it in the scatter plot.
- Clear the check box beside a statistical measure to hide it in the scatter plot.

4.8.2.5.2 Average and Standard Deviation

The statistical measure "Average" displays the X-axis and Y-axis standard deviation marking lines.

The standard deviation, s, is an indication of how dispersed the probability distribution is about its center. It is computed as follows:

$$s = \sqrt{\frac{\sum_{i=1}^{n} (x_i - \overline{x})^2}{n - 1}}$$

where

n is the number of values in the group and

 \overline{x} is the mean value of the group.

Note: In this application, the standard deviation is calculated for the data in the data set, as opposed to calculation of standard deviation for the mean value only.

User Interface

verage and Standard	Deviation X
Calculate average of • X values • Y values	Base calculation on Selected records All records
Number of standard de	viations: 2.0
Trellis plot options	atistics for each trellis panel
C Create statistics ba	sed on entire visualization
Line Color:	Width: 3
Help	OK Cancel
Option	Description
Calculate average of	Specifies whether the average of the X values or the Y values show be calculated.
Base calculation on	Specifies whether the statistical measure should be calculated base on All records in the data set regardless of any filtering done with query devices, or whether the calculation should be based on the Selected records so that filtering with the query devices will affect the result.
Number of standard deviations	Specifies how many standard deviations away from the (bolder) average line the deviation lines will be drawn.
Trellis plot options	
	Specifies whether the average displayed in each trellis panel will be calculated based on the records specific to that trellis panel only, of the average will be based on all records regardless of trellis condit and therefore be the same for every trellis panel.
Color	Specifies whether the average displayed in each trellis panel will be calculated based on the records specific to that trellis panel only, of the average will be based on all records regardless of trellis condit and therefore be the same for every trellis panel. The color of the displayed line.

4.8.2.5.3 Error Bars

Error bars are used to indicate the estimated error in a measurement. In other words, they indicate the uncertainty in the x and/or y values.

Unlike other statistical measures in Spotfire DecisionSite, no calculations are performed to produce the error bars. Instead the data needed is assumed to be in the data set, in the form of three columns representing an average value, a high error and a low error. The marker itself shows the average value, and the high and low error values make up the error bar.



User Interface

Error Bars 🔀
Column containing main values:
LogRatio1
Column containing upper errors:
LogRatio6
Column containing lower errors:
LogRatio7
Bars © Use marker color
C Use custom color:
Width: 1
Help OK Cancel

Option

Description

Column containing main values	Specifies which column contains the main (or average) values.
Column containing upper errors	Specifies which column contains the upper error values.
Column containing lower errors	Specifies which column contains the lower error values.
Use marker color	Select this option to use the marker color for the error bars.
Use custom color	Select this option to use a custom color for the error bars.
Width	The width (in pixels) of the error bars.

4.8.2.5.4 Orthogonal Straight Line Fit

Orthogonal straight line fit is calculated by choosing the line that minimizes the least square sum of the distance **d** perpendicular to the line, of all the selected markers (see picture below). It should be used when the distance between the markers along both the X-axis and the Y-axis varies.



User Interface

Orthogonal Straight Line Fit 📃 🔁	¢
Base calculation on Selected records All records	
 Trellis plot options Create separate statistics for each trellis panel Create statistics based on entire visualization 	
Color: Width: 1	
Help OK Cancel	

Option

Description

Base calculation on	Specifies whether the line should be calculated based on all records in the data set regardless of any filtering done with the query devices, or whether the calculation should be based on the selected records so that filtering with the query devices will affect the result.
Trellis plot options	Specifies whether the orthogonal straight line fit displayed in each trellis panel will be calculated based on only the records specific to that trellis panel, or if the fit will be based on all records regardless of trellis condition and therefore be the same for every trellis panel.
Color	The color of the displayed line.
Width	The width (in pixels) of the displayed line.

Results

If Orthogonal Straight line fit is active and the Legend is visible, information about Statistical measures will be displayed there. The correlation value, \mathbf{R} , which is displayed, is the standard Pearson's correlation and is calculated like this:

$$R = \frac{\sum_{i} (x_{i} - \bar{x})(y_{i} - \bar{y})}{\sqrt{\sum_{i} (x_{i} - \bar{x})^{2} \sum_{j} (y_{j} - \bar{y})^{2}}}$$

Note: The Legend will not display the R value if you have several Trellis panels.

4.8.2.5.5 Curve

The Curve feature allows you to specify a curve to be displayed on top of a scatter plot or pie chart, given that you have specified X- and Y-axes in the pie charts. You simply enter an expression where the curve is defined as "y as a function of x" and it will be drawn on top of the plot. To aid you in creating powerful expressions, you can use the Spotfire Expression Language (SXL). All the functions of SXL can be selected and inserted from the **Function** list in the dialog.

Examples:

y(x) = 10+xy(x) = Average(x)+100

y(x) = 10*sin(x*PI())+5

You can also select the color and width of the curve. In the **Status** field there is also a syntax verification of the entered expression, where you can easily see if the expression is correct. If the expression is valid, and the **Redraw curve while typing** check box is selected, the curve will be drawn and immediately updated on screen when you edit your expression, so you can always check to see if it looks like you intended.

Transformations

The x and y values are unaffected by transformations, but the mapping onto the plot will be affected. This means that a straight line equation such as y(x) = x, will turn into a curve if the X-axis column uses a Log transform.

Curve		<u>1</u>
Functions Category: All Function: + * /	•	Description: Adds the two arguments. Example: 3.5 + 2.5
Curve Expression: $y(x) =$ $30 \pm Co \le (x \pm 10) \pm 10 \pm x$		Redraw curve while typing
		T
Color:	Width: 2	▼ Status: OK
Help		OK Cancel

User Interface

Category

Select a category of functions to limit the choices in the Function list.

- All
- Operators
- Math Functions
- Statistical Functions
- Text Functions
- Logical Functions
- Date & Time Functions
- Conversion Functions

Function

Select a function by clicking on it, and click the **Insert Function** button to insert it to the **Expression** field. You can also double-click on a function to insert it.

If you place the cursor at a specific location in the **Expression** field, the function will be inserted there.

Description

This field provides a brief description of the selected function. For more detailed descriptions, please see Spotfire Expression Language (SXL).

Expression

This is the text field in which you build your expression. You can insert functions to it from the list, or enter text as in any standard text editor.

Cut/Copy/Paste works in the field using standard Ctrl+X / Ctrl+C / Ctrl+V.

Highlighting a section of the expression, and clicking Insert Function will add the selected function to the expression with the highlighted section as an argument.

Also, Undo/Redo functionality is available by pressing Ctrl+Z.

Note: Very long expressions will be displayed truncated in the Visualization Legend. To avoid this, insert a blank space with suitable distance. This will not affect the expression, but will allow the Legend to display it over several rows.

Color

Select the color of the curve by clicking on this button.

Width

Select the width (in pixels) of the curve by clicking on this drop-down list.

Status

This field shows if the current expression is valid or not. If the expression is correct, then **OK** will be shown.

If this field shows an **#EXPR!** error, there is a problem with the syntax of the expression. Moving the mouse pointer over the field or clicking on it, will display an explanation of what is wrong. Pressing **F5** will also display the error description. Pressing **F4** will move the cursor to the position in the expression where the error lies.

Redraw curve while typing

If this check box is selected, the curve will be drawn and updated in the plot while you edit the expression. This is useful to verify that the curve actually looks like you intended, but if you are using very large data sets and complex expressions for the curve, it may be a good idea to turn it off in order to improve performance.

4.8.2.5.6 Curve Fit

4.8.2.5.6.1 Curve Fit

Curve fit (regression analysis) allows you to summarize a collection of sample data points by fitting them to a model that will describe the data and display a curve or a straight line on top of a scatter plot or a pie chart. Unlike the Curve feature, Curve Fit is not a fixed curve, but rather a line that can be changed upon changing the input data during filtering or zooming.

Curve fitting can be used either to determine the parameter values of a known regression model or to find a model that fits the data better than other models.

Tip: If a curve fit is active and the Legend is visible, information about the curve fit will be displayed there. Select **View > Legend** to display it. More information is also available via View Result, see below.

Transformations

The x and y values are unaffected by transformations, but the mapping onto the plot will be affected. This means that a straight line equation such as y(x) = x, will turn into a curve if the X-axis column uses a Log transform.

Limitations on data

All types of input data cannot be used to calculate curves using all different types of models. All models require:

- more than one data point to use in the calculation
- that not all data points have the same x- and y-values (lie on top of each other)
- that not all data points have the same x-value

In addition, the logarithmic model, the power model and the logistic regression model require that all data points have positive x-values. The power model also requires that all y-values have the same sign (positive or negative).

The logistic regression requires that no values are lower than the specified min value or higher than the specified max value and that not all data points have the same y-value. If any of the above limitations occur, no curve will be drawn, and an error message will be displayed in the Legend.

User Int	erface
-----------------	--------

irve Fit		
Model:		
Logistic Regression		Properties
Base calculation on	_ Line — —	
Selected records	Color:	- I
O All records	Width:	2
Trellis plot options Create separate statistics for	each trellis pan	el
C Create statistics based on er	ntire visualization	ı
		View Result
Help Apply	ОК	Cancel

Model

Specifies the type of curve to display in your visualization. Choose from:

Straight Line	y=a+bx
Logarithmic	y=a+blnx
Exponential	y=ae ^{bx}
Power	y=ax ^b
ogistic Regression	y=min+(max-min)/(1+(X50/x) ^{Hill})
2nd order Polynomial	y=a+bx+cx ²
3rd order Polynomial	$y=a+bx+cx^2+dx^3$
4th order Polynomial	$y=a+bx+cx^2+dx^3+ex^4$
5th order Polynomial	$y=a+bx+cx^2+dx^3+ex^4+fx^5$

See Curve Fit Models for more information.

Properties...

Available for Logistic regression only. Lets you specify values for max and min. If no values are specified, they will be automatically calculated.

Note: If you specify max and min values within the range of your data, you must filter out all data points outside of your specified range using the query devices or zooming in order to obtain a curve. (For example, no curve will be calculated if the min value equals the lowest value of y in your data set, unless you filter out this value and base the calculation on selected values only.)

Base calculation on

Specifies whether the statistical measure should be calculated based on all records in the data set regardless of any filtering done with the query devices, or whether the calculation should be based on the selected records so that filtering with the query devices will affect the result.

Color

The color of the displayed line.

Width

The width (in pixels) of the displayed line.

Trellis plot options

Specifies whether the curve fit displayed in each trellis panel will be calculated based on only the records specific to that trellis panel, or if the fit will be based on all records regardless of trellis condition and therefore be the same for every trellis panel.

View Result

Opens the Curve Fit: Result dialog, where detailed results from the fit is shown and can be copied into other applications.

Apply

Applies the curve fit to the visualization. Allows you to test one or many curve fits in your visualization without having to close the Curve Fit dialog.

4.8.2.5.6.2 Curve Fit: Result Dialog

The Curve Fit Result dialog displays detailed information about all curve fits that were enabled when you clicked on the button. Click on a specific curve fit in the Visualizations tree to view its details.

Tip: Select all text in the gray part of the dialog and copy the information, if you want to include the results in a report.

Ourve Fit: Result				×
⊡ Visualizations i= Scatter Plot Straight Line 2nd order Polynomial	 Curve Fit, Straig y = a + b*x y = -11.35 + 46.76*x R2 = 0.8941 	ht Line, using selecte	d records only	
⊡····· Scatter Plot	Name	Value	StdDev	
Logistic	a	-11.35	7.873	
Hegression	Ь	46.76	4.646	
Help				<u>C</u> lose

User Interface

The left pane shows a tree view of the different visualizations that have one or more curve fits applied. Click on the desired curve fit to view the details in the right pane of the dialog.

The right pane displays detailed information about the used equations and parameters of the selected curve. See Curve Fit Theory and Curve Fit Models for more information about the various parameters.

To reach the Curve Fit: Result dialog:

Right-click in the scatter plot or pie chart where you have applied a curve fit and select **View Curve Fit Result** from the pop-up menu.

Tip: You can also reach this dialog from the Curve Fit dialog, e.g., if you are testing several different curves using the Apply-button. In the Curve Fit dialog, click on the **View Result** button to display the results.

4.8.2.5.6.3 Curve Fit Models

There are several different models available for curve fitting. See Curve Fit for information about how to apply the various curves. The Curve Fit models below can be used when there is no randomness for the markers along the X-axis.

Straight Line

The straight line fit is calculated by choosing the line that minimizes the least square sum of the vertical distance \mathbf{d} , of all the selected markers (see picture below) by using the following equation:

y = ax + b

where a is the slope and b is the intercept.

For example, you could plot days along the X-axis and have one marker for each day. The distance between the markers along the X-axis is the same, thus making straight line fit appropriate.



Logarithmic

The logarithmic fit calculates the least squares fit through points by using the following equation:

 $y = a + b \ln x$

where a and b are constants, and ln is the natural logarithm function. This model requires that x>0 for all data points. DecisionSite uses a nonlinear regression method for this calculation. This will result in better accuracy of the calculation compared to using linear regression on transformed values only.

Exponential

The exponential fit calculates the least squares fit through points by using the following equation:

 $y = ae^{bx}$

where a and b are constants, and e is the base of the natural logarithm.

Exponential models are commonly used in biological applications, e.g., for exponential growth of bacteria. DecisionSite uses a nonlinear regression method for this calculation. This will result in better accuracy of the calculation compared to using linear regression on transformed values only.

Power

The Power fit calculates the least squares fit through points by using the following equation:

 $y = ax^{b}$

where a and b are constants. This model requires that x>0 for all data points, and either that all y>0 or all y<0. DecisionSite uses a nonlinear regression method for this calculation. This will result in better accuracy of the calculation compared to using linear regression on transformed values only.

Logistic Regression

The logistic regression fit is a dose response ("IC50") model, also known as sigmoidal dose response. The four parameter logistic model is the most important one.

Dose-response curves describe the relationship between response to drug treatment and drug dose or concentration. These type of curves are often semi-logarithmic, with log (drug concentration) on the X-axis. On the Y-axis one can show measurements of enzyme activity, accumulation of an intracellular second messenger or measurements of heart rate or muscle contraction.

The current implementation of the logistic regression fit uses the following equation:

$$y = \min + \frac{\max - \min}{1 + \left(\frac{X50}{x}\right)^{\text{Hall}}}$$

where min and max are the lower and upper asymptotes of the curve, Hill is the slope of the curve at its midpoint and X50 is the x-coordinate of the inflection point (x, y). This model requires that x>0 for all data points and that you use at least four records to calculate the curve.



Note: The logistic regression model of DecisionSite does not assume logarithmic values of x and X50, unlike some other curve fitting software. Hence, if your input data is logarithmic you might want to create a column that is not logarithmic before you apply the logistic regression curve fit, in order to obtain similar results to the ones you are used to. (For example, by using Data > New Column > By Expression.) If you want the curve to be displayed on a logarithmic form, right-click in the Query Devices window and select Set Property > Log Scale.

2nd order Polynomial

The second order polynomial fit, or quadratic curve, calculates the least squares fit through points by using the following equation:

 $y = a + bx + cx^2$

where a, b and c are constants. This model requires that you use at least three records to calculate the curve.

3rd order Polynomial

The third order polynomial fit calculates the least squares fit through points by using the following equation:

 $y = a+bx+cx^2+dx^3$

where a, b, c and d are constants. This model requires that you use at least four records to calculate the curve.

4th order Polynomial

The fourth order polynomial fit calculates the least squares fit through points by using the following equation:

 $y = a + bx + cx^2 + dx^3 + ex^4$

where a, b, c , d and e are constants. This model requires that you use at least five records to calculate the curve.

5th order Polynomial

The fifth order polynomial fit calculates the least squares fit through points by using the following equation:

 $y = a+bx+cx^{2}+dx^{3}+ex^{4}+fx^{5}$

where a, b, c, d, e and f are constants. This model requires that you use at least six records to calculate the curve.

If you have a low number of unique x-values, a polynomial curve can be calculated in an unlimited number of ways. This means that you may end up with a curve that does not look like expected. If this should happen, you probably should not apply this model to your data. The polynomial models have all been partially solved by using the LAPACK software package, see References.

4.8.2.5.6.4 Curve Fit Theory

Generally, curve fit algorithms determine the best-fit parameters by minimizing a chosen merit function. In order to optimize the merit function, it is necessary to select a set of initial parameter estimates, and then iteratively refine the merit parameters until the merit function does not change significantly between iterations. The Levenberg-Marquardt algorithm has been used for nonlinear least squares calculations in the current implementation.

The goodness of fit is shown as an R2-value. A value of R2=1.0 indicates a perfect fit, whereas R2=0.0 indicates that the regression model might be unsuitable for this type of data.

The standard deviation (StdDev) shown in the Curve Fit: Result dialog is the standard deviation of the differences between the actual data points and the calculated curve. It approaches 0 if the selected model accurately describes the data.

R2

The R2-value measures how much of the variation in the data points that can be explained by the selected regression model:

where

$$SSR = \sum_{i=1}^{n} (\hat{Y}_{i} - \overline{Y})^{2}$$
(the regression sum of squares)
$$SSE = \sum_{i=1}^{n} (Y_{i} - \hat{Y}_{i})^{2}$$
(the residual or error sum of squares)

 $SST = \sum_{i=1}^{n} (Y_i - \overline{Y})^2$ (the total sum of squares, SST= SSE+SSR)

and \hat{Y}_i represents the ith fitted value (calculated using the selected model) of the dependent variable Y.

Limitations to curve fitting

Since the calculation of the curve is an iterative process, the calculation must stop somewhere. In some cases the maximum number of iterations might be reached before the best possible curve has been calculated. In that case, a message will inform you of this in the Legend (select View > Legend to display it). In some cases, for example if the data is widely scattered or too few data points are available, the iterative process might also result in a curve that converges on a false minimum.

When a model is applied during data analysis, it is important not only to look at the R2-value and how well the curve fits the current markers in the scatter plot. It is also good to consider

what the curve would look like for more extreme values and determine if the model is reasonable in a scientifical or statistical context. The number of unique x-values must be larger than, or equal to, the number of degrees of freedom in order to obtain a unique curve. If the curve can be solved in an infinite number of ways, it is not sure that the presented curve will be relevant to your data.

References

Heath, M.T., (2002), Scientific Computing: An Introductory Survey, 2nd ed., McGraw-Hill, New York.

Anderson, E., Bai, Z., Bischof, C., Blackford, S., Demmel, J., Dongarra, J., Du Croz, J., Greenbaum, A., Hammarling, S., McKenney, A., Sorensen, D., (1999), LAPACK Users' Guide, 3rd ed., Society for Industrial and Applied Mathematics, Philadelphia, PA, ISBN = 0-89871-447-8

4.8.2.6 Reference Lines in Bar Chart

4.8.2.6.1 Reference Line Dialog

This dialog is used to create vertical reference lines in a bar chart.

Reference Line		×	
Line Position			
Expression: x =			
150		Edit	
Result: 150			
Line Settings			
Line style:			
So	olid 💽 🔽	2 🔽	
Transparency:			
	j		
Place line in:			
Foreground	•		
T			
Show label:			
(expression	1): (value)	Te <u>m</u> plates ▼	
 Horizontal 	C Vertical		
_			
Adjust data rang	e to include line		
Help	UK	Lancel	
Ontion	Description		
option	Description		
Expression	Type the expression ye	ou want to be pres	sented as a reference line i

	the text field. If you want a line drawn at a specific number, you simply type that number in the text field. You can also type more complicated expressions, including a number of functions and variables such as mean and median directly in the field. For more information about the available functions and variables, click on Edit (see below). Note that variables such as median and mean are always calculated on all data and not on the data filtered by the query devices or zooming.
Edit	Opens the Edit Expression dialog, where you can combine different variables and functions into an expression, as well as read a short description of all available functions.
Result	Displays the result of the expression.
Line style	Allows you to change the color, style and line width of the reference line.
Transparency	Allows you to change the transparency of the reference line. A completely solid line is obtained by moving the thumb to the far right.
Place line in	Determines whether the line should be placed in the Foreground or in the Background of the bars.
Show label	Select this check box to show a label for the reference line. Clear the check box to remove the label. You can type a label text directly in the text field or, you can use one of the available templates, see below.
Templates	Displays a drop-down menu from where you can select a template for how the label should be presented. Choose from Value (which simply shows the x-axis value of the reference line), Expression (which shows the expression, e.g., "median+150"), Expression: Value (e.g., "median+150:328") or Display Name (which shows the name of the reference line as it is presented in the legend (e.g., "Vertical reference line: x = median+150").
Horizontal	Click this radio button for a horizontal label.
Vertical	Click this radio button for a vertical label.
Adjust data range to include line	Select this check box to adjust the data range so that the reference line becomes visible even if it is outside the data range for the current data set.

► To reach the Reference Line dialog:

- 1. Create a bar chart with a continuous column on the X-axis.
- 2. Select Edit > Properties.
- 3. Go to the **Data and Background** tab.
- 4. Click on Add and select Vertical Reference Line... from the drop-down menu.

4.8.2.6.2 Edit Expression Dialog

dit Expression	×
Variables: firstQuartile max	Function category:
mean median min stddev sum thirdQuartile	Function:
Insert Variable	Adds the two arguments. Example: 3.5 + 2.5
Expression: median+150	<u> </u>
	V
Target type: Real	Result: 328
Recent expressions: 1+4	✓ Insert
Help	OK Cancel

Option

Description

Variables	Lists the available variables which can be used to create your expression. Insert a variable into your expression with the Insert Variable button.
Function	Select a category of functions to limit the choices in the Functions list:
category	All
	Operators
	Math Functions
	Statistical Functions
	Text Functions
	Logical Functions
	Date & Time Functions
	Conversion Functions
Function	Select a function by clicking on it, and click the Insert Function button to insert it to the Expression field. You can also double-click on a function to insert it.
	If you place the cursor at a specific location in the Expression field, the function will be inserted there.

Description	Provides a brief description of the selected function. For more detailed descriptions, please see Spotfire Expression Language (SXL).
Expression	This is the text field in which you build your expression. You can insert variables and functions to it from the lists, or enter text as in any standard text editor.
	Cut/Copy/Paste works in the field using standard Ctrl+X / Ctrl+C / Ctrl+V .
	Highlighting a section of the expression, and clicking Insert Function will add the selected function to the expression with the highlighted section as an argument.
	Also, Undo/Redo functionality is available by pressing Ctrl+Z . Note: Very long expressions will be displayed truncated in the Visualization Legend. To avoid this, insert a blank space with suitable distance. This will not affect the expression, but will allow the Legend to display it over several rows.
Target type	Displays the data type of the result.
Result	This field displays the result of applying the current expression to the data set.
	If this field shows an error message, then there is a problem with the expression. Clicking on the field will display an explanation of what is wrong. Pressing F5 will also display the error description. Pressing F4 will move the cursor to the position in the expression where the error lies. There are three kinds of error messages:
	#EXPR! – there is a problem with the syntax of the expression.
	#NUM! - the expression evaluates to infinity or other illegal number.
	#ARG! – there is a problem with one or many arguments.
Recent expressions	This list contains the fifteen most recent expressions you have created.
Insert	Inserts the selected recent expression to the cursor position of the expression field.

4.8.3 Columns Tab

4.8.3.1 Columns tab

Edit > Properties > Columns tab

perties:	The depo	osit of	heavy m	etals ov	er Sweden			×
Trell Annotati	is ons	 Data	Axes and Back	 ground	3D Column:	s	Markers Details Columns	
Column: Column Chrome Copper Lead InChrome InCopper InLead Nickel Vanadin X Y	Type Integer Integer Integer Integer Integer Integer Integer Integer Integer	V 16 108 133 444 45 33 43 80 124 120 293	Visibility Hidden Visible Visible Visible Visible Visible Visible Visible Visible Visible	Index 4 5 7 10 6 8 11 9 12 1 2	Query Devir Full text set Radio butto Range slide Range slide Range slide Range slide Range slide Range slide Range slide Range slide		Query device type Check boxes Radio buttons Range slider Item slider Full text search Show empty value Show / Hide Rename Column	s
Annotation Indicator	: s w indicato	rs in qu	ery device:	\$	×		Format Scale Scale Delete Columns	

This dialog is used to set column properties columns—how they are viewed, what query device to associate with the column, annotations, name, scale, etc.

Option	Description
Column	Lists all the existing columns in the data set. Select a column name and use the controls described below to control that column. Click on the headers (e.g., Column, Type, etc.) to sort the columns accordingly.
Annotation	Enter any text that you want to associate with this column. This text will appear when you place the mouse pointer over the paper clip icon next to a query device.
Show indicators in query devices	Displays a paper-clip icon in the upper right corner of the query device when the column has an annotation, and displays the letter 'e' when the column contains empty values.
Query device type	Shows what query device type is assigned to the selected column in the list.
Show empty values	Shows (or hides) all records were a value is missing in the selected column.
Show/Hide	Toggles the query device associated with this column.
Rename Column	Allows you to enter a new name for the column.
Format	Configures how to display the format for various columns (Number Formatting, Date and Time Formatting, Date Formatting or Time Formatting). For example, how to represent negative values, number of decimal digits, etc.

	Select one or more columns from the list, click the Format button, and select a formatting option to access the formatting dialog.
	Note: Formatting may change the perceived type of a column. For example, a date column will be presented as a string column when week day formatting is applied. See Rearranging the Data by Formatting for more information.
	Selecting Format > None from the drop-down menu, resets the options to the default settings.
Scale	Sets the scale of the selected column or columns when mapped to an axis in the visualization. Scale options: Original , Ln (1+x), Log , Exp , Exp10 , Inverse Scale , and Reverse sorting .
New Column	Adds a new column either by Binning or from an Expression.
Delete Columns	Deletes the selected column from memory. The underlying file is not affected unless you save the data set.

This dialog can also be accessed by double-clicking in the upper right corner of any query device.

4.8.3.2 Annotating Columns

Edit > Properties > Columns tab

It is possible to annotate individual columns. This text will appear when you place the mouse pointer over the paper clip next to a query device.

To enter an annotation for a column:

- 1. Go to the Columns tab of the Properties dialog.
- 2. Select a column.
- 3. Enter your text in the Annotation field.

You can also edit annotations for a column by double-clicking the paper-clip next to the corresponding query device, or by selecting **Edit Annotations...** from the query device pop-up menu.

4.8.3.3 Transforming Axis Scale

A numerical column can be set to display its values using a variety of scales instead of the linear scale, which is default: Natural Log Scale (Ln (x+1)), Logarithmic Scale (Log), Exponential to the bases of e (Exp) and 10 (Exp10), Inverse Scale (1/x), and Reverse Scale. The last option changes the sort order for the selected column. This is accomplished by right-clicking on the query device representing the column, and from the **Set Property** sub-menu selecting the transformation desired.

Another way to change the scale is from the **Columns** tab of the **Properties** dialog, by marking the column to rescale and selecting the transformation from the Set Scale pull down box.

Properties: Correlati	ion		×
Trellis	Axes	3D	Markers
Annotations	Data and Backgrou	nd Columns	Details Columns
Column:			– Quero device tope –––
Column	Туре	Vā 🔺	Check boxes
Customer age Total	Integer Integer		C Radio buttons C Range slider
	String		C Item slider
Recency Date joined	Date Date		C Full text search
First buy Number of purchas	Date es Integer		Show empty values
Business location Groceries	String Integer	-	Show / Hide
liarden ■		Þ	Rename Column
Annotation:		-	Format 🔻
			Scale 🔻
		-	Original Scale
- Indicators	Ln(1+x) Scale		
Show indicato	Log Scale		
	Exp Scale		
			Exp10 Scale
			Inverse Scale
			Reverse Sorting

The transformation can be removed and the scale reset to linear by choosing Original Scale.

4.8.3.4 Number Format

You can specify how you want DecisionSite to display number formatting for integer and decimal columns. You can set the number of decimal digits, how to display negative numbers, to display numbers using scientific notation, select whether or not to use thousands separators, and also add a currency symbol to be displayed together with the actual value.

Note: If you prefer, you can set default number formatting for all Integer type columns and all Decimal type columns, instead of specifying this for each column individually. Such default settings will be applied every time you open a new data set in DecisionSite Client. Default settings are made in the Fonts & Numbers tab of the Options dialog.

► To set Number Formatting for a column:

- 1. Open the **Properties** dialog by selecting **Edit** > **Properties** and click on the **Columns** tab.
- 2. Select one or more columns you wish to set number formatting for.
- 3. Click on the **Format** button.

4. Select Number... which opens the Number Format dialog.

Number Format	X
Number of decimal digits:	2
Negative numbers:	-123
C Scientific notation	
🔲 Use thousands separator	
Currency symbol	
Left: \$	Right:
Example	
\$-123	34567.12
Help	OK Cancel

- 5. Specify the Number of decimal digits and how to display Negative numbers.
- 6. Specify whether or not you wish to display the numbers in **Scientific notation.** (For example: 1,23E+006.)

Note: When using Scientific notation, the Use thousands separator check box is cleared and grayed out, as it is no longer applicable.

- Decide whether or not to Use thousands separator. Note: The symbol used for thousands separator and decimal separator is determined by the Windows Locale setting.
- 8. If desired, enter **Unit labels** in the **Left** or the **Right** text field.
 - Comment: This could be a currency symbol or any other unit. The maximum length is 12 characters.
- 9. Click OK.

Selecting **Format** > **None** from the Format drop-down menu, resets the options to the default settings.

4.8.3.5 Date and Time Format

You can specify how you want DecisionSite to display date and time formatting for time stamp columns. You can set the date and time to be shown either according to regional settings, with or without milliseconds, or according to a number of other date and time formats.

By changing the date format for a date or time stamp column, you can obtain a whole new set of factors to filter your data by. See Rearranging the Data by Formatting for more information.

To set Date and Time Formatting for a column:

- 1. Open the **Properties** dialog by selecting **Edit** > **Properties** and click on the **Columns** tab.
- 2. Select one or more columns you wish to set time formatting for.
- 3. Click on the **Format** button.

4. Select Date and Time... which opens the Date and Time Format dialog.

Date and Time Format				
Туре:				
According to regional settings According to regional settings, long format According to regional settings, with milliseconds if available				
ISO formatted (YYYY-MM-DD HH:MM) ISO formatted, with seconds (YY-MM-DD HH:MM:SS) ISO formatted, with milliseconds (YYY-MM-DD HH:MM:SS.fff)				
ISO formatted, with milliseconds if available (YYYY-MM-DD HH:MM:SS[.ff] Excel compatible formatted, with milliseconds (YYYY-MM-DD HH:MM:SS.I Two digit year (YY-MM-DD HH:MM)				
Two digit year, with seconds (YY-MM-DD HH:MM:SS) Two digit year, with milliseconds (YY-MM-DD HH:MM:SS.fff) Compact (YYMMDD HHMM)				
Sample:				
2007-09-17 13:21:32				
Help OK Cancel				

5. Click on a format type.

Response: An example of what the selected date and time format would look like is shown in the Sample field.

6. When you are satisfied with the selected format, click **OK**.

Selecting **Format > None** from the Format drop-down menu, resets the format to the default setting.

Tip: If you want to change the date and time formatting for a single column you can also reach the Date and Time Format dialog from the pop-up menu of the Query Devices panel. Rightclick on the column of interest and select **Set Property > Format > Date and Time...** from the pop-up menu.

4.8.3.6 Date Format

You can specify how you want DecisionSite to display date formatting for time stamp columns. You can set the date to be shown either according to regional settings or according to a number of other date formats.

By changing the date format for a date or time stamp column, you can obtain a whole new set of factors to filter your data by. See Rearranging the Data by Formatting for more information.

► To set Date Formatting for a column:

- 1. Open the **Properties** dialog by selecting **Edit** > **Properties** and click on the **Columns** tab.
- 2. Select one or more columns you wish to set date formatting for.
- 3. Click on the **Format** button.
4. Select Date... which opens the Date Format dialog.

Date Format
Туре:
Date according to regional settings Date according to regional settings, long format USD formatted date (\CCCY-MM-DD)
Date with two digit year (YY-MM-DD) Compact date (YYMMDD) Compact date, with full year (YYYMMDD)
Year (YYY) Year, short (YY)
Year, week (ISO) (YYYYWww) Year, week (ISO) (YYYYWww) Year, day of year (YYYY-ddd)
Day of week, Monday first (day name)
07-09-17
Help OK Cancel

5. Click on a format type.

Response: An example of what the selected date format would look like is shown in the Sample field.

6. When you are satisfied with the selected format, click **OK**.

Selecting **Format > None** from the Format drop-down menu, resets the format to the default setting.

Tip: If you want to change the date formatting for a single column you can also reach the Date Format dialog from the pop-up menu of the Query Devices panel. Right-click on the column of interest and select **Set Property > Format > Date...** from the pop-up menu.

4.8.3.7 Time Format

You can specify how you want DecisionSite to display time formatting for time and time stamp columns. You can set the time to be shown either according to regional settings, with or without milliseconds, or according to a number of other time formats.

By changing the time format for a time column, you can change the number of unique values in your data set. See Rearranging the Data by Formatting for more information.

To set Time Formatting for a column:

- 1. Open the **Properties** dialog by selecting **Edit** > **Properties** and click on the **Columns** tab.
- 2. Select one or more columns you wish to set time formatting for.
- 3. Click on the **Format** button.

4. Select **Time...** which opens the Time Format dialog.

Time Format
Туре:
Time according to regional settings Time according to regional settings, with milliseconds if available 24 hour time (HH:MM) 24 hour time with seconds (HH:MM:SS) 24 hour time with milliseconds if available (HH:MM:SS.ff) 24 hour time with milliseconds if available (HH:MM:SS.ff) 24 hour time with two decimals (HH:MM:SS.ff) 24 hour time with one decimal (HH:MM:SS.ff) Compact 24 hour time (HHMM) Compact 24 hour time with seconds (HHMMSS) Compact 24 hour time with milliseconds (HHMMSS) 24 hour time, hour only (HH)
Sample: 08:05:03.180
Help OK Cancel

5. Click on a format type.

Response: An example of what the selected time format would look like is shown in the Sample field.

6. When you are satisfied with the selected format, click **OK**.

Selecting **Format > None** from the Format drop-down menu, resets the format to the default setting.

Tip: If you want to change the time formatting for a single column you can also reach the Time Format dialog from the pop-up menu of the Query Devices panel. Right-click on the column of interest and select **Set Property > Format > Time...** from the pop-up menu.

4.8.4 Trellis Tab

4.8.4.1 What is a Trellis plot?

Trellis plots enable you to quickly recognize similarities or differences between different subsets. Trellis plots provide the means to create a systematic layout for scatter plots, bar charts, profile charts and heat maps. Each individual pane in a Trellis plot displays a subset of the original data set, where the subset is defined by certain *conditions*. By this we mean that all the records in a particular subset have the same value for one or more attributes. A condition specifies one attribute.



A Trellis plot is a way of breaking up a visualization (scatter plot, profile chart or heat map) into several panels, each one displaying a particular sub set of the data. The example above displays a Trellis plot with two conditions: Sex and Dead/Alive.

► To create a Trellis plot:

- 1. Create a new scatter plot, profile chart or heat map.
- 2. Open the **Properties** dialog.
- 3. Go to the **Trellis** tab.
- 4. In the Conditions box, click Add...
- 5. In the **Trellis condition** dialog, select the variable (column name) by which you want to separate the plots.
- 6. Click OK.

4.8.4.2 Trellis Tab

Edit > Properties > Trellis tab

Properties: Correlation			×
Annotations [Trellis]) ata and Background Axes	Columns 3D	Details Columns Markers
Conditions	Values	Rind To	
Gender	2	Columns	Edit
			Move Down
Layout Bind dimensions to Columns: 2 Rows: 1 Pages: 1 Drop empty panels	Description	Headings Show hea Text: Background: Indicator:	idings
Conditions	A condition specifies a variable by which the data is divided into subsets. Each value of the conditioning variable will yield a separ subset. Adding a second condition will split each subset, etc.		
Layout	 ayout You can control the layout of the plots in terms of rows, column and pages. There are two ways of doing this: Automatically, by binding a dimension to each conditioning variable. Manually, by specifying the exact dimensions of the Trellis plot You can also select whether or not to show empty trellis panels clearing or selecting the Drop empty panels check box 		
leadings	Specifies whether or P You can also change	not to show head the colors used in	ings. 1 the headings.

4.8.4.3 Trellis Conditions

Edit > Properties > Trellis tab

A condition specifies a variable by which the data is divided into subsets. Each value of the conditioning variable will yield a separate subset. Adding a second condition will split each subset, etc.

If, for example, two Boolean variables are used as conditioning variables, this will result in four separate plots representing the combinations True-True, True-False, False-True and False-

False. If a Boolean variable is used in conjunction with a variable that has five different values, this will yield ten plots. From this follows that variables with a continuous distribution and a wide range of values (e.g. Real values) should be binned before forming a Trellis plot. Otherwise the number of plots quickly becomes unmanageable.

To add a condition:

- 1. In the Properties dialog, under the Trellis tab, click Add...
- 2. In the Trellis condition dialog, select a variable and a dimension to bind it to.
- 3. Optionally, use the radio buttons in the **Heading** box to control what information to show in the heading for this variable.
- 4. Click **OK**.

T	ellis condition
Γ	Condition
	Variable: Bioavailability
	Bind to: Rows
	Show empty values
[Heading
	C Show variable name
	C Show variable value
	Show variable name and value
Ļ	Help OK Cancel

Empty values

Selecting the **Show empty values** option will generate an extra trellis panel containing records for which the conditioning variable is undefined.

► To remove a condition:

- 1. Select a condition from the list on the **Trellis** tab.
- 2. Click Remove.

► To modify an existing condition:

- 1. Select a condition from the list.
- 2. Click Edit...
- 3. In the **Trellis condition** dialog, make the desired changes.
- 4. Click OK.

To change the order of conditions:

- 1. Select a condition from the list.
- 2. Click Move up or Move down.

Tip: The settings in the Trellis condition dialog can also be reached and changed by rightclicking on any trellis panel heading.

4.8.4.4 Trellis Layout

Edit > Properties > Trellis tab

You can control the layout of the plots in terms of rows, columns and pages. There are two ways of doing this:

- Automatically, by binding a dimension to each conditioning variable.
- Manually, by specifying the exact dimensions of the Trellis plot.



Example of three conditioning variables bound to rows, columns and pages.

► To arrange the plots automatically:

- 1. In the **Properties** dialog, under the **Trellis** tab, make sure the check box labeled **Bind dimensions to conditioning variables** is selected.
- 2. Click Add....
- 3. In the Trellis Condition dialog, select a variable and a dimension to bind it to. Comment: If Bind to: Columns is selected, all trellis panels will be displayed side by side with the title at the top. If Bind to: Rows is selected, the trellis panels will be under each other with the title on the right hand side of all rows. If Bind to: Pages is selected, each trellis panel will be displayed on a separate page and you will have to scroll down to see all panels.
- 4. Repeat steps 2 and 3 for any additional conditions.

Tip: Experiment with different layouts while still in the Trellis Condition dialog. The visualization is updated dynamically, so you can immediately see the results of your current settings.

► To set layout manually:

- 1. In the **Properties** dialog, under the **Trellis** tab, make sure the check box labeled **Bind dimensions to conditioning variables** is cleared.
- 2. Enter the number of trellis panels that you want to show next to each other simultaneously, both horizontally (columns) and vertically (rows). The number of pages is automatically updated to make sure there is room for the specified panels you can never change the number of pages directly.

4.8.4.5 Trellis Headings

Edit > Properties > Trellis tab

Show Headings

You can select whether or not to show trellis panel headings from the **Trellis** tab of the **Properties** dialog. Select the check box to show all headings. Clear the check box to hide all headings. You can also right-click on any trellis panel header and select **Heading > Hide All Headers** from the pop-up menu.

Heading Color

The colors used in the headings of columns, rows and pages can be set manually from the **Trellis** tab of the **Properties** dialog.

Text is the color of the text in all headings.

Background is the background color of all headings.

Indicator is the color of the bar that indicates the relative size and position of the range of values.



Note: The indicator bar represents the size of the range of values represented by a column, row or page, not the number of records with that value.

Heading Text

What to show in the heading text is specified from the Trellis condition dialog, reached by clicking Add... or Edit... on the **Trellis** tab of the **Properties** dialog. You can specify which of three options should be shown as the heading for the trellis panels.

- Show variable name
- Show variable value
- Show variable name and value

4.8.4.6 Empty Panels

It is possible to insert empty panels anywhere in the layout. This can be useful when manually configuring a multi-page layout. Normally in such a layout, a page flows to the next as soon as it is full. This may not always be appropriate.

Consider, for example, a situation with twenty-four panels arranged in a three-by-three layout. This would yield two pages with nine panels on each, and a final page with only six panes. By inserting an empty panel on each page, the result would be three pages with eight (non-empty) panels on each.

► To insert an empty panel:

- 1. In the **Trellis** tab of the **Properties** dialog, make sure **Bind dimensions to conditioning variables** is cleared.
- 2. Right-click in the heading field of the panel were you want the empty panel to be inserted.
- 3. Select Insert Empty Panel.

If an empty panel is inserted on the first page, it will appear at the same position on each subsequent page. An empty panel inserted on the second page will appear on even pages, etc.

You may also be in the situation where some of the combinations of variables used for the trellis panels result in panels without any records. These panels can easily be hidden.

► To hide empty panels:

- 1. Right-click in the heading field of any trellis panel.
- 2. Select **Drop Empty Panels** from the pop-up menu.
 - Comment: You can also select the Drop empty panels check box in the Layout field of the Trellis tab in the Properties dialog.

4.8.5 Axes Tab

4.8.5.1 Axes Tab

Edit > Properties > Axes tab

Axis labels for Scatter Plots are controlled from the **Axes** tab of the **Properties** dialog. For other plots see Axes.

Annotations Data and Background Columns Details Columns Trellis Axes 3D Markers Axis: Y Axis [Total] Range Min: -1314.375 Max: 57039.375 Default Ticks © Automatic Settings © Interval Every: 10000 From: 0 Fixed 0:10000;20000;30000;40000;50000; Grid Image: Show gid lines	Properties: Correlation				×
Axis: Y Axis [Total] Range Min: -1314.375 Max: 57039.375 Default Ticks Automatic Settings Automatic Settings Interval Every: 10000 From: Fixed ():10000;20000;30000;40000;50000; Grid Grid Show gid lines 	Annotations Trellis	Data and Background Axes	Colum 3D	ns Details Columns Markers	
Ticks ● Automatic Settings ● Interval Every: 10000 From: 0 ● Fixed 0;10000;20000;30000;400000;50000; Labels ● Horizontal ● Vertical Grid ♥ Show grid lines	Axis: YAxis (Tot Range Min: -1314.375	al) Max: 5	7039.375	Default	
	Ticks C Automatic Settings Interval Every: 10000 From: 0 Fixed 0;10000;2000	0;30000;40000;50000;	Gric	rels Show labels I Horizontal Vertical Show grid lines	

Option Description

Axis

Select the axis whose labels you want to edit. All other settings made in the **Axes** dialog are specific to the axis you have currently selected here.

Range	The minimum and maximum values specify the range of the axis labels. Default will set the range to encompass the entire data range.
Ticks	 There are three options for tick mark control: Automatic – this option will attempt to display a suitable number of labels at even intervals. You can modify this somewhat by clicking the Settings button, which opens the Ticks dialog. Select the Spacing you want, and the number of Ticks to be displayed. For spacing you can select to show axis labels in four ways: Even Distribution – will attempt to distribute labels evenly between the highest and lowest value At Values – will not place a label where there is no value At Even Values – will place labels at all values At Even Values – will attempt to place labels at evenly spaced whole numbers. Interval – this option lets you specify an exact interval for the labels, which you enter in the Every field. You may also specify from which value the labels should be drawn, in both directions. For example, if you set Every: 10 and From: 1920, labels would appear in steps of -10 and +10 originating from the value 1920. Fixed – this option lets you specify the exact values for which you want labels to appear. Simply type the values into the field separated by a carries of a compared with 1020:1022:1022:1020:1055:1001
	This can also be used to specify the number of decimals to be shown on the axes.
	Another feature of the Fixed option is that you may name a tick mark to display a string instead of the value, like this: 0.0;3.14=Pi;5.0;10.0 which would display the text "Pi" as a label instead of 3.14.
Labels	The Show labels check box sets whether or not to display labels for the current axis. The Horizontal or Vertical radio buttons sets whether the labels for the current axis should be displayed horizontally or vertically.
Grid	The Show grid lines check box sets whether or not to display grid lines for the current axis.

4.8.6 3D Tab

4.8.6.1 3D Tab

Edit > Properties > 3D tab

Annotations	Data and Background	Columns	Details Columns
Trellis	Axes	3D	Markers
Dimensions			-
C 2D Plot			
3D Plot			
·			
Rendering		- Perspective	
🔽 Lighting		Less	More
🔲 Smooth shadi	ng		<u> </u>
Navigation			
🔽 Show boundir	ng box		
🔽 Show axes			
Quick navigation	if more than 1000 🔹	visible records	
			Reset Navigation

Option	Description
Dimensions	You can chose whether to display a 2D Scatter Plot or a 3D Scatter Plot by selecting the appropriate radio button. A 3D visualization can be 'flattened' into a 2D scatter plot or, conversely, a 2D plot can be made into one with 3D attributes. In the latter case Spotfire DecisionSite will suggest a third axis using the same algorithm as with 2D scatter plots.
Rendering	With the Lighting check box cleared, the glyphs will be flat, as if illuminated evenly from all sides, a sphere will appear as a filled circle and a cube from certain angles will look like a hexagon and from other angles like a square. The Smooth Shading alternative will smooth edges of adjacent polygons on the surface of the glyphs; mostly useful when the filled sphere is used, this makes the sphere appear rounder.
Perspective	The perspective slider modifies the 'field of view' of the 3D visualization. Using the mouse, drag the slider towards the right for a 'wide angle' perspective.
Navigation	This section provides various helpful settings for quicker navigation of the 3D scatter plot.

4.8.6.2 3D – Perspective

Edit > Properties > 3D tab



The perspective slider modifies the 'field of view' of the 3D visualization. Using the mouse, drag the slider towards the right for a 'wide angle' perspective. With the slider in the left-most position the view becomes orthogonal, a projection where the size of the markers is retained no matter the distance. The keyboard arrow keys allow fine-tuning of the perspective when the slider has been activated.



Orthogonal view (left) and exaggerated perspective (right).

Note: When viewing 3D plots the perspective view will make markers that are 'closer' to the viewer look bigger and so care must be taken if you also want size to reflect some attribute. Orthogonal projection where markers retain size irrespective of distance may be preferable.

4.8.6.3 3D – Navigation

Edit > Properties > 3D tab

Navigation			
🔽 Show bounding box			
🔽 Show axes			
Quick navigation if more than	1000 🚦	visible records	
			Reset Navigation

Option

Show bounding box	This draws a dotted cube around the edges of the visualization volume, which often aids in locating a marker in the 3D space.
Show axes	This draws the arrows representing the X, Y and Z axes.
Quick navigation if more thanvisible records	This lets you speed up rotation, zooming, etc by drawing markers as dots while navigating. Markers are restored to their normal shapes as soon as you stop navigating. Use this feature if the lag times become too great during 3D navigation.
Reset Navigation	This button resets the orientation of the visualization—X (horizontal), Y (vertical), and Z (depth)—but does not affect zooming or perspective.

Note: The Reset button in the toolbar will reset not only navigation, but also all query devices.

4.8.7 Markers Tab of the Scatter Plot

4.8.7.1 Markers Tab of the Scatter Plot

4.8.7.2 Markers Tab of the Scatter Plot

Edit > Properties > Markers tab

Annotations Data and Background	Columns Details Columns
Trellis Axes	3D Markers
Color By: gender Fixed Continuous Categorical Customize Show deselected Shape Fixed Customize Per value	Size Min Max By: weight (kg) Drawing order By: (None)
By: eye color	None 🚽 Max
Labels Dynamic labels: Customize	Rotate By: (None)
Static labels: Reset None Marked Visible, max 200 Reset By: height (m)	Line connection By: (None) Order: (None) Arrows indicating direction

Option	Description
Color	Markers can be colored to reflect the value of a particular attribute. There are three modes for coloring: Fixed, Continuous and Categorical.
Shape	The shape of markers can be fixed, or made to reflect the value of a particular column. Click Fixed or Per value to alternate between these modes.
Labels	It is possible to tag each marker with a label, showing the value of a particular column. You can select to show both Dynamic labels (Highlight and/or Active) and Static labels (None/Marked/Visible) at the same time. Dynamic labels are always placed on top of any static labels. The static labels include the following options:

	None – No labels are visible.
	Marked – Only records that are marked will have labels next to them.
	Visible, max – All visible records (up to a specified maximum number) will have labels next to them, provided that the number of visible markers does not exceed the specified max number. If so, no labels are shown.
	Select the column you wish to label by, from the drop-down list By:
	Click on Customize to open the Customize Labels dialog, where you can change the color and line width of the label frames and lines, as well as the size available to labels.
	You can drag labels to any position within the visualization area. Click on Reset to return all marker labels to their original position.
	If you are running DecisionSite for Lead Discovery, you can also select to display the chemical structure for each record in the label. This is done by right-clicking in the scatter plot and selecting Structure Marker Labels from the pop-up menu.
	Select Structure Marker Labels > Remove to revert to the column selected here.
Size	The size of markers can be made to reflect the value of a particular column. Select a column from the drop-down list under Size . Moving the slider changes the size of all markers, while maintaining the size ratio of different markers.
Drawing order	It is possible to specify the order in which the markers of a scatter plot will be drawn. This is done by specifying a column that will determine the drawing order.
	Note: By setting both Size by and Drawing order by to the same column, the smaller markers will be drawn on top of the larger ones.
Jitter	Jittering displaces markers slightly and randomly, thereby making aggregations stand out visually. Attention is brought to areas where many records overlap.
Rotate	The rotation of markers can be made to reflect the value of a column. Using asymmetrical markers and rotating them according to a chosen variable takes advantage of the human ability to visually detect regions with different surface structure.
Line connection	Line connection means that a line is drawn between records that share some property. To follow a progression, markers can also be connected in ascending order according to some other property. The order of lines can be made clearer by use of arrows indicating direction (pointing from lower to higher value in the Order column).

4.8.7.3 Color

Edit > Properties > Markers tab

Color	
By: Hits	•
C Fixed 🖲 Con	tinuous 🔿 Categorical
Customize	Show deselected

Option	Description
Fixed	Fixed coloring means that all markers are the same color (except deselected and marked).
Continuous	Continuous coloring means that the maximum and minimum specified values in the selected column are each assigned a color. Intermediate values are then assigned colors on a scale ranging between the two extreme colors. In scatter plots, any column can be used for continuous coloring. Any values not included in the range are given a specific color.
	Colors, representing minimum and maximum values are set with the Customize dialog. Begin and End categories define the color limits.
	When one of the categories is selected, you can choose which color will represent that end of the value range. A line with the color scale is displayed below the corresponding query device.
Categorical	Categorical coloring means that each value in the chosen column is given its own color. However, categorical coloring makes most sense if there are less than ten unique values. To control which color is assigned to each value, click Customize .
Customize Colors	Regardless of coloring mode, the choice of colors can be controlled by clicking Customize on the Markers tab of the Properties dialog. Depending on the current coloring mode, the top-most list will display the fixed color, Begin and End colors (continuous mode), or the color associated to each category (categorical mode). The other list displays colors associated with deselected, empty and marked records. ("Empty" refers to records for which no value is specified in the column used for coloring.)

Markers can be colored to reflect the value of a particular attribute. There are three modes for coloring: Fixed, Continuous and Categorical. The mode is set in the **Properties** dialog.

4.8.7.4 Overlapping Color Ranges

It is possible to specify overlapping color ranges. This means that the value of a marker can be inside several ranges, but the marker will always only have one color. DecisionSite uses the following method to determine which color range will be used to set the color of the marker: If the value of a marker is included in several ranges, the gradient with the highest start value is selected. However, if multiple gradients exist with the same low start value, the gradient with the lowest end value is selected.

Also note that categorical values are more important than continuous ones. In other words, if you have a value that you have set to a specific categorical color, this color will be used even if the value is also defined within a color range.

Example:

min max Add 1 227 Delete min+19 max-157 Marked: 20 70 Marked:]
min max ▲ 1 227 Delete min+19 max-157 ▲ 20 70 Marked:]
1 227]
min+19	1
20 70 Marked:	
min+19 v max-197 v	1
20 30 Empty:	
]
min+29	
]
Deselected:	
]
Templates - Import Export	
Help Advanced Close	
Advanced	

If you have set the Ranges as above:

- Value 1 is colored according to the first range.
- Value 20 is colored according to the third range.
- Value 30 is colored according to the last range.

When the dialog is opened the color gradients are sorted such that the highest priority is at the bottom, next highest just above that, and so on. If new gradients are added, the order is changed, but you can restore the order by right-clicking and selecting **Sort gradients**, which will cause the list to reflect the drawing order.

4.8.7.5 Shape and Rotation

Edit > Properties > Markers tab

Shape		
• Fixed	Customize	
O By: IrP1		

The shape of markers can be fixed, or made to reflect the value of a particular column. Click **Fixed** or **By** to alternate between these modes. Only columns with less than 23 distinct values can be used for controlling shapes. Click **Customize** to choose appropriate shapes for each value.

There are twelve shapes available for 3D markers:

Solid Cube	Wire Cube	Arrow (Pyramid)	Minus
Solid Sphere	Wire Sphere	Diamond	Bar
Solid Tetrahedron	Wire Tetrahedron	Cross	Point

These shapes consist of polygonal surfaces or lines. They all show shading and other '3D' characteristics. Some shapes are particularly useful in conjunction with rotation. It is possible to customize the shape and size of the markers in a scatter plot.

► To customize markers:

- 1. Open a scatter plot.
- 2. Select **Edit > Properties**.
- 3. Select the Markers tab.
- 4. Select a column to determine the shape of the markers.

Shape—			
C Fixed		Customize	
● By:	Sex	•	
	Fatigue		
-Labels-	Malaise		1
None	Anorexia Liverbig		

5. Click on **Customize**.



- 6. Select a value ("no", "yes" or "Empty" in the example above).
- 7. Select a shape for that value.
- 8. Select the **Specify size** check box. When this option is selected, the custom size overrides the usual size slider in the properties Marker tab.
- 9. Enter **Width** and **Height**.

These values are relative to the scale used in the current visualization. Look at the scale used in the current visualization and determine how large you wish your markers to be.

Note: The horizontal and vertical scale may be different, which means that a perfect square might not have the same Width and Height values.

Note: Use Reverse sorting if you want the markers to be drawn in the opposite order. Rightclick in the Query Device you wish to sort by, select Set Property and Reverse sorting.

Rotation

- <u>R</u> otat	e		1
By:	Age group	•	
			-

The rotation of markers can be made to reflect the value of a column. Using asymmetrical markers and rotating them according to a chosen variable takes advantage of the human ability to visually detect regions with different surface structure. The maximum rotation is 90 and so the most useful shapes for this effect are the arrow, the minus, and the bar.

In 3D plots, the marker rotation is implemented around the Z-axis.

4.8.7.6 **Jitter**

Edit > Properties > Markers tab

_ <u>J</u> itter]
None	Мах
J	

Jittering displaces markers slightly and randomly, thereby making aggregations stand out visually (below, right). Attention is brought to areas where many records overlap. Such regions can then be investigated further, by zooming, changing axes, etc. Use the slider to increase or decrease jittering.

Scatter plots, line charts, profile charts and pie charts support jittering.



4.8.7.7 Line Connection

Edit > Properties > Markers tab



Line connection means that a line is drawn between records that share some property. To follow a progression, markers can also be connected in ascending order according to some other property. The order of lines can be made clearer by use of arrows indicating direction (pointing from lower to higher value in the **Order** column). To demonstrate the usefulness of line connection, in the example data above, the locations of two salespersons, indicated by red and blue, are plotted. The two salespersons visit various locations at different points in time. Without the lines and arrows indicating direction, we would be unable to see in which order the blue salesperson visited the different locations.

Setting the **By:** selection to (None) causes the Line connections to disregard which individual salesperson went to what location, and will instead plot a timeline showing which locations were visited by any salesperson in order of the date the locations were visited:



4.8.7.8 User Interface

4.8.7.8.1 Fixed Coloring Dialog



Option	Description
Fixed	Shows the color of the markers in the data set.
Marked	Shows the color of the records that have been marked.
Empty	Shows the color of the empty records. Empty refers to records that have at least one empty field. These records are not shown at all in visualizations where an axis corresponds to the missing field.
Undefined	Shows the color of values that are not included in a range (continuous).
Deselected	Shows the color of the deselected values. Deselected refers to records that do not fulfill the constraints of the query devices.

4.8.7.8.2 Continuous Coloring Dialog

Continuous Coloring		×
Ranges:		
min 🔹	🖌 max 👻 🗾	Add
Boston	Seattle	Delete
		Marked:
		Empty:
		-
		Other:
		· ·
		Deselected:
Templates 👻	Import Export	
		Class
	Advanced	Liose

Option	Description
Ranges	Displays the values in the chosen column, and the color for each value. Note: When the dialog is opened the color gradients are sorted such that the highest priority is at the bottom, next highest just above that, and so on. If new gradients are added, the order is changed, but you can restore the order by right-clicking and selecting Sort gradients .
Add	Adds a new item to the list of Color ranges. Using this, you can assign specific colors to values, and create your own coloring arrangement.
Delete	Removes a selected value. Ctrl+click to select multiple items for deletion.
Marked	Shows the color of the records that have been marked.
Empty	Shows the color of the empty records. Empty refers to records that have at least one empty field. These records are not shown at all in visualizations where an axis corresponds to the missing field.

Other	Shows the color of values that are not included in a range (continuous).		
Deselected	Shows the color of the deselected values. Deselected refers to records that do not fulfill the constraints of the query devices.		
Templates >			
> Two color gradient for all records	Applies a two-color color arrangement to your data, one color as your minimum value, and one as your maximum value.		
> Three color gradient for all records	Applies a three-color color arrangement to your data, one color as your minimum value, one as your maximum value, and the third color as a central value.		
> Two color gradient for visible records	Applies a two-color color arrangement to your visible data.		
> Three color gradient for visible records	Applies a three-color color arrangement to your visible data.		
> Two color gradient highlighting outliers	Applies a two-color color arrangement to your data, but outliers are highlighted in another color, rather than being included in the continuous coloration.		
> Two color gradient resisting outliers	Applies a two-color arrangement to your data in which all values before median-2*stddev are colored the first color (red), and all values after median+2*stddev are colored the final color (blue). Outliers are colored either red or blue. Values close to the median are easily distinguished.		
Import	Imports a color arrangement from a file.		
Export	Exports a color arrangement to a file. This enables you to save a color arrangement and reuse it.		
Advanced	Switches you to the Advanced Coloring dialog where you can have more control over the way you color your values and ranges.		

► To change a color in Continuous mode:

- 1. Click on the square of the color that you want to modify.
- 2. Select a color from the palette or click More colors... to see the complete color palette.

► To change the Marked, Empty or Deselected color:

- 1. Click the button of the color that you want to modify.
- 2. Select a color from the palette or click **More colors...** to see the complete color palette.

► To switch between the Compact and Extended color views:

Right-click in the Continuous Coloring dialog and select either **Compact color view** or **Extended color view**.

Compact color view is useful when you are creating a connected gradient, i.e., when there are overlaps or holes. If, for example, you have a connected gradient through the points min->median->max, and you wish to change median to average, you only need to change one item in the Compact color view, whereas you would have to change two items (min->median and median->max) in the Extended color view.



4.8.7.8.3 Categorical Coloring Dialog

Values:	
31	Add
32	Delete
70	
71	Marked:
72	
73	Empty:
77	
85	Other:
98	
100	
103	
110	
112	
114	
117	
119	
120	
Import Export	
Help Advanced	Close

Option

Description

ValuesDisplays the values in the chosen column, and the color for each value.Note: When the dialog is opened the values are sorted. If new values are
added, the order is changed, but you can restore the order by right-clicking
and selecting Sort gradients.

Add	Adds a new item to the list of Color values. Using this, you can assign specific colors to values, and create your own coloring arrangement.
Delete	Removes a selected value. Ctrl+click to select multiple items for deletion.
Marked	Shows the color of the records that have been marked.
Empty	Shows the color of the empty records. Empty refers to records that have at least one empty field. These records are not shown at all in visualizations where an axis corresponds to the missing field.
Other	Shows the color of values that are not specified in the Values list.
Deselected	Shows the color of the deselected values. Deselected refers to records that do not fulfill the constraints of the query devices.
Import	Imports a color arrangement from a file.
Export	Exports a color arrangement to a file. This enables you to save a color arrangement and reuse it.
Advanced	Switches you to the Advanced Coloring dialog where you can have more control over the way you color your values and ranges.

► To change a color in Categorical mode:

- 1. Click on the square of color that you want to modify.
- 2. Select a color from the palette or click **More colors...** to see the complete color palette.

► To change the Marked, Empty, Other or Deselected color:

- 1. Click the button of the color that you want to modify.
- 2. Select a color from the palette or click **More colors...** to see the complete color palette.

4.8.7.8.4 Advanced Coloring Dialog

Advanced Coloring			×
Name:			
Default			
	Preview Column:	×P1	
Values:		,	_
23			Add
			Add All
			Delete
			Delete All
Ranges:			
sharedMin	▼ sharedMiddl	le 👻	Add
0	525		Delete
sharedMiddle	✓ sharedMax 1050	-	Delete All
525	1000		
Other Color		Deselected:	Empty:
From palette	Edit	Marked:	
C Fixed:		-	
Templates 👻	Import	Export	
Help		Basic	Close

Option	Description
Name	Displays the name of the coloring arrangement. Type to enter a new name.
Preview Column	Lists the columns from which you can add values to the Values list.
Values	Displays the values in the chosen column (Preview Column), and the color for each value. If a value has a defined categorical color, this color will be used even if the value is also defined within a color range.
Add	Adds a new item to the list of Values. Using this, you can assign specific colors to values, and create your own coloring arrangement.
Add All	Adds all available values from the selected Color by column to the Values list.

Delete	Removes a selected value. Ctrl+click to select multiple items for deletion.	
Delete All	Deletes all items in the Values list.	
Ranges	Shows the color of the empty records. Empty refers to records that have at least one empty field. These records are not shown at all in visualizations where an axis corresponds to the missing field.	
Add	Adds a new item to the list of Ranges. Using this, you can assign specific colors to values, and create your own coloring arrangement.	
Delete	Removes a selected value. Ctrl+click to select multiple items for deletion.	
Delete All	Deletes all items in the Ranges list.	
Other Color >	Determines which color is used for markers that do not get a color from any other setting. The color a marker gets is decided in the following order: Markers associated with a data row with empty/null value in the color column are set to the empty color	
	Markers filtered out by query devices or zoom sliders are set to the deselected color.	
	Marked items are drawn using the marked color. Markers that are included in the value list are set to the color specified there. The value list may include values that are not part of the current data set, but you know those values could be included in a future data set, thus it is possible to set up color arrangements that have predefined colors for all anticipated values. Markers that are included in a color range (from the Ranges list) are set to a color from that range. Note: Because it is possible to specify overlapping ranges, a marker can be inside several ranges. See Overlapping Color Ranges for more information. Any other markers are set to either a fixed color, or a color from a palette, depending on your selections. A palette is a list of colors. If there are more unique values in the color column than there are colors in the palette, colors will be reused.	
> From palette	Causes each marker to get an individual color from the color palette list. Note: If there are more than 97 values, colors will be reused.	
> Edit	Launches the Edit Palette dialog where you can adjust the RGB values of individual colors.	
> Fixed	Lets you choose the color that the markers will get.	
Deselected	Shows the color of the deselected values. Deselected refers to records that do not fulfill the constraints of the query devices.	
Marked	Shows the color of the records that have been marked.	
Empty	Shows the color of the empty records. Empty refers to records that have at least one empty field. These records are not shown at all in visualizations where an axis corresponds to the missing field.	
Templates >		
> Two color gradient for all	Applies a two-color color arrangement to your data, one color as your	

records	minimum value, and one as your maximum value.		
> Three color gradient for all records	Applies a three-color color arrangement to your data, one color as your minimum value, one as your maximum value, and the third color as a central value.		
> Two color gradient for visible records	Applies a two-color color arrangement to your visible data.		
> Three color gradient for visible records	Applies a three-color color arrangement to your visible data.		
> Two color gradient highlighting outliers	Applies a two-color color arrangement to your data, but outliers are highlighted in another color, rather than being included in the continuous coloration.		
> Two color gradient resisting outliers	Applies a two-color arrangement to your data in which all values before median-2*stddev are colored the first color (red), and all values after median+2*stddev are colored the final color (blue). Outliers are colored either red or blue. Values close to the median are easily distinguished.		
Import	Imports a color arrangement from a file.		
Export	Exports a color arrangement to a file. This enables you to save a color arrangement and reuse it.		
Basic	Returns you to the basic Categorical or Continuous or Heat Map Coloring dialog.		

► To change a color of the Values or Ranges:

- 1. Click on the square of color that you want to modify.
- 2. Select a color from the palette or click **More colors...** to see the complete color palette.

► To change the Marked, Empty or Deselected color:

- 1. Click the button of the color that you want to modify.
- 2. Select a color from the palette or click **More colors...** to see the complete color palette.

4.8.7.8.5 Color Expression Dialog

Color Expression	×
Variables: firstQuartile markedMax markedMedian markedMin markedThirdQuartile max median min selectedFirstQuartile selectedMax selectedMin selectedThirdQuartile	Function category: All Function:
Expression: selectedMax Target type:	Result: C9 H9 N5 07
Recent expressions: markedSum	Insert OK Cancel

Option

Description

Variables	Lists the available variables which can be used to create your expression. Insert a variable into your expression with the Insert Variable button.
Function	Select a category of functions to limit the choices in the Functions list:
category	All
	Operators
	Math Functions
	Statistical Functions
	Text Functions
	Logical Functions
	Date & Time Functions
	Conversion Functions
Function	Select a function by clicking on it, and click the Insert Function button to insert it to the Expression field. You can also double-click on a function to insert it.
	If you place the cursor at a specific location in the Expression field, the function will be inserted there

Description	Provides a brief description of the selected function. For more detailed descriptions, please see Spotfire Expression Language (SXL).
Expression	This is the text field in which you build your expression. You can insert variables and functions to it from the lists, or enter text as in any standard text editor.
	Cut/Copy/Paste works in the field using standard Ctrl+X / Ctrl+C / Ctrl+V.
	Highlighting a section of the expression, and clicking Insert Function will add the selected function to the expression with the highlighted section as an argument.
	Also, Undo/Redo functionality is available by pressing Ctrl+Z . Note: Very long expressions will be displayed truncated in the Visualization Legend. To avoid this, insert a blank space with suitable distance. This will not affect the expression, but will allow the Legend to display it over several rows.
Target type	Displays the data type of the result.
Result	This field displays the result of applying the current expression to the first row of the data set. If this field shows an error message, there is a problem with the expression. Clicking on the field will display an explanation of what is wrong. Pressing F5 will also display the error description. Pressing F4 will move the cursor to the position in the expression where the error lies.
	There are three kinds of error messages: #EXPR! – there is a problem with the syntax of the expression. #NUM! – the row evaluates to infinity or other illegal number. #ARG! – there is a problem with one or many arguments.
Recent expressions	This list contains the twenty most recent expressions you have created.
Insert	Inserts the selected recent expression to the cursor position of the expression field.

4.8.7.8.6 Customize Labels Dialog

Customize Label	5		×
Layout-			
Maximum label s	ize:		
_Appearance		Transparent	Solid
Background:			
Border:	·		L
	🔲 Use marker c	olor	
	Frame width:	—j—	
	Line width:		
Text:	•		
Help		ОК	Cancel

Option

Description

Maximum label size	Allows you to change the maximum label size that you wish to allow.
Background	Allows you to change the color of the background on the label. You can also adjust the transparency of the background using the slider.
Border	Allows you to change the color of the frame surrounding the label as well as the line leading to the border. The transparency of the border can also be adjusted.
Use marker color	Select this check box to use the same color on the label frame and line as is used on each item. Note: In bar charts, only the segment labels will be affected by this setting, not the bar labels.
Frame width	Adjusts the thickness of the surrounding frame.
Line width	Adjusts the thickness of the line leading from the marker to the label.
Text	Allows you to change the color of the label text.

4.8.8 Details Columns Tab

4.8.8.1 Details Columns Tab

Edit > Properties > Details Columns tab

Pro	operties: Age Di	istribu	tion					×
	Trellis Annotations	s s Data and Ba		Bars ackground	Bar Columns	Chart Colu Detai	imns Is Columns	
Available columns:			Columns in D)etails-on-E)emand: Type	-		
	Age group Gender Customer age Recency Total Date joined	Intega String Intega Date Intega Date	er er	Add >> << Remove Remove All Move First Move Up Move Down Move Last	First buy Number of Business loo Groceries Garden Furniture Electronics Toys Receipt ave	purchases cation erage	Date Integer String Integer Integer Integer Integer	

Option Description

Available columns	These columns are not included in the bar chart. Note: You can right-click on the Name header to get a pop-up menu where you can select other attributes you would like to be visible.
Columns in Details-on- Demand	These columns are displayed as information in the Details-on-Demand window. Note: The Details-on-Demand table cannot display more than a few hundred columns (depending on the width the columns). This means that in a very wide data set you might not be able to view all columns in the Details-on-Demand simultaneously.
Add >>	Select a column from the left list and press the Add >> button to move it to the right list, and include it in the details-on-demand.
<< Remove	Select a column from the right list and press the <<remove< b=""> button to move it back to the available columns list, and remove it from the details-on-demand.</remove<>
Remove All	Removes all columns from the right list, and moves them to the available columns list.
Move First	Select a column from the right list and press the Move First button to move it to the top. This changes the order the columns are displayed in the details-on-demand.
Move Up	Select a column from the right list and press the Move Up button to move it a step up. This changes the order the columns are displayed in the details-on-demand.

Move Down	Select a column from the right list and press the Move Down button to move it a step down. This changes the order the columns are displayed in the details-on-demand.
Move Last	Select a column from the right list and press the Move Last button to move it to the bottom. This changes the order the columns are displayed in the details-on-demand.

4.8.9 Bars Tab

4.8.9.1 Bars Tab

Edit > Properties > Bars tab

roperties: Bar Chart		X
Annotations Data and Details Columns Trellis Color By: Region Fixed Categorical Customize Show deselected	Background Columns Bar Chart Columns Bars Layout Stacked bars Side-by-side bars 100% stacked bars 100% side-by-side bars	
C None Customize C Marked	 □ Drop empty bars X-axis □ Date of Sale □ Use binned values 	
 ● Horizontal ● Horizontal ● Vertical ● Vertical ● Width Min ▲ Max ✓ Show outline on bars 	Number of bins: Manual 10 Automatic 11 bins Create Binned Column	

Option

Description

Color	If fixed coloring is used, one color is assigned to the entire bar or, if you are using multiple columns, to the part of a bar that originates in a single column. When using categorical coloring for bar charts, the bars are divided into sections according to the column selected in the drop down menu. Categorical coloring is not available for multiple columns display.
Labels	You can select to display labels for the bars in the bar chart, to see the exact values they represent.
	None – No labels are displayed.
	Marked – Only the bars that are marked will display labels.
	Visible, max – All visible bars will have labels next to them, provided

that the number of visible bars does not exceed the specified max number. If so, no labels are shown.
Click on Customize to open the Customize Labels dialog, where you can change the color and line width of the label frames and lines, as well as the size available to labels.
Select the Bar labels check box to display labels above the bars. Select the Segment labels check box to display labels on bar segments. You can also specify whether you want Horizontal or Vertical labels.
Drag the slider to modify the width of the bars.
If you select the Show outline on bars check box, black outlines will be drawn around the bars.
When categorical coloring is applied, you can choose between four different ways of displaying the bars. Stacked bars will place all columns in a category on top of each other, in effect summarizing them. Side-by-side bars will place the bars beside each other for comparison. The 100%-options are used if you want to compare the proportions of different categories for, e.g., different time periods. With 100% stacked bars , all bars will be of equal height (100%), unless some negative values exist in the data. 100% side-by-side bars displays bars side by side, but proportionally so that each group sums up to 100% (if the Sum measure is selected). See Bar Chart Layout Details for more information. Selecting the Drop empty bars check box, will hide all bars containing no records from the visualization, letting the visible bars use the space along the horizontal axis. Filtering with the query devices will cause bars to appear/disappear dynamically if this option is selected.
Use the drop-down list to change the column to use on the X-axis. If the X-axis in your bar chart represents a numeric value, you can select to bin (group) the records from several bars into larger "binned" bars. Rather than showing a separate bar for say, 1987, 1988, 1989, etc., you can show a single bar for 1980-1989, another bar for 1990-1999, etc. Do this by first selecting the Use binned values check box. This setting can also be reached from the right-click menu of the axis selector. Then you can either can choose your own number of bins by typing the number into the Manual field, or, select Automatic and adjust the slider to display a suitable number of bars. Moving the slider sets a maximum number of bins (1-1000), and the bar chart displays a number of bars as close to this as possible depending on the range of the data. Note : Automatic binning of the bar charts uses a form of even interval binning, which is optimized for interactivity and has heuristics to automatically adjust to fit logical tick marks on the X-axis. Click on Create Binned Column to add a new column to the data set containing the binned values. Create Binned Column can also be reached from the right alight more of the avia selector

4.8.9.2 Bar Charts – Color

Edit > Properties > Bars tab

Fixed Coloring

If fixed coloring is selected, one color is assigned to all bars. If you are displaying Multiple Columns, the bars of each column will by default be a different color.

► To Specify the Fixed Color for a Column:

- 1. Select **Edit > Properties**.
- 2. Select the **Bars** tab.
- 3. Select the radio button called **Fixed**.
- 4. Click on the **Customize** button.
- 5. Select a column from the list, and pick a color for it in the palette to the right.
- 6. Click OK.

Categorical Coloring

In single column mode you can use categorical coloring for the bars, which means that each bar is divided into differently colored sections, representing another column of your data set. See Bar Chart Layout Details for more information about different layout options.

► To Specify Categorical Coloring:

- 1. Select Edit > Properties.
- 2. Select the **Bars** tab.
- 3. Select the radio button called **Categorical**. **Note:** You cannot set Categorical coloring when using Multiple Columns.
- 4. Select the column you want to color the sections by.
- 5. Optionally, you can also click the **Customize** button to set the specific colors used.



Bar chart with categorical coloring, displaying the Average Value line.

Total Sum Line / Average Value Line

When using categorical coloring and there are negative segments in the bar, it can still be very useful to see how high the bar would be if all the positive and negative segments were summed up. This is indicated by a black line crossing each bar. If the bars are set to show the Sum of the values the line indicates the Total Sum, and if the bars are set to show the average of the values the line indicates the Average Value. Such a value can be both positive and negative.

Show deselected

If you select the **Show deselected** check box, a gray shadow will appear behind the regular bars. This indicates how the bars would look if all the records in the data set are included. Filtering with a query device or zooming in another plot deselects records in bars, causing the bars to change, but you can always compare them to the background shadows which remain the same.



You can change the color of the shadow by clicking on the **Customize** color button in the **Bars tab** of the **Properties** dialog.

4.8.9.3 Bar Chart Layout Details

When categorical coloring is applied, you have the option to display the categories in four different ways:

- Stacked bars
- Side-by-side bars
- 100% stacked bars
- 100% side-by-side bars

The categorical coloring layout is changed in the Properties dialog (**Edit** > **Properties** > **Bars** tab). Different layout modes are more or less useful for different types of aggregations: Sum, Average and Count. Below is a description of what you will see when you use the different layout options and aggregations.

Count

With Count, the height of a bar represents the number of records with a particular value. All layout options will display positive bars and show the contribution of each category to the total of the group.

Example:

In a data set containing personal data, the different eye color categories contain a different number of people (4,5,5). Also, by using the 100% stacked bar option, it is easy to see that women are slightly over-represented in the blue eye color category.



Sum

With Sum, the height of the bar indicates the total sum of the values of all records in that bar. The various categorical coloring layout options show the contribution of all categories to the total sum.

Option	Height of each category
Stacked bars	Represents the sum of the values in that category.
Side-by-side bars	Represents the sum of the values in that category.
100% stacked bars	Represents how many percent of the total sum for the group that is constituted of the sum of the values in the category.
	The exact percentage of each category can be seen in the details-on- demand window, when clicking on a bar category.
100% side-by-side bars	Represents how many percent of the total sum for the group that is constituted of the sum of the values in the category.
	The exact percentage of each category can be seen in the details-on- demand window, when clicking on a bar category.

Example:

If you want to compare the proportions of different categories for, e.g., different time periods, you can use either of the 100% layout options in the Properties dialog. With 100% stacked bars, all bars will be of equal height (100%), unless some negative values exist in the data.



In the example above, one can see that the Seattle revenue (yellow) has affected the total revenue more during 2002 than in previous years, whereas the Dallas revenue (blue) has decreased in importance.

Average

Side-by-

side bars in that category (Avg_{cat}).

Note: The representation of the bars may be difficult to understand if your data contains both positive and negative values. Use this type of representation with moderation for data with mixed signs.

Click on a bar or a bar category and view the details-on-demand window for more information about the various bars and categories.

Option Height of each category **Details-on-Demand information**

Represents the average of the values Stacked in that category divided by the bars number of categories (Avg_{cat}/n).



The exact percentage of each category's average compared to the total average of the entire group ((Avg_{cat}/Avg_{group})*100).




Example:

When you are using Average to represent the height of the bars, the 100% side-by-side bars option will display the percentage of the category average compared to the group average. That means that if the average for the specific category is higher than the average for the whole group, the bars will reach a height of more than 100%, see below.



4.8.10 Bar Chart Columns Tab

4.8.10.1 Bar Chart Columns Tab

Edit > Properties > Bar Chart Columns tab

operties: Age Dis	tribution			2
Annotations Trellis Available columns:	Data and Ba	ackground Bars	Columns D Bar Chart (Columns in bar char	etails Columns Columns rt:
Name 1 Groceries Garden Furniture Electronics Toys Receipt aver	[ype Integer Integer Integer Integer Integer	Add >> << Remove Remove All Move First Move Up Move Down Move Last	Name Total Customer age Age group Number of purcha	Type Integer Integer ses Integer
•			•	

Option	Description
Available columns	These columns are not included in the bar chart. Note: You can right-click on the Name header to get a pop-up menu where you can select other attributes you would like to be visible.
Columns in bar chart	These columns are included in the bar chart. The order of this list corresponds to the order the columns are shown in the Bar Chart visualization.
Add >>	Select a column from the left list and press the Add >> button to move it to the right list, and include it in the bar chart.
<< Remove	Select a column from the right list and press the <<remove< b=""> button to move it back to the available columns list, and remove it from the bar chart.</remove<>
Remove All	Removes all columns from the right list, and moves them to the available columns list.
Move First	Select a column from the right list and press the Move First button to move it to the top. This changes the order the bars are displayed.
Move Up	Select a column from the right list and press the Move Up button to move it a step up. This changes the order the bars are displayed.
Move Down	Select a column from the right list and press the Move Down button to move it a step down. This changes the order the bars are displayed.
Move Last	Select a column from the right list and press the Move Last button to move it to the bottom. This changes the order the bars are displayed.

4.8.11 Pies Tab

4.8.11.1 Pies Tab

Edit > Properties > Pies tab

Properties: Pie Chart	×
Annotations Data and Background Columns	Details Columns Pies
Color By: Gender C Fixed Pies Average Customize Show deselected Number of color bands:	Size Min Max © Fixed size © By records count © By average: © Ru sum:
Labels Color band: Labels None All records, max 20 Labels Pie size Pie size Pie position Pie records count Color: Color:	Jitter None Max

Option Description

Color	A pie chart can consist of one or more bands, each reflecting the distribution of values in a certain column. Set Number of color bands to the desired number, then select one band at a time using Color band . Color settings are set for each band individually.
Labels	 Five different labels can be added to the pie charts: Pie size shows the number of records associated with the pie, or average or sum, depending on the settings under Size. Pie sector value shows the value associated with each sector in the outermost band. Pie sector percentage shows the percentage of the pie that each sector covers in the outermost band. Pie records count shows the number of records in the pie.
	Pie position shows the position of the pie. Requires the use of axes.
Size	The maximum size of the pies in the pie chart can be varied with the Size slider. Under the Size slider there are four options of radio buttons with the following functions:
	Fixed size – pies are sized all the same.
	By records count – pies are sized according to the number of records in each pie.
	By average – pies are sized according to the average value of the records in the pie.
	By sum – pies are sized according to the sum of the records in the pie.
Jitter	The Jitter function, at the bottom right of the Properties dialog, can be used in the same way with pie charts as when working with scatter plots.

The overlapping pies will be randomly displaced so that hidden information will be made visible. At least one axis has to be in use.

4.8.11.2 Pie Charts - Color

Edit > Properties > Pies tab

A pie chart can consist of one or more bands, each reflecting the distribution of values in a certain column. Set **Number of color bands** to the desired number, then select one band at a time using **Color band**. Color settings are set for each band individually. The image shows a pie chart with multiple color bands.



For whole pies or bands, three coloring modes are available:

- Fixed One color is assigned to the entire pie or band.
- **Pies** The normal way of coloring: the band to be colored is divided into sections whose size is determined according to the distribution of the selected column.
- Average Assigns one color to each band or pie. The color is given according to the average value of the records in the chosen column for that pie/band.

Use the **Customize** button to choose color.

Customize Colors	×
Settings for *P2	
0	
40	
80	
120	
160	
Special colors:	Other
Deselected	Default Colors
Empty	D'ordait Colors
Marked	ОК

► To change a color:

- 1. Select the category that you want to modify.
- 2. Select a color from the palette.

► To revert to default coloring, click Default Colors.

► To select a color from the complete palette, click Other....

Note: Empty refers to records that have at least one empty field. These records are not shown at all in visualizations where an axis corresponds to the missing field.

Use **Show deselected** if all records in the data set should be included in the pies. The deselected records are displayed as a separate sector. The color of this sector can be altered with the color selector under **Customize** the color of the sector representing empty markers and the marking color can be changed in the same way.

4.8.11.3 Pie Charts - Size

Edit > Properties > Pies tab

The maximum size of the pies in the pie chart can be varied with the **Size** slider. Under the **Size** slider there are four options of radio buttons with the following functions:

- **Fixed size** pies are sized all the same.
- By records count pies are sized according to the number of records in each pie.
- **By average** pies are sized according to the average value of the records in the pie.
- **By sum** pies are sized according to the sum of the records in the pie.



When high *negative* values are used for sizing (By average or By sum), pies will appear large. A red filled circle within the pie will indicate that the value used for sizing is negative. If the sum or average is zero, this will yield invisible pies.

4.8.12 Lines Tab

4.8.12.1 Lines Tab

Edit > Properties > Lines tab

Properties: Line Cha	rt			×
Annotations Lines	Data and Backgrou Markers	ind Col	umns Details Line Chart Colum	Columns ins
Column:				
Customer age		- Appearance Color: Line type:	Straight line	_
		Line width:		
		Relative	Numeric	
		Bottom	Vertical Position:	Тор
		Min	Vertical Scale:	Max
Cascade All	Maximize All			
Option	Description			
Appearance	Here you set the p column you want right. Adjusting th	properties for to edit, and vi te controls wi	each column, that is lew the properties in ll change the appear	, each line. Select the list boxes of ance of the select

Layout When Scale Mode is set to <i>Individual</i> (see Markers property page) possible to control the vertical position and amplitude of the plotted curves. This makes it easy to compare the shapes of the curves. Pos and scale can be set either using sliders, or by entering numerical values. You can at any time switch between the two modes by preseither of the two radio buttons labeled Relative or Numeric .		column.
	Layout	When Scale Mode is set to <i>Individual</i> (see Markers property page) it is possible to control the vertical position and amplitude of the plotted curves. This makes it easy to compare the shapes of the curves. Position and scale can be set either using sliders, or by entering numerical values. You can at any time switch between the two modes by pressing either of the two radio buttons labeled Relative or Numeric .

4.8.12.2 Line Charts – Appearance

Edit > Properties > Lines tab

On the **Lines** of the **Properties** dialog tab you set the properties for each column, i.e., each line. Select the column you want to edit, and view the properties in the list boxes on the right. Adjusting the controls will change the appearance of the selected column.

Color

The color used for this column. The column is used for lines and markers as well as for axis labels in the Individual Scale mode.

Line type

Determines the type of the line used to connect points. Alternatives:

None – no line will be drawn

Straight line - points will be connected with a straight line

Step – points will be connected with a right angle. The first line is horizontal

Line width

Indicates the width of the line in pixels. The default setting is 1.

Thick lines take considerably longer time to draw. It is therefore a good idea to use a low value for Line width when viewing large data sets.

Marker

Allows you to select a shape to use for markers. If **Marker** is set to None, no markers are shown in the plot.

Please note that no markers will be drawn unless **Show Markers** is turned on in the **Markers** tab.

4.8.12.3 Line Charts – Layout

Edit > Properties > Lines tab

When **Scale Mode** is set to *Individual* (see Markers property page) it is possible to control the vertical position and amplitude of the plotted curves. This makes it easy to compare the shapes of the curves. Position and scale can be set either using sliders, or by entering numerical values. You can at any time switch between the two modes by pressing either of the two radio buttons labeled **Relative** or **Numeric**.

Vertical Position (Relative)

Moves the selected curve up and down in the visualization window. This may be desirable when you want to compare two curves by superimposing them on one another.

Vertical Scale (Relative)

Scales the selected curve. If you move the slider to *Min* the curve will appear almost flat. When set to *Max* the curve amplitude will equal the window height of the visualization.

High (Numeric)

Sets the highest value of the visible range.

Low (Numeric)

Sets the lowest value of the visible range.

Cascade all

Sets the Scale and Position of all columns so that each of them will occupy a separate slot of the window height.

Maximize all

Set the Scale and Position on every column so they utilize the whole height of the window.

4.8.13 Line Chart Columns Tab

4.8.13.1 Line Chart Columns Tab

Edit > Properties > Line Chart Columns tab

roperties: Line Chart				x
Annotations Details Columns Lines	Data and Backgro Line C	und hart Columns	Columns Markers	
Available columns:		Columns in line cha	art:	
Name Type		Name	Туре	
First buyDateNumber of pIntegerBusiness locaStringGroceriesIntegerGardenIntegerFurnitureIntegerElectronicsIntegerToysIntegerReceipt averIntegerBinned CustoString	Add >> << Remove Remove All	Customer age Total Gender Age group Recency Date joined	Integer Integer String Integer Date Date	
	Move First Move Up Move Down			
	Move Last	•		·

Option

Description

Available columns	These columns are not included in the line chart.
	Note: You can right-click on the Name header to get a pop-up menu where you can select other attributes you would like to be visible.
Columns in line chart	These columns are included in the line chart. The order of this list corresponds to the order the columns are shown in the Line Chart visualization.
Add >>	Select a column from the left list and press the Add >> button to move it to the right list, and include it in the line chart.
<< Remove	Select a column from the right list and press the <<remove< b=""> button to move it back to the available columns list, and remove it from the line chart.</remove<>
Remove All	Removes all columns from the right list, and moves them to the available columns list.
Move First	Select a column from the right list and press the Move First button to move it to the top. This changes the order the lines are displayed.
Move Up	Select a column from the right list and press the Move Up button to

	move it a step up. This changes the order the lines are displayed.
Move Down	Select a column from the right list and press the Move Down button to move it a step down. This changes the order the lines are displayed.
Move Last	Select a column from the right list and press the Move Last button to move it to the bottom. This changes the order the lines are displayed

4.8.14 Markers Tab of the Line chart

Markers Tab of the Line chart 4.8.14.1

Edit > Properties > Markers tab

Properties: Line Chart	×
Annotations Data and Backgr Lines Market Color Marked color: Deselected color: Show deselected	round Columns Details Columns ers Line Chart Columns Markers Show markers Min Size Max
Scale mode One for all Individual	Jitter None Max
Labels None Marked records All records, max 20 # labels	Line connection Connect by (None)
Color:	 Break on deselected values

Option

Option	Description
Color	The colors used for drawing marked and deselected records are edited here. Whether deselected records should be drawn or not is determined with the Show Deselected check box.
	Note: the color used to plot the records is the same as the connecting line, and thus configured on a per column basis on the Lines tab.
Scale mode	The line chart works in two modes: one in which all columns are plotted against a common Y-axis, and one where each column has a Y-axis of its own. One for all In this mode there is a single Y-axis scale for all columns. The range of
	in this mode more is a single 1 with some for an obtained. The tange of

this axis is automatically adjusted to fit all the columns currently being visualized.
Note: Since the values of the plotted columns may be of different magnitude, some lines might not be visible due to their low amplitude in relation to the scale of the Y-axis. Select Individual scale mode, or use the zoom bar on the Y-axis to zoom in on curves with low amplitude.
Individual
In this mode each column has a Y-axis scale of its own. This is useful when you want to visualize data of different types and magnitude in one plot, or when the shapes of the curves are more interesting than the absolute values. In Individual mode you can control the vertical position and scale of each plotted column using the sliders on the Lines tab.
For line charts, labels show the values of the column being plotted. Functionality is otherwise the same as for scatter plots.
The markers check box determines if markers should be drawn or not. The size of markers is controlled with the Size slider. The shape and color of the markers are controlled on column basis on the Lines tab.
Jittering has the same functionality as for scatter plots. That is, the X and Y coordinates are slightly moved to make it possible to tell data points with the same coordinate apart. The slider sets the amount of random displacement.
You can choose which column to use for discriminating between lines (Connect by), and the order in which data points are connected within each line (Order by). The order can be set to any column, to <i>Row Number</i> , or to <i>None</i> . The column on the X-axis is used by default. Selecting <i>None</i> turns line connection off.

4.8.14.2 Line Charts – Line Connection

Edit > Properties > Markers tab

You can choose which column to use for discriminating between lines (**Connect by**), and the order in which data points are connected within each line (**Order by**). The order can be set to any column, to *Row Number*, or to *None*. The column on the X-axis is used by default. Selecting *None* turns line connection off.

Line connection works in a slightly different way for line charts compared to scatter plots. In scatter plots, points will be connected no matter how many intermediate points are deselected (filtered out). In a line chart, you can control how you want to handle values that are missing or deselected.



In the first chart, no values are deselected.

In the second, high values have been deselected and **Break on deselected values** has been turned on. Broken lines then extend half way to the deselected value.

In the third chart, high values have been deselected and **Break on deselected** values turned off.

4.8.15 Profile Tab

4.8.15.1 Profile Tab

Edit > Properties > Profile tab

operties: Profile Chart			
Annotations Details Columns	Data and B Trellis	ackground Profile Columns	Columns Profile
Color By: (None) © Fixed © Continuou Customize Scale mode © All columns use same © All columns use indiv Labels Dynamic labels: © Highlight ♥ Acti Static labels: © None © Marked © Visible, max 200 Due unciebt (ka)		Jitter None Lines Width ↓ Line width by: [None] I Break on empty	Max

Option	Description
Color	Markers can be colored to reflect the value of a particular attribute. There are three modes for coloring: Fixed, Continuous and Categorical. Coloring in profile charts is identical to scatter plots.
Scale mode	The vertical dimension in a profile chart represents the value of each attribute. The scale can either be the same for all columns, or individual for each column. In the first case, the scale used for all columns ranges from the lowest to the highest value in <i>all columns</i> being plotted. This should be used when the values in the plotted columns are of the same unit and similar magnitude. To use this mode, select All columns use same scale . In the second case, the scale for each column ranges from the lowest value in the column to the highest value in the column. To use this mode, select All columns use individual scales .
Labels	It is possible to tag each profile with a label, showing the value of a particular column. You can select to show both Dynamic labels (Highlight and/or Active) and Static labels (None/Marked/Visible) at the same time. Dynamic labels are always placed on top of any static labels. The static labels include the following options: None – No labels are visible. Marked – Only records that are marked will have labels next to them. Visible, max – All visible records (up to a configurable maximum number) will have labels next to them, provided that the number of visible records does not exceed the specified max number. If so, no labels are shown. Click on Customize to open the Customize Labels dialog, where you can change the color and line width of the label frames and lines, as well as the size available to labels. You can drag labels to any position within the visualization area. Click on Reset to return all profile labels to their original position. Select the column you wish to label by, from the drop-down list By:. If you are running DecisionSite for Lead Discovery, you can also select to display the chemical structure for each profile in the label. This is done by right-clicking in the profile chart and selecting Structure Marker Labels > Remove to revert to the column selected here.
Jitter	Jittering displaces markers slightly and randomly, thereby making aggregations stand out visually. Attention is brought to areas where many records overlap. Such regions can then be investigated further, by zooming, changing axes, etc. Use the slider to increase or decrease jittering.
Lines	The width of all lines is adjusted by moving the Width slider. Select a column under Line width by to associate the width of individual lines with the value of a particular attribute. Empty values can be dealt with in two ways: either by leaving a gap in the profile, or by connecting the values on each side with a straight line. To leave a gap select Break on empty
	0.F.,

Profile Columns Tab 4.8.16

4.8.16.1 **Profile Columns Tab**

Edit > Properties > Profile Columns tab

roperties: Profile Charl			×
Annotations Details Columns Available columns:	Data and Trellis	Background Profile Columns Columns in p	Columns Profile
Name Type Gender String Recency Date Date joined Date First buy Date Business loca String Toys Integ Receipt aver Integ	er << R er << R Rem Mov Mov	e Last	Type Integer Integer purchases Integer Integer Integer Integer Integer

Option

Description Available columns These columns are not included in the profile chart. Note: You can right-click on the Name header to get a pop-up menu where you can select other attributes you would like to be visible. Columns in profile These columns are included in the profile chart. The order of this list corresponds to the order the columns are shown in the Profile Chart chart visualization. Add >> Select a column from the left list and press the Add >> button to move it to the right list, and include it in the profile chart. << Remove Select a column from the right list and press the **<<Remove** button to move it back to the available columns list, and remove it from the profile chart. **Remove All** Removes all columns from the right list, and moves them to the available columns list. **Move First** Select a column from the right list and press the Move First button to move it to the top. This changes the order the lines of the profile chart are displayed.

Move Up	Select a column from the right list and press the Move Up button to move it a step up. This changes the order the lines of the profile chart are displayed.
Move Down	Select a column from the right list and press the Move Down button to move it a step down. This changes the order the lines of the profile chart are displayed.
Move Last	Select a column from the right list and press the Move Last button to move it to the bottom. This changes the order the lines of the profile chart are displayed.

4.8.17 Heat Map Tab

4.8.17.1 Heat Map Tab

Edit > Properties > Heat Map tab

Properties: Heat Map	×
Annotations Data and Backgro Details Columns Trellis Heat M Column colors	ound Columns App Columns Heat Map Row labels
ColumnColor rangeCustomerDefaultTotalDefaultAge groupDefaultNumberDefaultGroceriesDefaultGardenDefaultFurnitureDefaultElectronicsDefault	By: (None) Location: C Left Right Special colors Marked: Default
Color range Default Apply New Edit Show deselected	

The **Heat Map** tab of the **Properties** dialog is used to modify the color range of the heat map and to display or hide row labels and deselected records. The default color range is set to green for minimum values, black for intermediate values and red for maximum values.

Apply color range to column

To apply a specific color range to one or more columns, select the appropriate columns from the list, then choose a range from the **Color range** drop-down list, and finally click the **Apply** button.

Create new color scheme

To change the color range of one or more columns, you need to create a new range. Click on the **New** button to open the Create Color Scheme dialog.

Edit existing color scheme

You can also edit the coloring of an already existing color range. Select a certain color range from the **Color range** drop-down list and click on the **Edit** button to open the Edit Color Scheme dialog. Changes made to this color range will have effect on the columns already linked to the range.

Delete color range

To delete a color range, select the color range from the **Color range** drop-down list and click on the **Delete** button. Any columns linked to the deleted range will automatically be reset to the Default color range.

Show/hide deselected records

To hide records that have been deselected by using the query devices from the heat map, clear the **Show deselected** check box.

Note: If you have had a dendrogram associated to the heat map, this will no longer be valid after hiding the deselected values. In this case, the dendrogram tree will be removed. You can show the dendrogram again by selecting the Show deselected check box.

Show/hide row labels

To show row labels next to the heat map, select a column where appropriate labels are located from the **Row labels By:** drop-down list. Choose the location of the labels by clicking the **Left** or **Right** radio button.

Tip: If you want to include information from more than one column in the row labels, use the New Column from Expression tool to concatenate the columns prior to applying row labels on your heat map.

To remove the row labels, select [None] in the drop-down list.

4.8.17.2 Create/Edit Heat Map Coloring

Edit > Properties > Heat Map Tab > New/Edit Color Range

🧿 Continuous Coloring]		×
Name:			
Default			
Color mode: Continuous Categorical	Preview Column:	∫*P1	×
Ranges:			
sharedMin	▼ 0 525		Add
sharedMiddle			Delete
sharedMax	1050		Marked:
			Empty:
			Other:
			•
			Deselected:
Templates 👻	Import	Export	
Help		Advanced	Close

Type a Name of the new color scheme in the text field at the top. Then select **Categorical Coloring** or **Continuous Coloring**.

Categorical Coloring

Categorical Coloring means that each unique value in the heat map is represented by its own color. This is most useful when dealing with a smaller number of varying values, or when looking for identical values in a heat map.

You can change which color to represent a certain value by selecting a value from the list, and then choosing a new color for it from the palette.

Continuous Coloring

Continuous Coloring means that the color range is linear from one specific color to another color, via a third middle color. By default this is set to show low values in shades of green, intermediate values going towards black, and high values in shades of red.

Select new colors to represent the Min, Mid or Max values, by clicking on their corresponding color button and picking a new color from the palette that appears.

Continuous Coloring is divided into three sub-options:

• Shared custom range:

With this option, you can specify an exact Min, Mid and Max value for the color range instead of having these values being automatically determined. All selected columns will be colored according to these values regardless of their own individual Min and Max values.

• Shared auto range:

With this option, there is a separate shared auto range per data-type category:

- Date/DateTime
- Time
- Integer/Decimal

String columns are not grouped at all, and each column will get an individual range spanning from the first string to the last.

• Individual auto range:

With this option, the Min, Mid and Max values for the range are automatically set to the lowest, median and highest values respectively, that exist in each individual column. All selected columns will be colored according to their own individual Min and Max values.

4.8.17.3 Advanced Coloring Dialog

Advanced Coloring			×
Name:			
Default			
	Preview Column:	×P1	
Values	T TEVIEW Column.	1	
23			Add
			Delete
			Delete All
, Ranges:			
sharedMin		e 👻 📕	Add
0	525		Delete
sharedMiddle		-	
525	1050		
, Other Color		Deselected:	Empty:
 From palette 	Edit		-
		Marked:	
C Fixed:		•	
Templates -	Import	Export	
	import		
Help		Basic	Close

Option Description

Name	Displays the name of the coloring arrangement. Type to enter a new name.
Preview Column	Lists the columns from which you can add values to the Values list.
Values	Displays the values in the chosen column (Preview Column), and the color for each value. If a value has a defined categorical color, this color will be used even if the value is also defined within a color range.
Add	Adds a new item to the list of Values. Using this, you can assign specific colors to values, and create your own coloring arrangement.
Add All	Adds all available values from the selected Color by column to the Values list.

Delete	Removes a selected value. Ctrl+click to select multiple items for deletion.		
Delete All	Deletes all items in the Values list.		
Ranges	Shows the color of the empty records. Empty refers to records that have at least one empty field. These records are not shown at all in visualizations where an axis corresponds to the missing field.		
Add	Adds a new item to the list of Ranges. Using this, you can assign specific colors to values, and create your own coloring arrangement.		
Delete	Removes a selected value. Ctrl+click to select multiple items for deletion.		
Delete All	Deletes all items in the Ranges list.		
Other Color >	Determines which color is used for markers that do not get a color from any other setting. The color a marker gets is decided in the following order: Markers associated with a data row with empty/null value in the color column are set to the empty color Markers filtered out by query devices or zoom sliders are set to the deselected color. Marked items are drawn using the marked color. Markers that are included in the value list are set to the color specified there. The value list may include values that are not part of the current data set, but you know those values could be included in a future data set, thus it is possible to set up color arrangements that have predefined colors for all anticipated values. Markers that are included in a color range (from the Ranges list) are set to a color from that range. Note: Because it is possible to specify overlapping ranges, a marker can be inside several ranges. See Overlapping Color Ranges for more information. Any other markers are set to either a fixed color, or a color from a palette, depending on your selections. A palette is a list of colors. If there are more unique values in the color column than there are colors in the palette, colors will be reused.		
> From palette	Causes each marker to get an individual color from the color palette list. Note: If there are more than 97 values, colors will be reused.		
> Edit	Launches the Edit Palette dialog where you can adjust the RGB values of individual colors.		
> Fixed	Lets you choose the color that the markers will get.		
Deselected	Shows the color of the deselected values. Deselected refers to records that do not fulfill the constraints of the query devices.		
Marked	Shows the color of the records that have been marked.		
Empty	Shows the color of the empty records. Empty refers to records that have at least one empty field. These records are not shown at all in visualizations where an axis corresponds to the missing field.		
Templates >			
> Shared auto range	With this option, there is a separate shared auto range per data-type category: 3. Date/DateTime 4. Time 5. Integer/Decimal		

	String columns are not grouped at all, and each column will get an individual range spanning from the first string to the last.
> Individual auto range	Sets the Min, Mid and Max values for the range automatically to the lowest, median and highest values respectively, that exist in each individual column. All selected columns will be colored according to their own individual Min and Max values.
> Shared custom range	Lets you specify an exact Min, Mid and Max value for the color range instead of having these values being automatically determined. All selected columns will be colored according to these values regardless of their own individual Min and Max values.
Import	Imports a color arrangement from a file.
Export	Exports a color arrangement to a file. This enables you to save a color arrangement and reuse it.
Basic	Returns you to the basic Categorical or Continuous or Heat Map Coloring dialog.

► To change a color of the Values or Ranges:

- 1. Click on the square of color that you want to modify.
- 2. Select a color from the palette or click **More colors...** to see the complete color palette.

► To change the Marked, Empty or Deselected color:

- 1. Click the button of the color that you want to modify.
- 2. Select a color from the palette or click **More colors...** to see the complete color palette.

4.8.17.4 Color Expression Dialog

Color Expression	×
Variables: firstQuartile markedFirstQuartile	Function category:
markedMax markedMedian markedMin markedThirdQuartile max	Function:
min selectedFirstQuartile selectedMax selectedMedian selectedMin selectedThirdQuartile	Description: Adds the two arguments. Example: 3.5 + 2.5
Insert Variable	Insert Function
selectedMax	A
Target type: String	Result: C9 H9 N5 07
Recent expressions: markedSum	▼ Insert
Help	OK Cancel

Variables

Lists the available variables which can be used to create your expression. Insert a variable into your expression with the **Insert Variable** button.

Category

Select a category of functions to limit the choices in the Functions list.

- All
- Operators
- Math Functions
- Statistical Functions
- Text Functions
- Logical Functions
- Date & Time Functions
- Conversion Functions

Function

Select a function by clicking on it, and click the **Insert Function** button to insert it to the **Expression** field. You can also double-click on a function to insert it.

If you place the cursor at a specific location in the **Expression** field, the function will be inserted there.

Description

This field provides a brief description of the selected function. For more detailed descriptions, please see Spotfire Expression Language (SXL).

Expression

This is the text field in which you build your expression. You can insert variables and functions to it from the lists, or enter text as in any standard text editor.

Cut/Copy/Paste works in the field using standard Ctrl+X / Ctrl+C / Ctrl+V.

Highlighting a section of the expression, and clicking Insert Function will add the selected function to the expression with the highlighted section as an argument.

Also, Undo/Redo functionality is available by pressing Ctrl+Z.

Note: Very long expressions will be displayed truncated in the Visualization Legend. To avoid this, insert a blank space with suitable distance. This will not affect the expression, but will allow the Legend to display it over several rows.

Recent expressions

This list contains the twenty most recent expressions you have created. You can select one of these and click the Insert button to insert the expression into the **Expression** field. This will not replace the entire content of the field, only insert the selected expression at the cursor position.

Result

This field displays the result of applying the current expression to the first row of the data set. If this field shows an error message, there is a problem with the expression. Clicking on the field will display an explanation of what is wrong. Pressing F5 will also display the error description. Pressing F4 will move the cursor to the position in the expression where the error lies.

There are three kinds of error messages:

#EXPR! - there is a problem with the syntax of the expression.

#NUM! - the row evaluates to infinity or other illegal number.

#ARG! - there is a problem with one or many arguments.

4.8.18 Heat Map Columns Tab

4.8.18.1 Heat Map Columns Tab

Edit > Properties > Heat Map Columns tab

operties: Heat Map		×
Annotations Details Columns Trellis	Data and Background Columns s Heat Map Columns Heat Map	
Available columns:	Columns in heat map:	
Name Type	Name Type	
Gender String Recency Date Date joined Date First buy Date Business loca String Toys Integer Receipt aver Integer	Add >> Customer age Integer Add >> Total Integer Age group Integer Number of purchases Integer Groceries Integer Garden Integer Furniture Integer Electronics Integer	
I b	Move Up Move Down Move Last	

Option Description

Available columns	These columns are not included in the heat map. Note: You can right-click on the Name header to get a pop-up menu where you can select other attributes you would like to be visible.
Columns in heat map	These columns are included in the heat map. The order of this list corresponds to the order the columns are shown in the Heat Map visualization. You can also see this numerically in the X-axis selector of the Heat Map.
Add >>	Select a column from the left list and press the Add >> button to move it to the right list, and include it in the heat map.
<< Remove	Select a column from the right list and press the <<remove< b=""> button to move it back to the available columns list, and remove it from the heat map.</remove<>
Remove All	Removes all columns from the right list, and moves them to the available columns list.
Move First	Select a column from the right list and press the Move First button to move it to the top. This changes the order the lines are displayed.
Move Up	Select a column from the right list and press the Move Up button to move it a step up. This changes the order the columns are displayed in the heat map.
Move Down	Select a column from the right list and press the Move Down button to move it a step down. This changes the order the columns are displayed in the heat map.

Move Last Select a column from the right list and press the **Move Last** button to move it to the bottom. This changes the order the columns are displayed in the heat map.

4.8.19 Table Tab

4.8.19.1 Table Tab

Edit > Properties > Table tab

Properties: Table	×
Annotations Columns Details Columns Table Co	olumns Table
Color	Row height
Marked color:	Number of lines:
Deselected color:	
Show deselected	Header height
Sort rows by	Number of lines: 1
(None)	
C Ascending C Descending	Frozen columns
Then by	Number of columns:
C Ascending C Descending	
Then by	Grid
C Ascending C Descending	I▼ Show grid lines

Option	Description
Color	You can change the color that indicates marked and deselected markers by clicking on the corresponding button. You can also choose whether or not to display deselected records in the table by selecting or clearing the check box.
	Note: Deselected records cannot be marked or made active in any way. Even though it is possible to make them visible by selecting the Show deselected check box, they are not included when marking a group of records.
Sort rows by	You can sort the order of the rows in the table. From the Properties dialog this can be done by up to three columns, but if you wish to sort by more than three columns simply use the Shift+click functionality. In the Properties dialog, first select a primary column to sort the rows

	by, and select whether the order should be Ascending or Descending. You may then select a secondary column to sort by, and even a third if you so desire.
	Note: You can also sort the rows quickly by just clicking on the header of a column. Clicking several times will toggle between ascending or descending order. By holding down Shift and clicking on another column header you can sort by several columns.
Row height	This drop-down list box lets you choose how high each row in the table should be. Height is measured in number of lines. It can be useful to increase the number of lines if there is a great deal of information in each cell, as several lines makes the text wrap inside each cell.
Header height	This drop-down list box lets you choose how high the headers in the table should be. Height is measured in number of lines. It can be useful to increase the number of lines if there is a great deal of information in each column header, as several lines makes the text wrap inside each cell.
Frozen columns	In a table with many columns you often need to scroll horizontally. However, sometimes you may want certain columns to always be displayed regardless of scrolling. This is achieved by freezing one or more columns.
	Place the columns you want to freeze to the far left of the table, then use this drop-down list box to specify the number of columns you want to freeze.
Grid	Select this check box to show grid lines in the table.

4.8.20 Table Columns Tab

4.8.20.1 Table Columns Tab

Edit > Properties > Table Columns tab

Properties: Table			×
Annotations Columns Details Colu	imns Table Colum	nns Table	
Available columns:		Columns in table:	
Name Type		Name	Туре
Gender String		Recency Data (sized	Date
Total Integer		Pate joined First buv	Date
Age group Integer	Add >>	Number of purchases	Integer
	// Remove	Business location	String
	<td>Garden</td> <td>Integer</td>	Garden	Integer
	Remove All	Furniture	Integer
		Electronics	Integer
		Toys Receipt average	Inceger
	Move First		
	Move Up		
	Move Down		
	Move Last		
		•	

Option Description

Available columns	These columns are not included in the table.	
	Note: You can right-click on the Name header to get a pop-up menu where you can select other attributes you would like to be visible.	
Columns in table	These columns are included in the table. The order of this list corresponds to the order the columns are shown in the Table visualization.	
Add >>	Select a column from the left list and press the Add >> button to move it to the right list, and include it in the table.	
<< Remove	Select a column from the right list and press the <<remove< b=""> button to move it back to the available columns list, and remove it from the table.</remove<>	
Remove All	Removes all columns from the right list, and moves them to the available columns list.	
Move First	Select a column from the right list and press the Move First button to move it to the top. This changes the order the columns are displayed in the table.	
Move Up	Select a column from the right list and press the Move Up button to move it a step up. This changes the order the columns are displayed in the table.	
Move Down	Select a column from the right list and press the Move Down button to move it a step down. This changes the order the columns are displayed in the table.	
Move Last	Select a column from the right list and press the Move Last button to	

move it to the bottom. This changes the order the columns are displayed in the table.

4.9 Working with Visualizations

4.9.1 Changing Visualization Axes

To change the column to be mapped to each axis, click on an axis selector, and select a column name. For example, to see the Mendeleevian layout of the peroidic.csv example data set, select P1 for the X-axis and P2 for the Y-axis.



Note: You can also select which column to use as an X, Y or Z-axis by right-clicking on the Query Device representing that column, and selecting **Set Property > Axis** from the pop-up menu.

4.9.2 Zooming and Panning

Zooming can be done in two ways: by using the zoom bars or by using the mouse.

Mouse Shortcuts

2D Scatter Plots, Bar Charts, Pie Charts, Line Charts, Profile Charts, and Heat Maps.

Action	Mouse maneuver	Comment
Zoom in	Ctrl + Right-click	The scroll wheel has the same function
Zoom out	Ctrl + Shift + Right-click	
Zoom in Zoom out	Ctrl + Right-click Ctrl + Shift + Right-click	The scroll wheel has the same function

In 3D Scatter Plots, the zoom bars are used as in 2D. Additionally, the following means of navigation are available.

Action	Mouse action 1	Mouse action 2	Pointer icon	Comment
Rotate	Ctrl + drag using the right mouse button	Drag using the middle mouse button	¢	Rotation is around the visualization center

Zoom	Shift + drag using the right mouse button	Shift + drag using the middle mouse button	8	Moves in the direction of view
Roll	Shift + Ctrl + drag using the right mouse button	Shift + Ctrl + drag using the middle mouse button	C	Rotation is in the plane of the screen; down-wards and right cursor motion rotate clockwise
Zoom in on a specific marker	Click on a marker and use the mouse wheel	Ctrl + drag using the middle mouse button		Keeps the selected marker in the same place on screen

Note: Clicking the **Reset Navigation** button on the **3D** tab of the **Properties** dialog will undo all navigation adjustments.

Zoom bars

Dragging the end arrows of the zoom bars (along the edges of the visualization window) zooms in on a portion of the visualization. Dragging the bar itself (by placing the mouse pointer on the yellow bar and dragging) pans across different areas of the entire visualization.



Altering the length of the X-axis zoom bar

The pale yellow area represents the selected range of values, whereas the bright yellow area represents the range of existing values within the selected range.

The zoom bar can be adjusted to encompass only the currently selected data.

Setting the zoom bar span to the current selection:

1. Double-click on the bright yellow area.



Response: The scatter plot and the zoom bar are now adjusted to focus on the selected markers.



Tip: You can also right-click on the Zoom bar and select **Zoom to Selection** from the pop-up menu. To zoom in on one side but not on the other, double-click on the left or right drag box.

Resetting the zoom bar span:

1. Double-click on the center of the zoom bar.



Response: The zoom bar now expands to its full length.



Tip: You can also right-click on the Zoom bar and select **Reset Zooming** from the pop-up menu.

Note: By double-clicking on the left or right drag box of the zoom bar, you can narrow down the left or right span.

Setting the zoom bar to a specific value:

- 1. Click on an end arrow of the zoom bar.
- 2. Type the desired value.

The scatter plot and the zoom bar are now adjusted to show the value you entered.

Note: Note that no "edit field" will appear in which to type the value. Simply type the value after clicking, a temporary ToolTip will be displayed, and the slider will adjust itself to the specified number.

► Setting the Data Range to Selected records:

- 1. Move the drag box of the zoom bar to narrow the selection.
- 2. Right-click on the zoom bar.
- 3. Select Data Range from Zooming from the pop-up menu.

The zoom bar expands to its full width, but with the Data Range set to encompass only the selected records. Three dots are displayed to indicate that the range is not the original full range.

► To reset the Data Range:

1. Right-click the zoom bar and select **Reset Data Range**.

4.9.3 Axis Labels

Axis labels are by default displayed along both the horizontal and vertical axes. These can be adjusted in several ways.

► To adjust the axis label width/height:

1. Position the mouse pointer over the axis. The mouse pointer changes, as seen below.



2. Press down the mouse button and drag the axis to the width or height desired.

Note: If the axis labels are hidden, simply grab the axis and drag it to make the labels visible again.

Label options

By right-clicking in the axis label area, a pop-up menu appears. It contains several options: **Hide** – Hides the vertical or horizontal axis labels. Drag the axis (see above) to make the labels visible again.

Fewer Labels – Fewer labels are displayed on the axis.

More Labels – More labels are displayed on the axis.

Label Orientation – Sets the label text orientation to either Horizontal or Vertical (see below). **Properties** – Opens the Properties dialog in which you can set Label spacing and density.



4.9.4 Applying Templates

If you open many data sets of a similar nature in DecisionSite Client, you may wish to create a template of the usual visualizations you always create, certain query device settings you always initially make, etc. For information on how to save a template see Saving Spotfire Files.

A template file is basically a standard Spotfire file but without any data content. When you want to apply a template to a data set, you can therefore choose to apply the settings from either a Template file (SFT), a Spotfire Analysis File (SFS) or a Spotfire XML File (XSF, which is the same thing as an SFS file only in XML format).

► To Apply a Template:

- 1. Open your data set in DecisionSite Client.
- 2. Select File > Apply Template....
- 3. Select the template file you want to apply.
- 4. Click Open.

Response: The template is applied on your data.

4.9.5 Marking, Activating, and Highlighting Records

4.9.5.1 How to Mark, Activate and Highlight

In DecisionSite, there are three ways to interact with the data set: marking, activating and highlighting.



Note: An "object" can be a single record (as in scatter plots) or an aggregation of records (such as pie charts).

The effect of performing these actions varies with the tool and type of visualization. Go to the sections describing each tool to find out more, or click the Help window's **Back** button to return to where you were!

4.9.5.2 Marking

The purpose of marking records may be to view details, or to distinguish records in order to copy, erase, or in other ways manipulate them.

► To mark one or more records:

- 1. Click and hold the left mouse button, and drag the mouse: the pointer will delineate a rectangle.
- 2. Enclose the markers of interest in this rectangle. When the mouse button is released, the marked objects will be given a different color and outline.

Note: Marking a pie or bar is equivalent to marking all the records that are included in that pie or bar.

To add more records to the marked set:

- 1. Press and hold Ctrl.
- 2. Click on markers you want to add, one by one. Alternatively, use the mouse to draw a rectangle around several markers (while still pressing Ctrl).

Marking with the lasso

A set of graphical objects, be they pies, bars or scatter plot markers, can be "lasso selected", i.e., be surrounded by a line drawn in an arbitrary shape. Press the Shift key and the left mouse button, then draw a line capturing the markers. Note that a straight line connects the beginning and the endpoints of the lasso marquee. The line delineates the area that will be included in the selection.

Note: For a record to be marked, its exact coordinates must be within the bounds of the selecting line. Just slicing through part of an enlarged marker will not suffice.

Setting colors for marked objects

Marked records will be given an identifying color in all visualizations. You can define this color through the **Customize** color button of the **Properties** dialog.

Unmarking

Re-marking any marked object(s) while Ctrl is pressed will unmark them. If Ctrl is not pressed, only the new selection will be marked. Unmark all data by selecting **Edit > Marked Record(s) > Unmark**; or by pressing [**Ctrl+E**]. Alternatively you can unmark everything by marking an empty area of any visualization.

Message box when marking

If a set of markers is already marked, and you mark a new set, a message box will appear, warning you that you will loose the previous marking. You can turn this feature off by checking the box labeled **Never show alert again.** If, at a later time, you would like this feature back, select **Edit > Marked Record(s) > Unmark**, and check the box in the dialog. You can also use the **Customize** dialog.

4.9.5.3 Activating

Clicking on a single record will make a persistent circle surround the corresponding marker in all scatter plot visualizations. A record thus chosen is referred to as **active**.

The arrow keys will cause the nearest record in the direction of the arrow to become active. The Tab key will move the active record indicator to the next record in the data set. If you have a group of records marked, using the keys will only cycle through these.

The details of an active record are presented in the Details-on-Demand window. The record will continue showing details until another record is made active or a group of records marked with the lasso or rectangle method.

4.9.5.4 Highlighting

Moving the mouse pointer close to or on top of a graphical object will highlight it. A thin circle will cling to the marker until the pointer is moved a certain distance away.



Highlighted marker

Highlighting shows where in each visualization a data point lies, because the same record is highlighted in each visualization.

4.9.5.5 Actions Involving the Marked Set

The following commands concern the set of marked records. They can all be found via the **Edit** menu or in the right-click context menus of the visualizations.

Option	Description
Marked Record(s) > Unmark	Ctrl+E. Unmarks all records in the data set.
Marked Record(s) > Invert	Ctrl+I . Inverts the marking so that all unmarked records become marked and vice versa.
Marked Record(s) > Select	Ctrl+M . Sets query devices to include only the marked records. This hides the unmarked records.
Marked Record(s) > Undo Select	Shift+Ctrl+M. Undoes the previous selection.
Marked Record(s) > Delete	Delete . Removes corresponding records from the data set. The action is irreversible and immediately affects the loaded data set. However,

the data source (e.g., the file) will remain unchanged until you
explicitly overwrite it by saving.Data > New ColumnCreates a new column. By default, marked records will get the value
Yes, and unmarked records the value No.Records...Note: Found under the Data menu.

4.9.5.6 Resetting Visualizations

After having zoomed in, selected, deselected and performed a number of manipulations on the markers, pies and/or bars, the set of records shown in the visualizations may become disarrayed. The command **Reset to All** in the **Edit** menu (**Ctrl** + **R**) will get the visualization back in order again, resetting the query devices and restoring zoomed visualizations. Deleted records will be gone, however, and can only be restored by closing the visualization without saving it and then opening the original data set once again.

4.9.5.7 Copying Records

These commands under the **Edit** menu copy the data stored in the loaded data set, or a sub-set of it, to the clipboard. The copied information can then be exported, pasted into a spreadsheet program, such as Microsoft Excel or another program, e.g. Notepad.

Copy [Ctrl+C] copies the records corresponding to the markers, bars and pies marked with the lasso or rectangle marking tool to the Windows clipboard in text format. It also copies an image of the visualization to the clipboard, which can be pasted into other applications by using a Paste Special option.

Copy Special > Marked Records copies the records corresponding to the markers, bars and pies marked with the lasso or rectangle marking tool to the Windows clipboard in text format.

Copy Special > Selected Records copies only the records within the limits set by the query devices to the Windows clipboard in text format.

Copy Special > All Records copies all records to the Clipboard. Data in all the records in the data set is copied to the Clipboard in text format.

Copy Special > Visualization copies the active visualization display as a Windows Metafile image. This image can be pasted into other Windows compatible applications such as MS Word, Paint, PowerPoint etc. As Metafile images are vector-based graphics they can be enlarged or shrunk at will without loosing detail. Axes, labels and grid lines are included in the image. These images can be manipulated from within the new host applications.

4.9.5.8 Information About the Data Set

The record meter in the status bar at the bottom of the Spotfire DecisionSite gives continuous information about visualization statistics. You can see at a glance what portion of all the data is currently visible, marked, etc. The same information is displayed as text.



Colors should be read as follows:

Green – Records that are selected and marked.

Yellow - Records that are selected and unmarked.

Gray – Records that are selected, but lack a value required for representation on the current axes, and hence are invisible.

The sum of the above makes up the set of selected records. The length of the record meter in relation to the box in which it sits is an indication of the relative size of the current selection. To display or hide the status bar, use the **Status Bar** command in the **View** menu.

4.9.6 Organizing the Desktop

4.9.6.1 Arranging Visualizations

There are several ways to reposition windows; the commands governing these functions all reside in the **Window** menu:

Auto Hide Axis Selectors – when the visualization is small enough, this option automatically hides the zoom bars and the axis selectors.

Hide Window Frame – hides the title bar, giving more space to the visualizations—only available when several visualizations have been tiled.

Auto Tile – arranges all the windows on screen according to an internal algorithm. The active visualization will be made the largest, and placed in the upper left-hand corner.

Cascade – arranges the visualization windows so that they partially overlap each other, leaving each window accessible by clicking on the title bar.

Tile Horizontal – splits the window area horizontally, giving each visualization equal area. **Tile Vertical** – splits the window area vertically, giving each visualization equal area.

Tip: An alternative way of organizing visualizations is to use a Trellis plot. This allows you to split an existing plot into panes, and organize these in a grid. Note that this feature is currently available only for scatter plots (2D and 3D), bar charts, profile charts and heat maps. See What is a Trellis Plot? for more information.

4.9.6.2 Showing and Hiding Windows

Spotfire DecisionSite consists of several windows. It can be desirable to rearrange the application's layout to organize visualizations and information for more effective analysis. The **View** menu displays a list of the Spotfire DecisionSite windows. Each window can be shown or hidden by selecting or clearing the check mark next to the name of the window, respectively. The windows are listed and described below:

Toolbars – the row of clickable buttons right below the menus. See Toolbar Buttons for more information.

Status Bar – the information field at the bottom of the application window. The status bar displays information about pointer position, number and portion of records that are visible and marked, etc.

Full Screen – by selecting this option, all Toolbars are hidden and the Visualization, Query Device and Details-on-Demand window are maximized to fill the whole screen. By clicking on the small icon (below) the Toolbars are returned. You can also go to Full Screen mode by pressing **F11**.



Workbook – when this option is selected, each visualization is given a separate tab.

Details-on-Demand (Text) – the window where information about the marked records, the highlighted scatter plot marker, bar or pie object, etc., appears.

Details-on-Demand (HTML) – information about the highlighted or marked scatter plot marker(s), bar or pie object(s), etc., formatted according to the HTML templates stored in the current SFS file.

Details-on-Demand (External Browser) - as above, but launches a separate browser.

Query Devices – the window that contains all the query devices.

Legend – the window that explains the significance of the current visualization settings, e.g., which columns are used for size, rotation, color, etc.

Guides Toolbar – the row of clickable buttons pertaining to the Guides pane. **Guides Pane** – the browser window used to view Guides, and to run Spotfire DecisionSite applications (plug-ins).

4.9.6.3 Moving and Resizing Windows

Spotfire DecisionSite has a certain default setup; the Guides pane appears on the left, while the larger area in the centre is for the visualization(s). The right side is occupied by the Query Device window and the Details-on-Demand window.

Since this may not be the most effective layout for all purposes, it is possible to move and resize the windows.

To resize a window, click on a window border and drag it to the desired position.

To move a window, click on the title bar or gripper bar at the top of the window, and drag the window to the desired position. Alternatively, press the left mouse key while pointing at the left or right edge—there is a thin, 3 pixel band—to grab the window for repositioning.



4.9.6.4 Workbook Mode

Workbook mode can be used to put each visualization on its own tab. A click on a tab activates the corresponding visualization and allows manipulation and modification of its attributes.



To put Spotfire DecisionSite into Workbook mode, select Workbook from the View menu.

You can change the order of the tabs by right-clicking on a tab and selecting **Move** > **First/Left/Right/Last** from the pop-up menu.

Combining Workbook with Auto tile

With **Windows** > **Auto Tile** off, pages in the Workbook retain the size that they had been given; decreasing the size of the application window will crop portions of some visualizations. With the **Auto Tile** function on, clicking on a Workbook tab gives the chosen visualization priority position and size.

4.9.6.5 Duplicate Visualization

By selecting **Visualization > Duplicate Visualization** you can create a copy of the currently selected visualization. This is useful if you have created a visualization with different settings, and you wish to create an identical copy in which you then want to change some aspect and compare the two.
4.9.6.6 Customizing Visualizations

The **Tools > Options > Visualization Settings** tab allows you to control certain aspects of the visualizations.

Hiding axis selectors

Axis selectors can be made to automatically disappear when the visualization size is less than a certain threshold value. Click **Auto Hide Axis Selectors** and set threshold values to enable this function. The **Default** button restores default threshold values and disables Auto-hide.

Controlling default settings for new visualizations

The **Save** button on the **Visualization Settings** tab of the **Options** dialog allows you to set the preferred initial settings for new visualizations.

The settings of the current visualization are used as a template for initial visualizations of similar type. In this context, 2D and 3D scatter plots are linked, i.e., default settings for 3D visualizations will also apply to 2D scatter plots.

The following settings are saved for all visualizations:

- **Color** e.g., categorical or continuous coloring, beginning and ending colors for continuous coloring, marked and deselected marker color, etc., but not which column governs coloring.
- Size the size of markers (but not which column governs size).
- **Labels** the label mode (None, Marked, All), the number of labels displayed and their color, displacement, orientation, positioning and density.
- **Gridtype** show grid or not.
- Append axis names to visualization title
- Show deselected whether or not deselected records should be displayed.

In addition, marker shape is also saved for scatter plots, outline or no outline is saved for bar charts, scale mode is saved for profile charts and line charts as well as the show marker option for line charts.

No column-specific settings are saved, e.g., **Rotate by** is not saved since it refers to a specific column. Settings from the **3D** tab such as navigation, rendering and perspective are not saved; neither are **Data and Background** tab settings as they are column specific.

The **Reset** button will remove the configuration that you have previously saved and restore the default values.

4.9.6.7 Customizing Toolbars

Tools > Customize > Toolbars tab

You can tailor Spotfire DecisionSite's toolbars to allow you to rapidly access features that you use regularly.

► To customize toolbars:

- 1. Select **Tools > Customize...**.
- 2. Go to the **Toolbars** tab.
- 3. Click New....
- 4. Enter a name for the new toolbar and click **OK**.
- 5. Make sure the new toolbar is selected in the list. Your toolbar should be visible as a small box on your screen:



- 6. Go to the **Commands** tab.
- 7. Select a category of commands.

Customize	×
Toolbars Commands Categories: Buttons Default Import Export Import View Visualizations Window Spotfire. T ableVist	
Select a category, then click a button to see its description. Drag the button to any toolbar Description Creates a new 3D scatter plot visualization	
OK Cancel Apply Help	

- 8. Drag any button to your new toolbar (or to any of the standard toolbars).
- 9. Click OK.

4.9.6.8 Fonts & Numbers Tab

► To change the fonts:

Select **Tools > Options > Fonts & Numbers**. This opens the **Fonts & Numbers** tab of the **Options** dialog in which you can specify which font should be used for different categories of the application:

- Annotations the font used for the annotation when printing.
- Details on Demand on screen.
- Headers and Footers shown when printing.
- Legend on screen, when printing or exporting.
- Query Devices on screen.
- Title when printing.
- Visualization labels and texts in visualizations, on screen, when printing or exporting.

Select one or more categories and click on the Change Font button. This displays the Font selection dialog in which you can select which font, font style and font size should be used for the selected categories.

► To reset the fonts:

- Select one or more categories and click on the **Reset** button, to reset the font for these categories to the default font.
- Click on the **Reset All** button to reset all categories to the default font.

You can specify how you want DecisionSite Client to display number formatting for all Integer type values and Decimal type values. You can set the Number of decimal digits, how to display Negative numbers, and whether or not to use Thousands separators. The settings you make in this dialog will be set as default, and take effect when you load a new data set in to DecisionSite Client.

You can set other number formatting for specific columns later if you want to. See Number Format for Columns.

► To set Number Formatting:

1. Select Tools > Options > Fonts & Numbers.

Options		×	
Fonts & Numbers Visualization Settin	ngs Advanced Opt	ions	
Category			
Annotations	Sample:		
Details-on-Demand Headers and Footers Legend Query Devices Title Visualizations	AaBbCo	:XxYyZz	
		Change Font	
Reset			
exporting.	nen pinang or	Reset All	
Default numeric format			
Integer columns: Format			
OK Car	ncel Apply	Help	

2. Click on either the **Integers...** or **Decimals...** button and select either **None** formatting or a custom one under **Number...**.

Number Format	×			
Number of decimal digits:	2			
Negative numbers:	-123 💌			
Scientific notation				
🔲 Use thousands separator				
Currency symbol				
Left: \$	Right:			
Example				
\$ -1234567.12				
Help	OK Cancel			

 Specify the Number of decimal digits, how to display Negative numbers, and whether or not to Use thousands separators. Note: The symbol used for thousands separators and decimal separator is determined

Note: The symbol used for thousands separators and decimal separator is determined by the Windows Locale setting.

4. Click OK.

4.9.6.9 Advanced Options Tab

The **Advanced Options** tab of the **Tools > Options** dialog provides some options for finetuning your Spotfire DecisionSite environment. Use the check boxes to enable or disable any of the following features (the first four only take effect after Spotfire DecisionSite is restarted):

Option	Description
Show grippers on docked windows	Displays a small banner in docked windows, which can be used when dragging the window to a new position. Drag the banner to move the docked window. Examples of docked windows are the Details-on-Demand window and the Legend window.
Show full column names in query devices	When this option is selected, column names are displayed on a separate row inside each query device. Clearing the check box will display the column names and the values on the same row, in some cases truncating the column name, but instead the query devices will be more compact, thus displaying more query devices in the window.
Show warning when changing marked records	Displays a dialog each time you mark a new set of records.
Use OpenGL hardware acceleration	If you experience problems displaying 3D Scatter Plots, try turning off the OpenGL acceleration.

Use DirectX9 for smooth line rendering, if available	Enables the use of hardware-accelerated DirectX 9 for smooth line rendering. (This setting only has effect if there is a DirectX 9 capable graphics card available in your computer.)
Ignore case in full text search	This sets the default behavior for full-text search query devices. This means that when you import a new data set or change a query device into a full-text search, it will be either case sensitive or not, depending on this setting. However, you can also specify whether or not each individual full- text search query device should be case sensitive by right-clicking on it. In the pop-up menu that appears, select Set Property > Search options > Ignore Case . By using this alternative, different query devices can have different settings.
Use Regular Expression in full text search	This sets the default behavior for full-text search query devices. This means that when you import a new data set or change a query device into a full-text search, it will either use regular expressions or not, depending on this setting. However, you can also specify whether or not each individual full- text search query device should use regular expressions by right- clicking on it. In the pop-up menu that appears, select Set Property > Search options > Use Regular Expression . By using this alternative, different query devices can have different settings. Note: When you save the visualization, the settings for each query device are saved in the SFS file and will remain when you open the file again. However, since the case sensitivity and regular expression settings are not available in versions older than DecisionSite 7.1, the full-text search query devices in older SFS files that are opened in DecisionSite 7.1 or later, will be based on the default settings in the Advanced options tab.
Show Bar Chart version 7.x toolbar button	In DecisionSite 8.0 a new improved bar chart was introduced. For legacy reasons it is still possible to create a version 7.x bar chart. Select this check box and restart DecisionSite Client to display a toolbar button which lets you create a version 7.x bar chart.
Export data using column formatters	Select this option to use the current formatting of all columns upon export. See Export Data for more information.

You can also set:

- The default width of the query device window
- Vertical or horizontal auto-tiling
- Default file location; this is the directory you want Spotfire DecisionSite to open when you select **File > Open**. Entering a single period character in this field means that Spotfire DecisionSite's *Spotfire/DecisionSite/Data/* directory will be the default.

4.9.7 View Tip

4.9.7.1 What is View Tip?

View Tip is a tool for rapid assessment of potentially interesting visualizations. It suggests visualizations based on the correlation between data in the columns, the number of unique values, and the distribution of data. In some cases the View Tip also suggests colors where this is appropriate.

View Tip is a convenient way of quickly getting to know a data set. As you browse through the different miniatures plots, you realize that View Tip is a natural first step when you start exploring unknown data.

To use the View Tip function:

Open the data set in Spotfire DecisionSite, and select **View Tip...** from the **Visualization** menu. Click on an item in the Scatter plots or Histograms list, or use the arrow keys to quickly browse either list.

When you have found an interesting visualization that you want to investigate further, click **Create View** to generate the corresponding visualization in Spotfire DecisionSite.

Click Close.

Note: Selecting a Histogram will create a "Version 7.x Histogram".

4.9.7.2 View Tip Algorithms

Ordering of scatter plots

View Tip calculates the correlation between different combinations of columns, and orders the suggested visualizations according to the degree of linear correlation.

The most common measure of correlation is the Pearson Product Moment Correlation (called Pearson's correlation for short). When computed in a sample, it is designated by the letter r and is sometimes called Pearson's r. Pearson's correlation reflects the degree of linear relationship between two variables. Pearson's ranges from +1 to -1.

Positive correlation

A correlation of +1 means that there is a perfect positive linear relationship between variables. This scatter plot depicts such a relationship. It is a positive relationship because high scores on the X-axis are associated with high scores on the Y-axis.



Negative correlation

A correlation of -1 means that there is a perfect negative linear relationship between variables. This scatter plot depicts such a relationship. It is a negative relationship because high scores on the X-axis are associated with low scores on the Y-axis.



Zero-correlation

A correlation of 0 means there is no linear relationship between the two variables, as shown in this graph. Correlation is rarely, if ever 0, 1, or -1.



With behavioral data, there is almost never a perfect linear relationship between two variables. The more the points tend to fall along a straight line, the stronger the linear relationship. View Tip calculates the absolute value for r, and then determines the rank of the scatter plots accordingly.

5 Query Devices

5.1 What is a Query Device?

A query device works like a filter, imposing constraints on the loaded data set. For example, a query device may exclude all records with values above a certain threshold. Only records that comply with the query device settings are visible in visualizations. When manipulating a query device, you can instantly see how the current setting affects the visible data. The visible data (and any empty values for the active axis) is also referred to as **selected**.

When a data set is loaded, each column in the underlying data set becomes associated with one query device. The type of device depends on the type of data in the column. Spotfire DecisionSite has five types of query devices: range sliders, item sliders, full-text search, check box query devices, and radio button query devices. (Also, the zoom bars work like range sliders.)

Searching for a Query Device

When using a data set with many columns, you often have just as many query devices. Sometimes it can be hard to find the query device you wish to manipulate by scrolling through the query device panel. A quick way to find a certain query device is to use the search function at the top of the query device panel. If you know the name of the column (Query Device) you want, simply begin typing it into the search box and the desired query device should come into focus. Any columns with names that do not match this are hidden from the query device panel. As you enter text, the query device panel is continuously updated with the query devices that begin with the current substring. To show all query devices again, just clear the search box. The query device search expression is based on case-insensitive substring matching of the column name. For example: Typing in "a" will match a column named "Apple" as well as a column named "Pear" but it will not match a column named "Lemon".

You can also navigate between the query devices using your keyboard. F3+up arrow or F3+down arrow will move you up or down one query device. F3+home or F3+end will move you to the first or last query device, and F3+page up or F3+page down will move you up or down one screen length among the query devices.



You can also navigate between the query devices using your keyboard. F3+up arrow or F3+down arrow will move you up or down one query device. F3+home or F3+end will move you to the first or last query device.

5.2 Range Sliders

Range sliders allow the selection of a range of values. The left and right drag box can be used to change the lower and upper limit of the range, meaning that only records with values within the chosen range are selected and therefore visible in the visualization. Labels above the slider indicate the selected span. The range can also be adjusted with the arrow keys when the query device is active: left and right arrows move the lower limit (left drag box), and up and down arrow keys move the upper limit. The slider automatically jumps to values in the data set (not necessarily the visible or selected records).

The currently selected interval of the range slider can be grabbed and moved to pan the selected range—this provides a powerful way of sweeping over different "slices" of a data set. Click and drag the yellow portion of the range slider to do this. Observing the reactions the other sliders to such a sweep can give some interesting clues to correlation between parameters in the data set.



An important feature of the range slider is that the values are distributed on a linear scale according to the values of the data. Thus if values are unevenly distributed, this will be reflected in the range slider.

Note: This is not the case with item sliders, where values are evenly distributed along the range of the slider, regardless of what values appear in the column.

Note: For more information on how strings are sorted in a query device please see Strings.

Adjusting the Range Slider span

The range slider can easily be adjusted to encompass only the currently selected data.

► Setting the range slider span to the current selection:

1. Double-click on the center of the range slider.



2. The range slider is now adjusted so as to show only the effective area:



3. To reset the range slider, double-click on the center of it again. The range slider is then reset to its maximum width.

Setting the left range slider span:

1. Double-click on the left drag box.



2. The range slider is now adjusted:



3. To reset the left range slider span, double-click on the left drag box of it again. The range slider is then reset to its maximum width.

Note: This function also applies to the zoom bars functionality.

Sometimes you might wish to filter the data in a column using a smaller range than the full range of the column. If so, you can set a range slider to encompass only a smaller range.

Setting the Data Range to Selected records:

1. The original Range Slider span is 0 to 40.

Home Runs	
0	40
Þ	

2. Move the drag box to narrow down the selection.



- 3. Right-click on the Range Slider to bring up the Query Device pop-up menu.
- 4. Select **Data Range > From Selected**. The Range Slider expands to its full width, but with the range 27 to 40. Three dots are displayed to indicate that the range is not the original full range.

Home Runs	
27	40
▶	🔳

5. To reset the span, right-click the Range Slider and select **Data Range > Reset**.

5.3 Item Sliders

In an item slider query device, data items are represented by their numerical values on a continuous linear scale. However, the item slider selects only a single item at a time. The selected value is displayed as a label above the slider. As a special case, all items are selected when the slider handle is at the extreme left of the scale.



The item slider features two levels of granularity-a coarse grain slider for moving rapidly between items, and a fine grain slider for moving more slowly between adjacent items.

Note: The scope of an item slider is dependent on the settings of other query devices. This means that the item slider range constantly changes as you manipulate the query devices. Items that fall outside of the current selection or zooming become unavailable and will be grayed out.

Note: For more information on how strings are sorted in a query device please see String. If you are working with large data sets—consisting of perhaps several hundreds of thousands of records—it can be quite tricky to get the slider to stop at the desired value. The solution to this problem is to use the fine-resolution handle together with the keyboard.

To pin-point a certain entry with the item slider:

Click the upper handle of the slider, and drag the box to the approximate position of the entry by keeping an eye on the currently selected value above the slider.

Fine tune with the fine resolution handle.

When the input focus is set on the slider (marked by a dotted line), you can use the arrow keys on your keyboard to adjust the slider to the exact position of the entry. Up and right arrows move to the next value, down and left to the previous one.

When the item slider drag box is moved to its leftmost position, all values for the slider are selected. This is indicated by the label (All) above the slider.

5.4 Full-text Search

5.4.1 Full-text Search

The full-text search query device allows you to search for (sub)strings within columns. It also allows you to search for a pattern by using Regular Expressions. For example, you can enter a pattern that means "a letter followed by two digits".

By *normal-text search*, we refer to search strings that don't contain regular expressions. The search can be made arbitrarily complex by use of logical operators AND (&) and OR (blank space). Search expressions are evaluated from left to right.

Once the search string has been entered, press Enter on your keyboard to execute the search. All records matching the search criteria will be shown in the visualization window.

The operators allowed in normal searches are:

white-space	logical OR
&	logical AND
" "	search for the exact sub-string within double quotes

The full-text search query device also supports Cut/Copy/Paste of text strings using the CTRL+X, CTRL+C and CTRL+V.

You can specify whether a full-text search query device should use regular expressions or not, by right-clicking on it. In the pop-up menu that appears, select or deselect **Set Property** > **Search Options** > **Use regular expression**.

Case sensitivity

When importing a new data set or changing a query device into a full-text search, the resulting full-text search query device(s) will be either case sensitive or not. This is determined by a setting in the **Tools > Options > Advanced options** tab called **Case sensitive full-text search**. If this check box is selected then searches done with the query devices will be case sensitive. However, you can also specify whether or not each individual full-text search query device should be case sensitive by right-clicking on it. In the pop-up menu that appears, select **Set Property > Search Options > Ignore case**. By using this alternative, different query devices can have different settings.

When you save the visualization, the settings for each query device are saved in the SFS file and will remain when you open the file again. However, since the case sensitivity and regular expression settings are not available in versions older than DecisionSite 7.1, the full-text search query devices in older SFS files opened in DecisionSite 7.1 or later, will be based on the default settings in the **Advanced options** tab..

Note: When a query device is changed into a full-text search query device, the "Show Empty Values" option from the Properties dialog is automatically set to False. This means that empty values are not included in the search result.

5.4.2 Using the Full-text Slider

The slider integrated in the full-text search query device is really just an item slider with one important difference: the *scope* of the slider corresponds to the result of the full-text search. This means that if you set the slider in its leftmost position (All), all items *that match the search criteria* will be shown (which doesn't necessarily mean all the records in the data set). Use the slider to select individual items among those that match the search criteria. Drag the upper portion and the scrolling will be rapid. If the search has resulted in many hits, some will not appear with the coarse selector. When in the appropriate region of hits, drag the fine-tuning lower portion to locate the specific value you want.

As with other sliders, once activated they can be adjusted with the keyboard arrows. Keyboard selection is always fine-grained, value by value.

generic name
ox & "pine \[inn\]" & zep
(ALL)
E

Let's look at the example in the figure above. Note that the brackets must be preceded by a backslash since brackets have a special meaning in regular expressions (see Regular Expressions below).

carb ox & "pine \[inn\]" & zep

Spotfire DecisionSite will evaluate the search expression in the following way

(carb OR ox) AND ("pine [inn]") AND zep

In plain English this means: "Show me all items where the column Generic Name contains names that include the sub-strings **carb** or **ox**, and also contains the full string **pine [inn]** as well as the sub string **zep**.

This means that OXCARBAZE<u>PINE [INN]</u> would be matched, but not AMOXAPINE [U;INN] or CARBAMAZEPINE [U;INN].

Note: The scope of a full-text slider is dependent on the settings of other query devices. This means that the slider range constantly changes as you manipulate the query devices. Items that fall outside of the current selection or zooming become unavailable and will be grayed out.

5.4.3 Introduction to Regular Expressions

Regular expressions constitute the standard pattern matching language, used heavily for searching and parsing text in most UNIX and Perl software.

Regular expressions allow you to construct a template or pattern for what you're searching for. You can then use your pattern template to determine whether a given text fragment matches your pattern.

For example, suppose you wanted to find all records beginning with the letter n. You would then want to construct a regular expression that would have the meaning "has a letter n as the first character on the line". The regular expression for this is:

^n

The h in regular expression syntax means "beginning of line". Therefore n means "line beginning with the letter n".

Next, we want to find records whose first word begins with n, and whose second word begins with the letter g. Let's say we also don't care whether the letters are upper or lower case. Here is the regular expression meaning "all lines whose first word begins with n and whose second word begins with g":

^n.+\s+g.+

The three main components of the pattern are 'n', '\s', and 'g'. The n means the letter n, the g the letter g, and the \s is a special character meaning "white space", or "any spaces", which could be a space, a tab, or a line break. Notice that both the n and the g are followed by a period. The period in regular expression syntax means "any character". Therefore, n. or g. means n followed any character and g followed by any character, respectively.

Finally, notice the 3 plus signs. A plus sign (+) in regular expressions means "one or more" and it always applies to the character immediately preceding it. Therefore, a+ means "one or more a's", "\s+" means "one or more white spaces", etc. Since . means "any character", then, .+ means "one or more of any character", and "n.+" means "the letter n followed by one or more letters.

Therefore, $^n.+\s+g.+$ means "an n at the beginning of the line followed by one or more characters followed by one or more spaces, tabs, etc., followed by a g, followed by one or more characters".

For a more thorough tutorial on regular expressions, a good source is the *O'Reilly & Associates nutshell guide* to either *Sed & Awk* or *Perl*. These are UNIX programming languages which are based heavily on regular expression pattern matching, and the O'Reilly guide for each of these languages contains a chapter devoted to regular expressions.

Microsoft's MSDN web site offers a complete reference to the symbols that can be used with Spotfire DecisionSite full text query devices.

5.4.4 List of Regular Expression Symbols

Symbol	Description
	Positions
^	Only match the beginning of a string. "^T" matches the first "T" in "To Be Or Not To Be"
\$	Only match the ending of a string. "t\$" matches the last "t" in "A cat in the hat"
\ b	Matches any word boundary "ly\b" matches "ly" in "probably not"
	Literals
Alphanumeric	Matches alphabetical and numerical characters literally.
\ n	Matches a new line
\ f	Matches a form feed
\ r	Matches carriage return
\ t	Matches horizontal tab
\ v	Matches vertical tab
\?	Matches ?
* 	Matches *
/+	Matches +
١.	Matches .
V	Matches
\{	Matches {
}	Matches }
11	Matches \
/[Matches [
/]	Matches]
)(Matches (
$\langle \rangle$	Matches)
	Character Classes
[xyz]	Match any one character enclosed in the character set. "[a-e]" matches "b" in "basketball".

[^xyz]	Match any one character not enclosed in the character set "[^a-e]" matches "s" in "basketball".
•	Match any character except \n.
\w	Match any word character. Equivalent to [a-zA-Z_0-9].
\ W	Match any non-word character. Equivalent to [^a-zA-Z_0-9].
/d	Match any digit. Equivalent to [0-9].
\D	Match any non-digit. Equivalent to [^0-9].
\s	Match any whitespace character. Equivalent to [\t\r\n\v\f].
\S	Match any non-whitespace character. Equivalent to $[^tr_nvf]$.
	Repetition
{ x }	Match exactly x occurrences of a regular expression. " $d{5}$ " matches 5 digits.
(x,}	Match x or more occurrences of a regular expression. "\s{2,}" matches at least 2 space characters.
{ x , y }	Matches x to y number of occurrences of a regular expression. "\d{2,3}" matches at least 2 but no more than 3 digits.
?	Match zero or one occurrences. Equivalent to {0,1}. "a\s?b" matches "ab" or "a b".
*	Match zero or more occurrences. Equivalent to $\{0,\}$.
+	Match one or more occurrences. Equivalent to {1,}.

5.5 Check Boxes

The Check box query device presents a set of check boxes—one for each unique value present in the column. One or several boxes may be selected or cleared to determine which values are to appear in the visualizations. If all records with a certain value are deselected by some other query device the label of that value becomes red.



A check box query device applied to the column Subject of the Film database. Coloring is set to categorical; ticking a check box causes all records of that particular color to show (unless they are deselected by another query device).

By default Spotfire DecisionSite assigns check boxes to any column containing ten values or less. Initially boxes all are selected, which makes all records in the data set visible. For quick selecting or clearing of all the values, right click on the check boxes query device, and select **All** or **None** from the pop-up menu.

Like radio buttons, check boxes provide options that are either On or Off. Check boxes differ from radio buttons in that you typically use check boxes for independent or nonexclusive choices.

5.6 Radio Button

In a radio button query device, a radio button represents each data item. Radio buttons, also referred to as option buttons, represent a single choice within a limited set of mutually exclusive choices. That is, in any group of option buttons, only one option in the group can be set at a time. However an "All" option is always present among the radio buttons, which lets you select all records. Items that are selected in the global context are marked with black labels, while globally deselected items have red labels.

The radio buttons query device, like the check boxes, presents a list of all values stored in a column, but allows only one value to be selected at any given time. When a new value is selected, the old one is deselected.

```
Malaise
ⓒ All
ⓒ no
ⓒ yes
```

5.7 Changing the Type of Query Devices

Spotfire DecisionSite makes an initial suggestion of what query device to use for each column in the data set. The type of query device to use for the column can then be changed, with one restriction: check boxes and radio buttons can only be used for columns having less than 500 unique values.



The query device pop-up menu. The currently selected query device is marked with a bullet.

► To change the type of query device:

- Right-click the query device to make the pop-up menu appear. Select the appropriate query device option from the pop-up menu, or
- select the Columns tab of the Properties dialog. This tab contains a list of all the columns in the data set. Mark a column and select the type of query device to use for that column.

5.8 Moving Individual Query Devices

Working with data sets containing a large number of columns does not necessarily mean that you need to manipulate them all at once. A more useful strategy is to select a few parameters, to see how they interact with each other. For this reason you may want to regroup them and rearrange their order, so that you do not have to scroll up and down to keep track of the changes.

The initial order of the Query Devices depends on the structure of the data set loaded into Spotfire DecisionSite or the SQL query that was used to acquire data. You can change this as needed by rearranging columns in the originating spreadsheet program or writing the SQL query in a certain order.

► To change the order of the query devices:

1. Right-click on the query device to be moved. A pop-up menu will open.



- 2. Place the cursor over the **Move** option. A submenu will appear.
- 3. Choose the command that reflects the direction in which to move the device. The options **Up** and **Down** move it one step upwards or downwards respectively. The options **To the top** and **To the bottom** make the query device the topmost or bottommost device respectively.

5.9 Sorting the Query Devices

The order of the query devices can be sorted in four ways: by original order, by annotation, by name, or by type. For example, you can group all range sliders together, or sort the query devices in alphabetical order.

► To sort the query devices:

1. Right-click on a query device.

2. Select **Sort** from the pop-up menu.



3. Select Original, by Annotation, by Name, or by Type.

Note: Sorting **by Type** means the type of Query Device, not the type of the column itself (Integer, String, etc.).

5.10 Hiding a Query Device

Right-click on the query device to be hidden. From the **Move** sub-menu of the pop-up menu that appears, choose **Hide**. Or deselect **Show Query Device** in the **Columns** tab of the Properties dialog, while having the correct column marked. A hidden query device can only be brought back by reselecting the **Show Query Device** option in the **Columns** tab.

Ou	erv Devices					x
Pla	atelD					
	Check Boxe Radio Butto Range Slider Item Slider Full Text Se	s ns r arch				
PI A	None All Data Range			н	•	
PI 2	 ✓ Show Empty ✓ Show Full Na 	[,] Values ame		11		
	Sort		×			
Pŧ	Move		Þ	To the Top		
0.	New Column 🔹 🕨		Up			
	Set Property	/	Þ	Down	Ч	-
De	Edit Annotal	Edit Annotation		To the Bottom		×
Co	olumn	Value		Hide		
Pla	atelD	41 510		15		

To hide the Query devices window altogether, either clear the check mark next to Query devices in the View menu or click on the small X beside the parallel bars at the edge of the window.

Que	ery Devices	•	×	
Plat	elD			l

5.11 Entering a Value for a Slider

A minimum or maximum value can be typed into a **range slider**, **item slider** or the **full-text search slider**. There are two ways of doing this:

► To enter a minimum value:

- 1. Double-click on the number above the left drag box.
- 2. Type the desired minimum value, and press ENTER.



► To enter a minimum value:

- 1. Click on the left drag box.
- 2. Type the desired minimum value.



► To move the full-text search slider:

- 1. Click on the drag box.
- 2. Type the desired value.

Country	
land	
Ireland	
E.	
English	
Population	

Note the difference between entering a value in the full-text search field (which filters out a subset of the data set, in this example all countries containing the letters "land"), and entering a value on the drag box (which moves the slider, in this example the first country containing the letters "Eng").

Note: Note that no "edit field" will appear in which to type the value. Simply type the value after clicking, and the slider will adjust itself.

Note: An item slider or full-text search slider will adjust itself to the existing value nearest possible to the value you typed, where as a range slider will adjust to the exact value you typed.

5.12 Indicators

The Query Devices can display two types of indicators: a paper clip icon which indicates that the column has an annotation, and a letter 'e' which indicates that the column contains empty values.

In order to see these indicators you must switch on this option. Do this by opening the **Columns** tab of the **Properties** dialog. Then select the check box marked **Show indicators in query devices**.

Annotating columns

See Annotating Columns for more information.

Empty values

By default, the query device shows records with null or empty values. When a column contains empty values a black colored letter 'e' is displayed in the upper right corner of the query device. You can choose to hide records with empty values by clearing the check box **Show Empty** values from the **Columns** tab of the **Properties** dialog, or by deselecting the menu item **Show Empty Values** from the query device pop-up menu. The 'e' will then turn red.

5.13 Changing Column Name

You can easily change the name of a column and its corresponding query device by doubleclicking on the query device.

To change the column name:

- 1. Double-click on the name of the query device you wish to rename.
- 2. Type a new column name in the text field that appears, and press Enter.

5.14 Quick Access to Color and Size Properties

A quick way of setting the color or size property in the current visualization is to right-click on the query device representing the column, and selecting the appropriate property from the **Set property** sub menu that appears.

5.15 Initial Query Device Selection

Spotfire DecisionSite's default choice of query devices is based on the column content and the number of unique values present in the data set for that attribute.

If a column contains 10 unique values or less, check boxes will be assigned as query device.

For columns containing more than 10 values, an item slider is chosen for alphanumeric (string) attributes, such as names and descriptions. Range sliders are assigned to numeric columns like date, time, and decimal or integer values.

6 Details-on-Demand and Legend

6.1 Details-on-Demand

The Details-on-Demand window displays the actual values of marked or active records. For objects that consist of multiple records (such as pies, bars, etc.) the Details-on-Demand window displays information appropriate to that object, such as average value, number of values, etc.

Presenting the Details-on-Demand

There are three different ways in which the information can be presented:

- As plain text in the details frame (default).
- As an HTML document based on Microsoft Internet Explorer displayed in the Detailson-Demand window.
- As an HTML based document in an external browser.

The HTML based details information can be formatted using the templates in the **Data and Background** tab of the **Properties** dialog. The bar chart and the pie chart have their own HTML templates. Details for the other visualizations are controlled by a set of templates working on active or marked records. The HTML based presentation can use all functions provided by modern browsers, e.g., images, tables, links to the Internet and Java applets. Further manipulation of the HTML template is described below.

6.2 Plain Text

Details-on-Demand 🛛 🛛		
Element	Atomic Number	Atomic Mass
Os	76	190
Pd	46	106
Pt	78	195
Re	75	186
Rh	45	102
Ru	44	101
Sc	21	45
•		► I

By default, Details-on-Demand displays data in plain text. The details window is placed in the lower right corner of the main window. It can of course be moved to another location if desirable. The details for a single active record are presented in a vertical table, those for several marked records in a horizontal table.

Adjusting column width

The width of the columns in the Details-on-Demand text display can be adjusted. By default the width is as wide as the header of the column. To change the width, place the mouse pointer on the separating line in the column header. The mouse pointer will change shape as shown in the illustration below. Click-and-drag the separator to the desired position. If you double click on the separator, the column width will collapse or expand to fit the longest value in the table.

Element	Atomic Numbe s D	Atomic Mass
Os	76	190
Pd	46	106
Pt	78	195
Re	75	186
Bh	45	102
Ru	44	101

Note: Columns can be completely hidden from view. To find a column that accidentally has been minimized, move the separator along the column headers until it is changed into a double separator as seen below, then click and drag to resize the hidden column.

Element	Δ 4 Atomic Number
Os	76
Pd	46
Pt	78
Re	75
Bh	45

Sorting values in columns

The values in all columns in the Details-on-Demand window can be sorted alphabetically and/or numerically. You can use either increasing or decreasing sort order.

► To sort a Details-on-Demand column:

1. Click on a column heading.

Element	Atomic Number	Atomic Mass
los ki	ີ 76	190
Pd	46	106
Pt	78	195
Re	75	186
Bh	45	102

2. The column is now sorted in increasing order. Click on the column heading again to toggle between increasing and decreasing order. Note the small arrow beside the column title, showing the sorted order.

Element Δ	Atomic Num	Atomic Mass
Os	76	190
Pd	46	106
Pt	78	195
Re	75	186
Rh	45	102

3. To revert to the original order, right-click in the Details-on-Demand window and select **Reset > Row Order** from the pop-up menu.

✓ Auto-Switch	
Selected Record(s) Marked Record(s) Active Record(s)	
Reset 🕨 🕨	Row Order
	Column Order 🔨

Rearranging column order

The horizontal order of the Details-on-Demand columns can be rearranged.

To rearrange column order:

- 1. Place the mouse pointer on a column heading.
- 2. Drag-and-drop the column heading to the left or right, to the desired place among the other column headings.
- 3. To revert to the original order, right-click in the Details-on-Demand window and select **Reset > Column Order** from the pop-up menu.

✓ Auto-Switch	1
Selected Record(s) Marked Record(s) Active Record(s)	
Reset 🕨 🕨	Row Order
	Column Order
	h

6.3 Locking the Details-on-Demand Window

The Details-on-Demand information can be locked to always show a certain category of records; Selected, Marked or Active. This "lock function" is controlled by the **Auto-Switch** option. (See Marking, Activating and Highlighting in the Visualizations chapter for more information.)

By turning Auto-Switch **on**, the Details-on-Demand window automatically updates the Detailson-Demand window if you mark new records or make one record active.

However, if you turn Auto-Switch **off**, the Details-on-Demand window will only show information about a certain category of your choice.

Example: You choose to display only *Selected* records by turning Auto-Switch off, and selecting the Selected Records option. Then you click on a record, which makes it *Active*. This will not cause the Details-on-Demand window to show information about that particular record, but instead it continues to display information about the currently *Selected* records.

To always show selected records:

- 1. Right-click in the Details-on-Demand window. A pop-up menu appears.
- 2. Clear the Auto-Switch option. (No checkmark should be shown to the left of the option).

Auto-S <u>w</u> itch	
Selected Record(s) Marked Record(s) Active Record(s)	
<u>R</u> eset	۲

3. Select Selected Records from the same pop-up menu.

Making a record active in the visualization will now have no effect on the Details-on-Demand window. The Details-on-Demand window will always display information about the currently selected records. If you use the Query Devices or zoom bars to change the selected records, the information in the window will be updated.

Note: The **Limit maximum number of records shown** option that can be found in the Data and Background tab of the Properties dialog applies only to the HTML Details-on-Demand, not to the text Details-on-Demand.

6.4 HTML

Spotfire DecisionSite can display the data for active or marked records as an HTML formatted document in the details frame. This is initialized by selecting **View > Details on Demand** (**Html**).

Spotfire DecisionSite uses the HTML template specified for the data set to lay out the information. If no template has been defined, the application will provide a default template for the type of visualization that is active.

Details-on-Demand (Html)	×
Pb	<u> </u>
Name :	Pb
Atomic number:	82
Atomic mass:	207
Atomic radius:	146
Ionic radius:	133
Ionization energy:	74
Electronegativity:	20
	-

It is also possible to launch an external browser, such as Netscape or Internet Explorer, to view the details of the data. To do so, select **View > Details on Demand (External Browser)**.

6.5 Editing HTML Templates

The HTML templates used for formatting record details are accessed and edited through the **Data and Background** tab of the **Properties** dialog box. There are six editable templates, one each for:

- Pie highlighted pie details.
- Bar highlighted bar details.
- Active Marker these are individual records in scatter plots, profile charts, line charts, tables or heat maps that have been clicked on.
- Marked Records Header the header part of the Details-on-Demand (DoD) shown for marked records in all types of plots.
- Marked Records Body the body part of the DoD shown for marked records in all types of plots.
- Marked Records Footer the footer part of the DoD shown for marked records in all types of plots.

When some records have been marked or activated, the details of those records are presented according to the three marked records templates.

The **Edit...** button brings up an edit box in which you can edit the selected template. In the HTML editing window you have several possibilities for creating and modifying the template.

E	dit Details-on-Demand	x
	<l- by="" code="" generated="" html="" is="" spotfire="" this=""></l->	
	<head> <title>Spotfire: \$(DBNAME)</title> </head>	
	Set colors to white background, black text, blue links <body bgcolor="#ffffff" text="#000000" link="#000088" vlink="#000055" alink="#0000ff" ></body 	
		
	Create a table with one line for each marked row	•
	Load Save As Default OK Cancel	

The HTML Edit window for the Marked records Header.

The **Load** button allows you to browse for an external file and use it as the template. Here, you can also load a template file that you previously have edited for the current or for a different data set. The **Save As...** button saves the changes in an external HTML file that can be used to format information in other DecisionSite sessions. The **Default** button will revert to the default settings and remove any changes made to the open template. **OK** applies the editing changes to the Details-on Demand window. **Cancel** removes any changes you have made since opening the **Edit** window.

When a new data set is loaded into Spotfire DecisionSite, the program creates default HTML templates that can be edited to suit your needs.

Tip: The HTML templates made for another data set will also be applied to the presently loaded data set if you apply the previously created data set as a template (**File > Apply Template**). In this case, not only the HTML Details-on-Demand, but also any visualization settings, query device settings and general settings will be applied. See Applying Templates for more information. For a template file to work properly, it should only be applied to data with a structure similar to the one used to create the template.

Variables

In the HTML templates, variables that refer to the value of a specific column or to other information can be used, which will then be replaced with current values from any active or marked record:

HTML variable	Refers to
\$(Name)	Value of a particular record in column 'Name'.
\$Format(Name)	Value of a particular record in column "Name", formatted according to the configured number formatting for the column and the Windows locale.
\$(DBDIR)	The full path to the location of the directory of the current database (file), including a trailing backslash.
\$(DBPATH)	The full path, including the file name, of the currently loaded database.

\$(DBFILE)

The name of the currently loaded database, including the file extension (.skv, .csv, etc.).

\$(DBNAME)

The name of the currently loaded database, excluding the file extension.

Additional variables for displaying descriptive statistics about the data set are described below.

6.6 **Descriptive Statistics for HTML Templates**

The following variables may be added into the HTML template to display information about the records.

Measurement	Variable	Explanation
VISIBLE	\$(VISIBLE)	# of visible points
MARKED	\$(MARKED)	# of marked points
SELECTED	\$(SELECTED)	# of selected points
ALL	\$(ALL)	# total

6.7 Editing HTML: An Example

There is a plethora of literature on HTML programming. This example is merely a short demonstration of changing the colors and typeface of the displayed details.

► To alter the appearance of the Details-on-Demand presentation:

- 1. Load a data set. In this example we will use the periodic.csv data set.
- 2. Select Edit > Properties, then click on the Data and Background tab.
- 3. From the **Template** drop-down list in the middle of the tab, select **Marked Records Header** and click on the **Edit...** button.
- 4. Add the following lines of code inside the header of the HTML page to present text in a straight typeface:

```
<style>
td {font: 10pt 'Helvetica'}
</style>
```

Note: This should be placed above the body of the template to affect the entire presentation. Notice also the use of 'curly brackets'.

5. Further down in the body, change the background color of the body to light blue by changing the color definition from #ffffff - white - to light blue:

bgcolor="#ddeeff"

6. Add the following line of code above the titles to make the title line appear with a light yellow background:

E	dit Details-on-Demand	X
	>	•
		
	Create a table with one line for each marked row	
	set title background to light vellow	
	*P1 *P2 /td>	
		_1
		<u> </u>
	Load Save As Default OK Cancel	

7. Click OK.

Select View > Details-on-Demand (External Browser).

Each time you mark a number of records the details will be presented in a horizontal table in your web browser.

6.8 Information About the Data Set

The record meter in the status bar at the bottom of the Spotfire DecisionSite gives continuous information about visualization statistics. You can see at a glance what portion of all the data is currently visible, marked, etc. The same information is displayed as text.



Colors should be read as follows:

Green – Records that are selected and marked.

Yellow - Records that are selected and unmarked.

Gray – Records that are selected, but lack a value required for representation on the current axes, and hence are invisible.

The sum of the above makes up the set of selected records. The length of the record meter in relation to the box in which it sits is an indication of the relative size of the current selection. To display or hide the status bar, use the **Status Bar** command in the **View** menu.

6.9 Legend

The markers of various plots can be colored to indicate a certain parameter. By showing the Legend window you can easily see what the color of a marker means. For Scatter Plots the

Legend also explains the significance of other visualization settings, that is, which columns are used for size, rotation, etc.

For other plots the Legend displays information about their relevant parameters. For example, in Bar Charts the Legend states what the height of the bars represents, and in Pie Charts the Legend states if the size of a pie corresponds to a certain parameter.

Also, if the plot has any active Statistical Measures, these will be described in the Legend.



► To display the Legend window:

Select View > Legend.

7 Working with the Data

7.1 Add Columns

7.1.1 Add Columns Overview

The Add Columns tool allows you to incorporate new columns into your current data set. Data can be added from a file, from the clipboard or by being opened and conditioned using advanced data import. The new columns are appended to the data set.

Note: When you are using the Add Columns tool, it is not possible to save the resulting data set as linked data. Only embedded data is supported. See Saving Spotfire files for more information.

7.1.2 Using Add Columns

7.1.2.1 Adding Columns from a File

Note: The matching of values in the selected ID columns is case sensitive. If existing record IDs are missing in the file which is merged into the data set, the values in the new column will be empty for these records. Records with IDs that do not exist in the original data set will not be added at all.

▶ To add columns from a file to an open data set:

- 1. Select **Data > Add Columns...**.
 - Response: The Add Columns Select Source dialog is opened.
- 2. Click the **File** radio button.
- Click Browse... and open the file from which you want to add columns. Comment: You can also type the path and file name directly in the text box. Comment: Common formats like CSV, TXT, XLS, SKV, SFS, SFA or XSF can be opened.
- 4. Click to select a **Column match method**. (In this step instruction it is assumed that you select **Manual**.)

Comment: If **Automatic** is selected, identifier columns with identical names (not case sensitive) must exist in both the old and the new data set. All columns with identical names will be used as identifier columns (implicit primary key matching). The new data set must also contain at least one new column. Clicking Finish in the first step of the wizard will add all columns with names that do not exist in the current data set. Clicking **Next** > will take you to the Add Columns - Select Columns dialog where you can select which columns to add.

Manual allows you to select which columns to use in the matching of identifiers (explicit primary key matching). Use this option if you want to make sure that the matching is correct.

5. Click Next >.

Response: The Add Columns - Select Matching Columns dialog is displayed.

- 6. If you have selected a Microsoft® Excel file, a second dialog is opened where you can choose the table or data sheet where the desired information is located. When you are done with your selections, click **OK** to reach the Add Columns Select Matching Columns dialog.
- 7. Click to select a column from the **Columns in new data set** that you want to use to map against your current data.

Comment: This should be some kind of ID column (preferably containing unique identifiers). If a record in this column is missing in the current data set, the record will not be added to the data set. For information about how non-unique values are handled, see Details on how data are added.

Comment: If a column has already been used in a matching, it will not be available in the *Columns in new data set* list. Select a column pair in the *Matching columns* list and click on **Remove** to make the columns available in the two selection lists again.

8. Click to select a column from the Columns in current data set.

Comment: This should be some kind of ID column (preferably containing unique identifiers). For information about how non-unique values are handled, see Details on how data are added.

9. Click Add Match.

Comment: The selected column pair is moved to the *Matching columns* list box. If desired, it is possible to use multiple key pairs. In this case, only records that have identical values in all of the selected column pairs will be added to the data set. For more information, see Details on how data are added.

10. Click Next >.

Response: The Add Columns - Select Columns dialog is displayed.

Comment: Clicking Finish in the second step of the wizard will perform the addition of columns by adding all columns from the new data set that were not selected among the Matching columns above to the current data set.

- 11. Click to select the columns to actually include in your data set. Comment: If a column to include has the same name as one of the columns already in the data set, it will be added with the suffix (1), (2), etc.
- 12. Click Finish.

Response: The new columns are added and query devices representing the new columns are shown in Spotfire DecisionSite. (You may have to scroll down in the Query Devices window to see the new query devices.)

7.1.2.2 Adding Columns from the Clipboard

Note: The matching of values in the selected ID columns is case sensitive. If existing record IDs are missing in the file which is merged into the data set, the values in the new column will be empty for these records. Records with IDs that do not exist in the original data set will not be added at all.

▶ To add columns from the clipboard to an open data set:

- 1. Copy the columns that you want to add (e.g., from an Excel data sheet) together with one or more ID columns to be used in the matching against the current data set.
- 2. Select **Data > Add Columns...**.
 - Response: The Add Columns Select Source dialog is opened.
- 3. Click the Clipboard radio button.
- 4. Click to select a **Column match method**. (In this step instruction it is assumed that you select **Manual**.)

Comment: If **Automatic** is selected, identifier columns with identical names (not case sensitive) must exist in both the old and the new data set. All columns with identical names will be used as identifier columns (implicit primary key matching). The new data set must also contain at least one new column. Clicking **Finish** in the first step of the wizard will add all columns with names that do not exist in the current data set. Clicking **Next** > will take you to the Add Columns - Select Columns dialog where you can select which columns to add.

Manual allows you to select which columns to use in the matching of identifiers (explicit primary key matching). Use this option if you want to make sure that the matching is correct.

5. Click Next >.

Response: The Add Columns - Select Matching Columns dialog is displayed.

6. Click to select a column from the **Columns in new data set** that you want to use to map against your current data.

Comment: This should be some kind of ID column (preferably containing unique identifiers). If a record in this column is missing in the current data set, the record will not be added to the data set. For information about how non-unique values are handled, see Details on how data are added.

Comment: If a column has already been used in a matching, it will not be available in the *Columns in new data set* list. Select a column pair in the *Matching columns* list and click on **Remove** to make the columns available in the two selection lists again.

7. Click to select a column from the Columns in current data set.

Comment: This should be some kind of ID column (preferably containing unique identifiers). For information about how non-unique values are handled, see Details on how data are added.

8. Click Add Match.

Comment: The selected column pair is moved to the *Matching columns* list box. If desired, it is possible to use multiple key pairs. In this case, only records that have identical values in all of the selected column pairs will be added to the data set. For more information, see Details on how data are added.

9. Click Next >.

Response: The Add Columns - Select Columns dialog is displayed.

Comment: Clicking Finish in the second step of the wizard will perform the addition of columns by adding all columns from the new data set that were not selected among the Matching columns above to the current data set.

10. Click to select the columns to actually include in your data set.

Comment: If a column to include has the same name as one of the columns already in the data set, it will be added with the suffix (1), (2), etc.

11. Click Finish.

Response: The new columns are added and query devices representing the new columns are shown in Spotfire DecisionSite. (You may have to scroll down in the Query Devices window to see the new query devices.)

7.1.2.3 Adding Columns using Advanced Data Import

The Advanced Data Import option in the Add Columns tool can be used to add columns to a data set from a different source than a file or the clipboard (e.g., from a database). It can also be used if the delimiter or data type must be modified to retrieve the data properly.

Note: The matching of values in the selected ID columns is case sensitive. If existing record IDs are missing in the file which is merged into the data set, the values in the new column will be empty for these records. Records with IDs that do not exist in the original data set will not be added at all.

► To add columns using advanced data import:

- 1. Select Data > Add Columns....
 - Response: The Add Columns Select Source dialog is opened.
- 2. Click the Advanced Data Import radio button.
- 3. Click to select a **Column match method**. (In this step instruction it is assumed that you select **Manual**.)

Comment: If **Automatic** is selected, identifier columns with identical names (not case sensitive) must exist in both the old and the new data set. All columns with identical names will be used as identifier columns (implicit primary key matching). The new data set must also contain at least one new column.

Manual allows you to select which columns to use in the matching of identifiers (explicit primary key matching). Use this option if you want to make sure that the matching is correct.

4. Click **Next** >.

Response: The Import Data - Select Data Source dialog is displayed.

- 5. Click to select whether to add data from a **File**, a **Database** or the **Clipboard** or use one of the **Advanced** options.
- 6. Click Next >.

Response: The Import Data - Data Conditioning dialog is displayed. (If you have selected one of the Advanced options you may be Guided through other wizards prior to reaching this dialog. See the online help for the wizard you are using for more information).

7. If desired, select a data conditioning method from the drop-down list.

Comment: It is possible to pivot data using a Tall/Skinny => Short/Wide converter or to use the Case normalizer to remove duplicate strings based on case insensitive comparison. For more information about the conditioning methods, see Data Conditioning.

8. Click Finish.

Response: The Add Columns - Select Matching Columns dialog is displayed. Comment: If you have selected Automatic as the Column Match method you will go straight to the Add Columns - Select Columns dialog where you can select which columns to add.

9. Click to select a column from the **Columns in new data set** that you want to use to map against your current data.

Comment: This should be some kind of ID column (preferably containing unique identifiers). If a record in this column is missing in the current data set, the record will not be added to the data set. For information about how non-unique values are handled, see Details on how data are added.

Comment: If a column has already been used in a matching, it will not be available in the *Columns in new data set* list. Select a column pair in the *Matching columns* list and click on **Remove** to make the columns available in the two selection lists again.

10. Click to select a column from the Columns in current data set.

Comment: This should be some kind of ID column (preferably containing unique identifiers). For information about how non-unique values are handled, see Details on how data are added.

11. Click Add Match.

Comment: The selected column pair is moved to the *Matching columns* list box. If desired, it is possible to use multiple key pairs. In this case, only records that have identical values in all of the selected column pairs will be added to the data set. For more information, see Details on how data are added.

12. Click Next >.

Response: The Add Columns - Select Columns dialog is displayed.

Comment: Clicking Finish here will perform the addition of columns by adding all columns from the new data set that were not selected among the Matching columns above to the current data set.

13. Click to select the columns to actually include in your data set.

Comment: If a column to include has the same name as one of the columns already in the data set, it will be added with the suffix (1), (2), etc.

14. Click Finish.

Response: The new columns are added and query devices representing the new columns are shown in Spotfire DecisionSite. (You may have to scroll down in the Query Devices window to see the new query devices.)

7.1.2.4 Adding Columns if Case Mismatches

Since the matching of values in the ID columns is based on a case-sensitive comparison, adding a column where the IDs are in lower case to a data set where the IDs are in upper case will not result in any values being added to the existing data. In this case, it can be useful to add a new column with all values expressed in lower case (or upper case) prior to the merge of new columns.

▶ To create an all lower case ID column in the current data set:

1. Select **Data > New Column > From Expression...** from the menu bar in Spotfire DecisionSite.

Response: The New Column from Expression - Enter Expression: Step 1(2) dialog is displayed.

- 2. Click to select the column you want to convert to lower case.
- 3. In the **Category** drop-down list on the right, select **Text Functions**.
- 4. In the **Function** list box, select **Lower**.
- 5. Click Insert Function.

Response: The function Lower () is inserted into the Expression box.

- 6. Click **Insert Columns** to use the column selected in step 1 as an argument to the function.
- Click Next >. Response: The New Column from Expression - Specify Column: Step 2(2) dialog is displayed.
- 8. Type a suitable name for the new column.
- 9. Click Finish.

Response: The column is added to the data set.

10. Use this column to match against the ID column of the new data set in the Add Columns wizard.

7.1.3 User Interface

7.1.3.1 Add Columns - Select Source Dialog

🚰 Add Columns - Select Source: Step 1 (3)			
Add columns fro	om:		
🖲 File 🛛	D:\Program Files\Spotfire\DecisionSite\Data\Employee_data.xls Browse		
C <u>C</u> lipboard			
⊂ <u>A</u> dvanced	data import		
Column match r	method:		
C A <u>u</u> tomatic			
⊙ <u>M</u> anual			
<u>H</u> elp	< <u>Back N</u> ext > Einish Cancel		
Option	Description		
File	Click this radio button and enter a path and a file name in the	Click this radio button and enter a path and a file name in the text	

	or click Browse to locate a file containing the data that you want to add.
Browse	Opens the Choose file dialog where you can select which file to open.
Clipboard	Click this radio button to add columns from a data set on the clipboard.
Advanced Data Import	Click this radio button to add data from a source other than a file or the clipboard (e.g., from a database). This option can also be used if the delimiter or data type must be modified to retrieve the data properly. Clicking Next > will display the Import Data wizard. For more
	information about the Import Data wizard, see Importing Data.
Automatic	Spotfire DecisionSite will automatically match columns with identical names (implicit primary key matching). Note: If you have columns with identical names that do not contain the same identifiers, this option might result in that no data is added. In that case, it is probably better to use the Manual option (see below), and match on columns that contain correct identifiers.
Manual	Select this option if you want to be able to select which columns to use in the matching of IDs (explicit primary key matching). Use this option if you want to make sure that the matching is correct.
Next >	Takes you on to the next step of the wizard. If Automatic has been selected as the Column match method you will go straight to the Add Columns - Select Source dialog. If Manual has been selected you will be Guided to the Add Columns - Select Matching Columns dialog.
Finish	Only available if the Automatic Column match method has been selected. All columns in the new and old data set that have identical names (not case sensitive) will be used as identifier columns. This means that all values in all of the identifier columns must match for the data to be added. All columns with names that do not exist in the current data set will be added.

► To reach the Add Columns - Select Source dialog:

Select Data > Add Columns....

7.1.3.2 Add Columns - Select Matching Columns Dialog

This dialog is used to specify which columns should be used as keys in the merging of the new columns with the columns in the original data set. Normally, one column pair containing IDs is enough, but in some cases it may be necessary to use two or more column pairs to create unique mappings between the two data sets.

Note: If the data types of your ID columns mismatch, click < **Back** and use the *Advanced data import* option to specify your data types manually (or add a type definition row to your data set prior to using the Add Columns tool).
Add Columns - Select Match	ing Columns: Step 2 (3	3)		×	1
Select how the new data will be m	erged with the current da	ta.		☑ <u>S</u> how ToolTips	
Columns in new <u>d</u> ata set:		Columns in <u>c</u> urrent o	lata set:		
Last name	String 🔺	Last name		String	
First name Salary	String Real	First name Job title		String String	
	Y				
	Add Match	<u>H</u> emove			
Matching columns:				A	
Help	< <u>B</u> ack	<u>N</u> ext >	<u>F</u> inish	Cancel	
Option	Description	n			
Show ToolTips	If selected, a To together with th upon hovering Columns in new data Last name First name Alce John Anastasia Jane Displaying Too a remote or slov the check box a	(String)	ing the name he first five un name with th ke some time In that case, aying ToolTi	and type of the c nique records is s ne mouse pointer e if you are conne you might want t ips.	ected to clear
Columns in new data set	Displays the co in a matching c A column can o time and will th been included i	olumns in the n columns pair. conly be used in herefore be gra in the Matching	ew data set th a single coluyed out in thi g columns lis	hat are available umn pair matchin is list box after it t box.	for use g at a has
Columns in current data set	Displays the couse in a column A column can of time and will the been included it	olumns in the c n pair. Sonly be used in herefore be gra in the Matching	urrent data se a single colu yed out in thi g columns lis	et that are availab umn pair matchin is list box after it t box.	le for g at a has
Add Match	Select an ID co to add the pair	lumn in both l to the Matchin	ist boxes abo g columns lis	ve and click Add st box.	Match

Remove	Select one or more column pairs in the Matching columns list box and click this button to remove the pairs from the list. This will return the columns to the list boxes of available columns above.
Matching columns	Displays the selected column pairs that specify how the merge between the two data sets will be made. If more than one pair is selected, only records that have identical values in all of the selected column pairs will be added to the data set. For more information, see Details on how data are added.
Finish	If Finish is clicked in the second step of the wizard, all columns in the new data set that are not used as identifiers in the Matching columns list will be added to the data set.

To reach the Add Columns - Select Matching Columns dialog:

- 1. Select **Data > Add Columns...**.
- 2. Make your choice in the Add Columns Select Source dialog, make sure that you have selected **Manual** as the Column match method, and click **Next** >.

7.1.3.3 Add Columns - Select Columns Dialog

Add Coldmins - 2	Select Columns, Step 3 (3)	
Select the columns	from the new data set to add to your data:	
Last name		
First name		_
Salaly		
1		
<u>H</u> elp	< <u>B</u> ack <u>N</u> ext> <u>F</u> inish Car	ncel

The list box shows the columns available for import. All columns in the new data set are listed. Per default, all new columns that are not included among the *Matching columns* in the previous dialog will be selected. Click the name of the column you want to add. For multiple selection, press **Ctrl** and click on the desired columns. You can also use **Shift** or drag the mouse over the desired columns.

► To reach the Add Columns - Select Columns dialog:

- 1. Select Data > Add Columns....
- 2. Make your choices in the Add Columns Select Source dialog and click Next >.
- 3. Make your choices in the Add Columns Select Matching Columns dialog and click **Next** >.

7.1.4 Theory and Methods

7.1.4.1 Details on How Data are Added

The merging is based on the selected ID fields of the current and the added data sets. The matching of names is case sensitive. If existing record IDs are missing in the data which are merged into the data set, the values in the new column will be empty for these records. Records with IDs that do not exist in the original data set will not be added at all.

If multiple IDs exist in the data to be added, the value in the added column will be the first record from the top in the data columns used for adding. See Example of adding columns with multiple IDs for more information.

If multiple IDs exist in the current data set, all of the entries will receive the value from the added column (the first in the column if there are multiple IDs in the column to be added (see above)).

If several matching column pairs are selected in the Add Columns - Select Matching Columns dialog, all values in the pairs must match for the data to be added. Multiple key pairs can be used to create unique identifiers from several ID columns with multiple IDs.

Note: Empty values work in the same way as other values. Hence, if empty values exist in the key column of the current data set and other records have empty values in the key for the columns to be added, there is a major risk that values are added to the wrong records. Therefore, it is advisable to not use columns containing empty values as key columns. See Example of adding columns with empty values for more information.

7.1.4.2 Example of Adding Columns with Multiple IDs

Imagine that you have a data set with the following columns and records loaded into Spotfire DecisionSite:

Last name	First name	Job title
Scott	Alice	Analyst
Ford	Henry	Analyst
Miller	John	Clerk
Smith	Jane	Clerk
Smith	George	Clerk

Note that there are two employees with the last name "Smith". Hence, the "Last name" column does not contain unique identifiers.

Now you want to add information about the salary of each employee which is located in a separate file or data sheet:

Last name	First name	Salary
Scott	Alice	3200
Miller	John	1300
Smith	Anastasia	4400
Smith	Jane	800
Smith	George	750

In this data set, the employee "Henry Ford" is missing and a person called "Anastasia Smith" is included who was not a part of the original data set.

The Add Columns tool can add the Salary column with the following results, depending on your selections in the Add Columns - Select Matching Columns dialog.

Matching columns:	Result:				
Last name <-> Last name	Last name	First name	Job title	Salary	
	Scott	Alice	Analyst	3200	
	Ford	Henry	Analyst		
	Miller	John	Clerk	1300	
	Smith	Jane	Clerk	4400	
	Smith	George	Clerk	4400	
	All employe in the Salar last name S not be adde Ford (since	ees with the y column, sin mith in the n d to the data he was not p	last name nce that w new data so set. No va present in t	Smith ge as the fir et. Anast alue is ad the new o	et the value 4400 rst record for the asia Smith will lded for Henry data set).
Last name <-> Last name	Last name	First name	Job title	Salary	
First name <-> First name	Scott	Alice	Analyst	3200	
	Ford	Henry	Analyst		
	Miller	John	Clerk	1300	

Smith Jane Clerk 800 Smith George Clerk 750 With both last name and first name used as key pairs, the identification is unique and the correct salary is entered for Jane and George Smith. This would be the correct way of

Example of Adding Columns with Empty Values 7.1.4.3

If you have empty values in the ID column of the current data set and other records have empty values in the ID column of the new data set, there is a major risk that values are added to the wrong records. Take a look at this simple example where the current data set contains an empty value:

performing the merge.

Last name	First name	Job title
Scott	Alice	Analyst
Ford	Henry	Analyst
	John	Clerk
Smith	Jane	Clerk

Now you want to add information about the salary of each employee which is located in a separate file or data sheet:

Name	First name	Salary
	Alice	3200
Ford	Henry	2800
Miller	John	1300
Smith	Jane	800

Note that there is another record that contains the empty value in this data set.

L Fi

Adding the column using *Last name* and *Name* as matching columns will produce the following result:

Last name	First name	Job title	Salary
Scott	Alice	Analyst	
Ford	Henry	Analyst	2800
	John	Clerk	3200
Smith	Jane	Clerk	800

The name Scott is missing in the new data set and Alice Scott will therefore not receive any value in the Salary column. The person in the original data set where no last name was entered (John) will be matched with the empty value in the new data set and, hence, receive the Salary 3200, even though this number has nothing to do with him. Selecting both last name and first name as key columns would have produced empty values for both Alice Scott and John X, which in this case would have been the correct procedure (unless it was possible to add the correct last names to the data sets prior to import).

7.2 New Column by Binning

7.2.1 Different Binning Methods

Depending on the type of values in the columns (numeric or alphanumeric, continuous or discrete) you may need to resort to different methods to rearrange the data. Spotfire DecisionSite provides a variety of binning methods:

Specific Limits

This option allows you to explicitly enter the values of the limits to use for each bin. Enter the value you wish to use for the limits of your bins and separate them with a semicolon. Do not use a space character after the semicolon.

Even Intervals

The subranges suggested are equal in scope. This is the default method, dividing the value range into equal intervals, and works for all data types except string. The current data range is divided up into the desired number of bins. Empty values will be empty in the new column, and when loading data sets from external sources (linked data) new values will be placed inside the bin, or in the upper and lower bin respectively.

Even Distribution

The suggested division works for all data types and is made so that the bins each contain an equal number of unique values. Extra values are placed in the final bins, so if you have four values and you want three bins with one value in each bin, your final value will be placed in the third bin. Empty values will be empty in the new column, and when loading data sets from external sources (linked data) the even distribution will be recalculated.

Cherry Picking

This method works for all data types and allows you to manually select which value to put in each bin. A list of all values in the column is shown. Cherry picking is useful when you want to be very specific with how you group your values. It is not recommended to use cherry picking when loading data sets from external sources (linked data) as the new values will become empty values.

► To bin a column by Cherry Picking:

- 1. Select **Data > New Column > By Binning...**.
 - Response: The New Column by Binning dialog is launched.
- 2. Select a **Column** to bin.

- 3. Select **Cherry Picking** as method and click the **Settings...** button. Response: The Cherry Picking dialog is launched.
- 4. To create a new bin, click New Bin.
- 5. Select the desired values in the **Available values** field, and click **Add** >> to add the values to a bin.
- 6. Use the **Rename Bin** button (or **F2**) to rename bins.
- 7. When all values have been assigned a bin, click **OK**.
- 8. Type a New column name for the binned column or use the default name.
- 9. Click OK.

Based on Standard Deviation

This method works for numeric columns. The range is divided into sections as described by the selected standard deviation multipliers. Bins are created using standard deviations +/- 0.5, 1, 2, 3, 6. In the example below, the range is divided into the following six subsections (μ denoting the average value for the column and s the corresponding standard deviation):

lower limit \rightarrow (μ -3s)

 $(\mu-3s) \rightarrow (\mu-s)$ $(\mu-s) \rightarrow \mu$ $\mu \rightarrow (\mu+s)$ $(\mu+s) \rightarrow (\mu+3s)$ $(\mu+3s) \rightarrow$ upper limit

Empty values will be empty in the new column, and when loading data sets from external sources (linked data) the standard deviation will be recalculated.

Substring

This method works for all data types. It groups the records by the first or last characters of the values in the column to be binned – the exact number of characters to take into account must be supplied. Suppose the column to be binned contains family names, beginning with Adams and ending with Winter. To bin the records according to the first letter in the name, use Divide by Substring considering one character from the beginning. Bin names are generated from the substring, and if **Ignore case** is used, the bin names are all formatted as upper case.

► To bin a column by substring:

- Select Data > New Column > By Binning.....
 Response: The New Column by Binning Dialog is launched.
- 2. Select a Column to bin.
- 3. Select the **Substring** radio button.
- 4. Decide whether to compare from the **Beginning** or **End** of the column value.
- 5. Set **Positions** to the number of characters that should be equal in each bin.
- 6. Select whether to **Ignore case**, that is whether "adams" and "Adams" would be considered the same or not.

Note: If the Positions is three and Ignore case is selected, the bin name in this example would be ADA.

- 7. Type a **New column name** for the binned column or use the default name.
- 8. Click OK.

Response: The Edit Bin Names dialog is launched.

- 9. Give the bins new names, if desired.
- 10. Click **OK**.

Empty values will be empty in the new column, and when loading data sets from external sources (linked data) the new values will be placed in new bins, taking the substrings into consideration.

7.2.2 Performing Binning

► To perform binning:

- Select Data > New Column > By Binning.... Response: The New Column by Binning dialog in launched. Note: You can also reach this dialog by right-clicking in the Query Device window and selecting New Column > By Binning....
- 2. From the drop-down list, select the name of the column that you want to bin.
- 3. Select the desired binning method and enter the respective values.
- 4. Type a **New column name** for the binned column or use the default name.
- 5. Click OK.
 - Response: The Edit Bin Names dialog is launched.
- 6. Enter the desired bin names and click **OK** to create the new column. This column can now be used as any other Spotfire DecisionSite column.

7.2.3 User Interface

7.2.3.1 New Column by Binning Dialog

New Column by Binning	×
Column:	
MOLREGNO	•
- Bin method	
C o	
Specific limits (for example -1;0,5;10;40)	-
0;1250;3500;5250;6800	-
C Even intervals	
Number of bins: 5	
C Even distribution	
Number of bins: 5	
Cherry picking Settings	
C Based on standard deviation	
+/- std dev to include: 🔽 0,5 🔽 1 🔽 2 🖾 3 🔽 6	
C Substring	
Compare from:	
Positions:	
I Igruie case	
New column name:	
Binned MOLREGNO	_
Help OK Cancel	

Option	Description
Column	Displays the available columns on which you can perform binning. The values from this column will be sorted into several bins or categories based on your selections.
Specific limits	Allows you to explicitly enter the desired values of the limits to use for each bin. Enter the value you wish to use for the limits of your bins and separate them with a semicolon.
Even intervals	Allows you to specify the desired number of bins and divides the value range into equal intervals.
Even distribution	Allows you to specify the desired number of bins and divides the bins so that each one contains an equal number of unique values.
Cherry picking	The Settings button opens the Cherry Picking dialog where you can manually select which value to put in each bin.

Based on standard deviation	The range is divided into sections as described by the selected standard deviation multipliers.
Substring	Groups the records by the first or last characters of the values in the column to be binned. Note: The exact number of characters to take into account must be supplied
	oupp
New column name	Here you supply the binned column with an appropriate name.

► To reach the New Column by Binning dialog:

Select **Data > New Column > By Binning...** or right-click in the Query Device window and select **New Column > By Binning...**.

7.2.3.2 Cherry Picking Dialog



Option	Description
Available values	The values available for use in the binning. Click a value in the list to select it. To select more than one value, press Ctrl and click the values in the list.
Add >>	Moves selected columns from the Available values field to the selected bin in the Bins field.
<< Remove	Removes a column and brings it back to the Available values field.
New Bin	Creates a new bin into which you can add values from the Available values field.
Rename Bin	Allows you to rename the bins with names of your choosing.

7.2.3.3 Edit Bin Names Dialog

Edit Bin Names	×	
A new column has t	been created: Binned Carbon	
Double-click to cha	nge the bin names in the new column.	
Bin Name	Name to Display	
x ≤ 15	Lower Values	
15 < x ≤ 19 19 < x < 23	Middle	
23 < x ≤ 27		
27 < X		
I		
1.5		
Help	UK	
Option	Description	
Bin name	Displays the default names from the New Column by Binning dialog.	
New name	Allows you to rename the bins with names of your own choosing.	
	Double-click on a bin to change the name.	
	Note: You are not required to change the names of the bins. If you	

7.3 New Column from Marked Records

7.3.1 New Column from Marked Records Dialog

When you have found an interesting subset in the data, you can mark these records and then create a new column indicating for each record whether it is part of the subset or not. By doing so, you will be able to toggle the subset, and also the records excluded from the subset. **Note:** Columns created from marked records cannot be saved in templates (SFT files) and

the default names are sufficient, simply click **OK**.

cannot be saved as linked data.

New Column from Marked Re	cords	×
Properties for the new column-		
Name:		
Marked 1		
Label for marked records:	Label for unmarked records:	
Yes	No	
	OK Cancel	

Option	Description
Name	Type a suitable name for the column to be created.
Label for marked records	Type a name for the value associated with marked records.
Label for unmarked records	Type a name for the value associated with unmarked records.

To reach the New Column from Marked Records dialog:

Select **Data > New Column > From Marked Records...** or right-click in the Query Device window and select **New Column > From Marked Records...**.

7.4 New Column from Expression

7.4.1 Calculating Columns

New columns can be computed from the current data set by using mathematical and logical expressions. This chapter describes how to create and evaluate such expressions using the New Column from Expression tool.

7.4.2 Workflow of the New Column from Expression Tool

Occasionally the columns included in a data set do not allow you to perform all necessary operations, or to create the visualizations needed to fully explore the data set. Still, in many cases the necessary information can be computed from existing columns. Spotfire DecisionSite provides the option to calculate new columns by applying mathematical and logical operators to existing values.

The following section explains the basic workflow of using the New Column from Expression tool. More detailed explanations on how to use the user interface and specifications of the various functions follows later in the chapter.

► How to use the New Column from Expression tool:

- 1. Start DecisionSite and load a data set.
- 2. Select Data > New Column > From Expression....

The first step of the wizard is displayed. You can also reach the tool by right-clicking a query device.

- 3. If you have previously created a suitable expression, you may select it from the **Recent Expressions** list and click the **Insert** button.
- 4. If you need to create a new expression, proceed to specify the expression by either typing it directly into the **Expression** text area or by selecting columns and functions from the lists.

By selecting columns and functions, and clicking the **Insert Columns** or **Insert Function** buttons, you can gradually build the expression you want. You can always modify the expression by editing the text in the Expression field, using cut&paste or typing text.

An example of an expression could be: [Exports m\$]/[Population]

5. Verify that the result seems reasonable by looking at the **Sample result** field. This field will display the result of applying the expression to the first row of the data set.

If this field shows an error message, there is a problem with the expression. Moving the mouse pointer over the field or clicking on it, will display an explanation of what is wrong.

6. When you are satisfied, press the **Next** > button.

The second step of the wizard is displayed.

- 7. Fill in the new Column name if the default name is not acceptable.
- 8. Change the **Column type** if you want to.
- 9. Watch the preview and verify that the result is what you want. If not, click on the < **Back** button to go back and modify the expression until the desired result is achieved.
- 10. Click on the **Finish** button.
- 11. The expression is now evaluated for each row in the data set and a new column is created. A new query device will appear with the name of the new column you created.

If the new column data still is not what you intended, delete the column from the **Properties** dialog, and invoke the **New Column from Expression...** tool again.

7.4.3 User Interface Description

7.4.3.1 Enter Expression Dialog

The dialog can be resized to provide more space for editing and for the lists.

• New Column from Expression - Enter Expression: Step 1(2)		
Columns Column:	Functions Category:	
*P2 Element Atomic Number Atomic Radius Ionic Radius Ionization Energy Electronegativity *C1	Function:	
*C2 Selected columns: Types: [Atomic Mass] Integer Insert Columns Expression:	Divides Arg1 by Arg2. Example: 3.5 / 2.5	
[Atomic Mass]/[Ionic Radius]	Ă	
Recent expressions:	Sample result: 1.8015873015873	
Help < Back Next >	<u> </u>	

Columns

Select a column by clicking on it, and click the **Insert Columns** button to insert it to the **Expression** field. You can also double-click on a column to insert it. You can select several columns by pressing **Ctrl** or **Shift**.

If you place the cursor at a specific location in the **Expression** field, the column will be inserted there.

If you have many columns you can use the scrollbar to find them, or click on any column and type in the first letter of the desired column name to jump to it.

You can see the Type of the selected column in the field below the list.

Category

Select a category of functions to limit the choices in the Function list.

- All
- Operators
- Math Functions
- Statistical Functions
- Text Functions
- Logical Functions
- Date & Time Functions
- Conversion Functions

Function

Select a function by clicking on it, and click the **Insert Function** button to insert it to the **Expression** field. You can also double-click on a function to insert it.

If you place the cursor at a specific location in the **Expression** field, the function will be inserted there.

If you have many columns you can use the scrollbar to find them, or click on any function and type in the first few letters of the desired function name to jump to it.

Description

This field provides a brief description of the selected function. For more detailed descriptions, please see Spotfire Expression Language (SXL).

Expression

This is the text field in which you build your expression. You can insert columns and functions to it from the lists, or enter text as in any standard text editor.

Cut/Copy/Paste works in the field using standard Ctrl+X/Ctrl+C/Ctrl+V.

Highlighting a section of the expression, and inserting a new function will cause that function to encompass the highlighted section within parenthesis.

Also, Undo/Redo functionality is available by pressing Ctrl+Z/Ctrl+Y respectively.

Recent expressions

This list contains the twenty most recent expressions you have created. You can select one of these and click the Insert button to insert the expression into the **Expression** field. This will not replace the entire content of the field, only insert the selected expression at the cursor position.

Sample result

This field displays the result of applying the current expression to the first row of the data set. If this field shows an error message, there is a problem with the expression. Moving the mouse pointer over the field or clicking on it, will display an explanation of what is wrong. Pressing **F5** will also display the error description. Pressing **F4** will move the cursor to the position in the expression where the error lies.

There are three kinds of error messages:

#EXPR! – there is a problem with the syntax of the expression.

#NUM! - the row evaluates to infinity or other illegal number.

#ARG! - there is a problem with one or many arguments.

7.4.3.2 Specify Column Dialog

The dialog can be resized to provide more space for editing and for the lists.

New Colum	n from Expression -	Specify Column: Ste	p 2(2)		×
<u>C</u> olumn name:	umn name: Calculated Column				
Column <u>t</u> ype:	Column type: Real (Decimal)				
Expression:					
[Populatio	n]+[Pop.growthr	. (ppm)]			×
Preview:					
Population	Pop	.growthr.(ppm)		Calculated C	olumn
3273131	19			3273150	
3335044	18			3335062	
3285224	11			3285235	
3333839	12			3333851	
7867541	7			7867548	
7915145	5			7915150	
10373881	5			10373886	
10370269	3			10370272	
9909285	1			9909286	
9921910	1			9921911	
10016623	30			10016653	
Help	1	< Back	Nevts	Finish	Cancel
			Tileur /	<u></u> .	Cancer

Column name

Enter the name for the new column in this field.

Column type

This drop down box lets you select which Type the new column should have:

- String
- Integer
- Decimal
- Date
- Time
- DateTime

Expression

This field displays the expression which will be used to evaluate the new column. You cannot edit this field. Click the **< Back** button if you want to modify the expression.

Preview

This table provides a preview of how the first rows in the data set will be evaluated using the current expression. It displays the columns that are used in the expression and the resulting column. You can resize the window to show more rows.

Move the mouse pointer over the column headings to display a ToolTip stating the Type of the columns.

If the resulting column shows an error message, there is a problem with the expression for that row. Moving the mouse pointer over the field or clicking on it, will display an explanation of what is wrong.

There are three kinds of error messages:

#EXPR! – there is a problem with the syntax of the expression.

#NUM! - the row evaluates to infinity or other illegal number.

#ARG! - there is a problem with one or many arguments.

7.4.4 Spotfire Expression Language (SXL)

7.4.4.1 General Syntax

Spotfire DecisionSite uses an Expression Language which is described in this chapter. Some notes on the general syntax are:

Variables, functions and keywords are case insensitive:

SUM(C1) = Sum(C1) = sum(C1)

Column references are case sensitive.

The default null handling behavior is that operations on null return null.

7.4.4.2 Data Types

The data types with built in language support are:

- Integer
- Real
- Boolean
- String

Integer

Integer values are written as a sequence of digits, possibly prefixed by a + or - sign. If used where a decimal value was expected, they are automatically converted to a decimal value. **Note:** Hexadecimal formatted values have a size limitation of 8 characters.

Examples:

```
0

101

-32768

+55

0xff = 255

0x7ffffff = 2147483647

0x80000000 = -2147483648
```

Real

Real values are written as standard floating point numbers with a period for a decimal point and no thousands separator. The real values that can be specified range from

-1.79769313486231e+308 to 1.79769313486231e+308.

The exponent of real value constants may range from -307 to 308.

Math operations on real values that produce results that can't be represented by the real data type generate numeric errors. In the resulting data set, these special cases will be filtered out and replaced by null.

Examples:

0.0 0.1 10000.0 -1.23e-22 +1.23e+22 1E6

Boolean

True or false. Booleans are used to represent true and false values returned by comparison operators and logical functions.

Examples:

true false 1 < 5

String Literals

String literals are surrounded by double quotes or single quotes. A string literal can contain any sequence of UNICODE characters. A double quote can't be used within the string unless it is escaped. Backslash is used to escape special characters, so it must also be escaped. The basic escaping rules are that only the characters defined below can be used after a \; everything else will generate an error.

Escape sequence	Result
\иНННН	Any Unicode character expressed as four hexadecimal characters
\0000	A character in the range 0-255 expressed as three octal digits 0-7
\b	\u0008: backspace (BS)
\t	\u0009: horizontal tab (HT)
\n	\u000a: linefeed (LF)
\f	\u000c: form feed (FF)
\r	\u000d: carriage return (CR)
\"	\u0022: double quote "
٧'	\u0027: single quote '
//	$u005c: backslash \$

Examples:

"Hello world" "25\"23" "1\n2\n" "C:\\TEMP\\image.png"

Column References

Accessing columns are done by either simply writing the column name, or enclosing the column name in square brackets. The brackets are needed when the column name contains characters other than letters, digits or _ (underscore), or if the column name begins with a digit. If a column name is bracketed; any end brackets and backslashes in the column name must be

escaped by $\]$ or $\$ respectively. The same backslash escaping rules as for strings are followed, except that double quotes (") may not be escaped.

Examples: Column1 [Column1] [Binned Column1]

[1] [!@#\$%^&*()[\]\\]

Time, Date, TimeStamp

- Time A time of day type, range 0:00 to 24:00.
- Date Date type ranging from January 1st, 100 to December 31st, 9999.
- TimeStamp A combination of Time and Date.

Mathematical operations on date, time and timestamp data types are supported in DecisionSite 9.0 and forward.

For example, it is possible to calculate how many days it differs between two date columns. When a date, time or timestamp column is subtracted from another date, time or timestamp column, the corresponding result column will show the number of days as a real (decimal) column. For example, "2006-10-10 7.00 AM minus 2006-10-10 1.00 AM" equals 0.25 since 6 hours is a quarter of a day.

7.4.4.3 Operators

7.4.4.3.1 Operators Overview

Please select which type of Operators you are interested in: Unary Operators (Operators with only one argument) Binary Operators (Operators with two arguments) Trinary Operators (Operators with three arguments) Operator Precedence

7.4.4.3.2 Unary Operators

A unary operator takes one argument following the operator.

Operator	Description
- Argl	Negates the argument. The argument and the result are of type real.
! Arg1	Returns the logical Not of <i>Arg1</i> . The argument and the result are of type boolean. See also function Not.
Example: !true -> false !false -> true	

7.4.4.3.3 Binary Operators

A binary operator takes two arguments, one preceding and one following the operator.

Operator	Description
Arg1 + Arg2	Adds the two arguments. The arguments and the result are of type real. See operator & for string concatenation.

Arg1 – Arg2	Subtracts <i>Arg2</i> from <i>Arg1</i> . The arguments and the result are of type real.
Arg1 * Arg2	Multiplies the two arguments. The arguments and the result are of type real.
Arg1 / Arg2	Divides <i>Arg1</i> by <i>Arg2</i> . The arguments and the result are of type real. Division by zero results in an error. Example: 7/2 -> 3.5 0/0 -> #NUM! -1/0 -> #NUM!
Arg1 & Arg2	Appends <i>Arg2</i> to the end of <i>Arg1</i> . The arguments can be of any type, but are converted to strings. The result is of type string. See also function Concatenate. Example: "April " & (20+1) & "st" -> "April 21st" null & "Ape" -> #NULL!
Arg1 < Arg2	Returns true if <i>Arg1</i> is less than <i>Arg2</i> . The arguments are of type real and the result is of type boolean. The function is defined for comparing normal numbers to each other and to \pm Infinity. It is also defined for comparing Infinity to -Infinity. Other combinations result in errors or null. Example: $1 < 2 \rightarrow$ true $1 < $ null \rightarrow #NULL! $1 < 1/0 \rightarrow$ true $1/0 < 1/0 \rightarrow$ true $1 < 0/0 \rightarrow$ true $1 < 0/0 \rightarrow$ #NUM!
Arg1 > Arg2	Returns true if $Arg1$ is greater than $Arg2$. The arguments are of type real and the result is of type boolean. See operator < for the definition of valid arguments.
Arg1 <= Arg2	Returns true if $Arg1$ is less than or equal to $Arg2$. The arguments are of type real and the result is of type boolean. See operator < for the definition of valid arguments.
Arg1 >= Arg2	Returns true if $Arg1$ is greater than or equal to $Arg2$. The arguments are of type real and the result is of type boolean. See operator < for the definition of valid arguments.
Arg1 = Arg2	Returns true if <i>Arg1</i> is equal to <i>Arg2</i> . The arguments can be of any type, but must both be of the same type. The result is of type boolean. If any argument is null, the result is null. See function IsNull for comparing nulls. For arguments of type real, see operator < for the definition of valid arguments. Example: "Hello" = "hello" -> false "" = null -> #NULL! null = null -> #NULL!
Arg1 $>$ Arg2	Returns true if $Arg1$ is not equal to $Arg2$. The arguments can be of any type, but must both be of the same type. The result is of type boolean. If any argument is null, the result is null. See function IsNull for comparing nulls. For arguments of type real, see operator < for the definition of valid arguments.

Expr1, Expr2 Evaluates both expressions and returns *Expr2*. The expressions can be any valid expression, including expressions that evaluate to null.

7.4.4.3.4 Trinary Operators

A trinary operator takes three arguments.

Operator

Arg1? Arg2: Arg3	Returns Arg2 if Arg1=true, and Arg3 if
	Arg1=false. Arg1 is of type boolean, usually
	the result of a comparison. Arg2 and Arg3 can
	be of any type, but must both be of the same
	type or null. If Arg1 is null, the result is also
	null. See also function If.

Description

Example:

([Count] > 3)? "many": "few" true? null: null -> #NULL! true? 1: null -> 1 false? null: 2 -> 2 null? 1: 2 -> #NULL!

7.4.4.3.5 Operator Precedence

Below is a table showing the hierarchy of SXL operators with the highest precedence operator shown first.

Expressions inside parentheses are evaluated first; nested parentheses are evaluated from the innermost parentheses to the outer.

Operators in the same row in the chart have equal precedence

Туре	Order of Evaluation
Parentheses	left to right
Not	right to left
Unary minus and plus	right to left
Multiplicative	left to right
Additive	left to right
Concatenation	left to right
Relational	left to right
Equality	left to right
	TypeParenthesesNotUnary minus and plusMultiplicativeAdditiveConcatenationRelationalEquality

7.4.4.4 Functions

7.4.4.4.1 Math Functions

Function	Description
Abs(Arg1)	Returns the absolute value of <i>Arg1</i> . The argument and the result are of type real.
ACos(Arg1)	Returns the arccosine of $Arg1$ as an angle expressed in radians in the interval $[0, \pi]$. $Arg1$ must be in the interval $[-1.0, 1.0]$, otherwise NaN is returned. The

	argument and the result are of type real.
ASin(Arg1)	Returns the arcsine of <i>Arg1</i> as an angle expressed in radians in the interval
	$[-\pi/2, \pi/2]$. Arg1 must be in the interval $[-1.0, 1.0]$, otherwise NaN is returned. The argument and the result are of type real.
ATan(Arg1)	Returns the arctangent of <i>Arg1</i> as an angle expressed in radians in the interval $[-\pi/2, \pi/2]$. The argument and the result are of type real.
Ceiling(Arg1)	Rounds <i>Arg1</i> up to the nearest natural number. The argument and the result are of type real. Example: Ceiling(1.01) -> 2.0 Ceiling(-1.99) -> -1.0
Cos(Arg1)	Returns the cosine of <i>Arg1</i> where <i>Arg1</i> is an angle expressed in radians. The argument and the result are of type real.
Exp(Arg1)	Returns e (2.718281) raised to the <i>Arg1</i> power. The argument and the result are of type real.
Floor(Arg1)	Rounds <i>Arg1</i> down to the nearest natural number. The argument and the result are of type real. Example: Floor(1.99) \rightarrow 1.0 Floor(-1.01) \rightarrow -2.0
Ln(Arg1)	Returns the natural logarithm of $ArgI$. The arguments and the result are of type real. If $ArgI$ is negative, the result is a NaN error. If $ArgI$ is zero, the result is Infinity error.
Log(Arg1, Arg2)	Returns the logarithm of $Arg1$ expressed in the base specified by $Arg2$. Equivalent to $Ln(Arg1)/Ln(Arg2)$. The arguments and the result are of type real. See function Ln for the definition of valid arguments.
Log10(Arg1)	Returns the 10-based logarithm of $Arg1$. Equivalent to $Ln(Arg1)/Ln(10)$. The arguments and the result are of type real. See function Ln for the definition of valid arguments.
Mod(Arg1, Arg2)	Returns the reminder of the division of $Arg1$ by $Arg2$, The arguments and the result are of type real. If $Arg2$ is 0, the result is NaN. Mod($Arg1$, $Arg2$) is defined as: Arg1 – Arg2*Floor(Arg1/Arg2)
PI()	Returns the numerical constant π . The result is of type real.
Power(Arg1, Arg2)	Returns <i>Arg1</i> raised to the <i>Arg2</i> power. The arguments and the result are of type real. Example: Power(10, 3) -> 1000 Power(10, -3) -> 0.001 Power(0, 0) -> 1

Product(Arg1,)	Returns the product of the arguments. The arguments and the result are of type real. Null arguments are ignored and do not contribute to the product. Example: Product(-1) -> -1 Product(1.5, -2, 3) -> -9 Product(1, null, 3) -> 3 Product(null) -> #NULL!
Round(Arg1, Arg2)	Rounds <i>Arg1</i> to the number of decimal places specified by <i>Arg2</i> . The arguments and the result are of type real, but for <i>Arg2</i> , only the integer part is used. Note that <i>Arg2</i> can be negative to round to even 10s, 100s etc. 0.5 is rounded upwards to a number with higher magnitude (ignoring the sign). Example: Round(PI(), 3) $>$ 3.142 Round(-0.5, 0) $>$ -1 Round(25, -1) $>$ 30
Sin(Arg1)	Returns the sine of <i>Arg1</i> where <i>Arg1</i> is an angle expressed in radians. The argument and the result are of type real.
Sqrt(Arg1)	Returns the square root of <i>Arg1</i> . The argument and the result are of type real. If <i>Arg1</i> is negative, the result is a NaN error.
Sum(Arg1,)	Returns the sum of the arguments. The arguments and the result are of type real. Null arguments are ignored and do not contribute to the sum. Example: Sum(-1) -> -1 Sum (1.5, -2, 3) -> 2.5 Sum (1, null, 3) -> 4 Sum (null) -> $\#$ NULL!
Tan(Arg1)	Returns the tangent of <i>Arg1</i> where <i>Arg1</i> is an angle expressed in radians. The argument and the result are of type real.

7.4.4.2 Statistical Functions

Function	Description
Average(Arg1,)	Returns the average (arithmetic mean) of the arguments. The arguments and the result are of type real. Null arguments are ignored and do not contribute to the average.
	Example: Average(-1) -> -1 Average (1.5, -2, 3.5) -> 1 Average (1, null, 3) -> 2 Average (null) -> #NULL!
Max(Arg1,)	Returns the largest of the arguments. The argument and the result are of type real. Null arguments are ignored.

Example:
Max(-1) -> -1
$Max (1.5, -2, 3) \rightarrow 3$
Max (1, null, 3) -> 3
Max (null) -> #NULL!
Returns the smallest of the arguments. The argument and the result are of type real. Null arguments are ignored.
Example:
Min(-1) -> -1
Min (1.5, -2, 3) -> -2
Min (1, null, 3) -> 1
Min (null) -> #NULL!

7.4.4.3 Logical Functions

Function	Description
And(Arg1,)	Returns the logical And of the arguments. If any argument is false, the result is false. Otherwise, if any argument is null, the result is null. If all arguments are true the result is true. The arguments and the result are of type boolean. Example: And(true, false, true) -> false And(false, null) -> false And(true, null) -> #NULL!
If(Arg1, Arg2, Arg3)	Returns <i>Arg2</i> if <i>Arg1</i> =true, and <i>Arg3</i> if <i>Arg1</i> =false. <i>Arg1</i> is of type boolean, usually the result of a comparison. <i>Arg2</i> and <i>Arg3</i> can be of any type, but must both be of the same type or null. If <i>Arg1</i> is null, the result is also null. See operator ? : Example: If([Count] > 3, "many", "few") If(true, null, null) -> #NULL! If(true, 1, null) -> 1 If(false, null, 2) -> 2 If(null, 1, 2) -> #NULL!
IsError(Expr1)	 Returns true if <i>Expr1</i> evaluates to an error, and false if Expr1 evaluates to a proper value or null. Errors are e.g. numeric errors (NaN, ±Infinity), conversion errors and indexing errors. <i>Expr1</i> can be of any type and the result is of type boolean. Example: IsError(0/0) -> true IsError(null) -> false IsError(Left("A", -1)) -> true IsError(Real("Hello")) -> true (conversion)
IsNull(Arg1)	Returns true if <i>Arg1</i> is null, false otherwise. <i>Arg1</i> can be of any type and the result is of type boolean. Example:

	IsNull(0) -> false IsNull(null) -> true IsNull(0/0) -> #NUM!
Not(Arg1)	Returns the logical Not of <i>Arg1</i> . The argument and the result are of type boolean. See also unary operator ! Example: Not(true) -> false Not(false) -> true
Or(Arg1,)	Returns the logical Or of the arguments. If any argument is true, the result is true. Otherwise, if any argument is null, the result is null. If all arguments are false the result is false. The arguments and the result are of type boolean. Example: Or(false, true, false) -> true Or(false, null) -> true Or(false, null) -> #NULL!
Xor(Arg1, Arg2)	Returns the logical Xor of the arguments. If exactly one argument is true, the result is true, otherwise false. If any or both arguments are null, the result is null. The arguments and the result are of type boolean. Example: Xor(true, false) -> true Xor(true, true) -> false Xor(true, null) -> #NULL!

7.4.4.4 Text Functions

Function	Description
Concatenate(Arg1,)	Concatenates (appends) all the arguments into a string. The arguments can be of any type, but are converted to strings. The result is of type string. Null arguments are ignored. Example: Concatenate("April ", 20+1, "st") -> "April 21st" Concatenate(null, "Ape") -> "Ape" Concatenate (null, null) -> #NULL!
Find(Arg1, Arg2)	Returns the 1-based index of the first occurrence of the string <i>Arg1</i> in <i>Arg2</i> . If not found, 0 is returned. The search is case- sensitive. The arguments are of type string and the result is of type integer. If <i>Arg1</i> is the empty string, 0 is returned. Example: Find("lo", "Hello") -> 4 Find("a", "Hello") -> 0 Find("", "Hello") -> 0 Find("", null) -> #NULL! If(Find("Pri 1", [Col1])>0, "Important", "Not important")
Left(Arg1, Arg2)	Returns the first $Arg2$ characters of the string $Arg1$. $Arg1$ and the result are of type string. $Arg2$ is of type real, but only the integer part is used. If $Arg2 >$ the length of $Arg1$, the whole string is returned. If $Arg2$ is negative, an error is returned. Example:

	Left("Daddy", 3.99) -> "Dad" Left("Daddy", 386) -> "Daddy" Left("Daddy", -1) -> #ARG!
Len(Arg1)	Returns the length of the string <i>Arg1</i> . <i>Arg1</i> is of type string and the result is of type integer. Example: Len("Hello") -> 5 Len(null) -> #NULL!
Lower(Arg1)	Returns <i>Arg1</i> converted to lowercase. <i>Arg1</i> and the result are of type string.
Mid(Arg1, Arg2, Arg3)	Returns the substring of $Arg1$ starting at index $Arg2$ with a length of $Arg3$ characters. $Arg1$ and the result are of type string. $Arg2$ and $Arg3$ are of type real, but only the integer part is used. If $Arg2 > \text{Len}(Arg1)$, an empty string is returned. Else, if $Arg2+Arg3 > \text{Len}(Arg1)$, $Arg3$ is adjusted to 1+Len $(Arg1)$ - Arg2. If either $Arg2$ or $Arg3$ is negative or if $Arg2$ is zero, an error is returned. Example: Mid("Daddy", 2, 3) -> "add" Mid ("Daddy", 4, 386) -> "dy" Mid ("Daddy", -1, 2) -> #ARG! Mid ("Daddy", 2, -1) -> #ARG!
Right(Arg1, Arg2)	Returns the last $Arg2$ characters of the string $Arg1$. $Arg1$ and the result are of type string. $Arg2$ is of type real, but only the integer part is used. If $Arg2$ > the length of $Arg1$, the whole string is returned. If $Arg2$ is negative, an error is returned. Example: Right("Daddy", 3.99) -> "ddy" Right("Daddy", 386) -> "Daddy" Right("Daddy", -1) -> #ARG!
Upper(Arg1)	Returns <i>Arg1</i> converted to uppercase. <i>Arg1</i> and the result are of type string.

7.4.4.4.5 Date and Time Functions

Function	Description
AddDays(Arg1, Arg2)	Adds Arg2 number of days to Arg1. Arg2 is of type Real and Arg1 is of type Date or TimeStamp. The result is of the same type as Arg1.
	Example: AddDays(2002-03-04, -2) -> 2002-03-02
AddSeconds(Arg1, Arg2)	Adds Arg2 number of seconds to Arg1. Arg2 is of type Real and Arg1 is of type Time or TimeStamp. The result is of the same type as Arg1.
	Example: AddSeconds([Time col], 30) AddSeconds([Time col], 0.010)
Date(Arg1, Arg2, Arg3)	Creates a Date. The arguments are year, month and day and are of type Real. The year must be between 100

	and 9999. The month must be between 1 and 12. The day must be between 1 and 31). See also conversion functions. Example: Date(2003, 4, 9) -> 2003-04-09 Date(2000, -1, 1) -> #ARG! (conversion error)
DateDiff(Arg1, Arg2)	Returns the difference in milliseconds in between two Date, Time or TimeStamp values. Example: DateDiff([Time col 1],[Time col 2])
Day(Arg1)	Extracts the day from a Date or TimeStamp. The result is of type Integer. Example: Day(2002-03-04) -> 4
Days(Arg1, Arg2)	Returns the number of days between two dates. The arguments can be either of type Date or of type TimeStamp. If the arguments are of type TimeStamp, the time part is ignored. The result is of type Integer. Example: Days(2002-03-04, 2002-03-02) $\rightarrow 2$
Hour(Arg1)	Extracts the hour from a Time or TimeStamp. The result is of type Integer. Example: Hour(11:38:02) -> 11
Millisecond(Arg1)	Extracts the millisecond part of a Time or TimeStamp. The result is of type Integer. Example: Millisecond([Time col])
Minute(Arg1)	Extracts the minute from a Time or TimeStamp. The result is of type Integer. Example: Minute(11:38:02) -> 38
Month(Arg1)	Extracts the month from a Date or TimeStamp. The result is of type Integer. Example: Month(2002-03-04) -> 3
Second(Arg1)	Extracts the second from a Time or TimeStamp. The result is of type Integer. Example: Second(11:38:02) -> 2
Seconds(Arg1, Arg2)	Returns the number of seconds between two times. The arguments can be either of type Time or of type TimeStamp. The result is of type Integer. Example: Seconds(11:38:02, 11:37:00) -> 62
Time(Arg1, Arg2, Arg3)	Creates a Time. The arguments are hours, minutes and seconds and are of type Real. The hours, minutes and seconds must be valid (0-23, 0-59, 0-59). See also conversion functions. Example: $Ti = (14.4.01) \ge 14.04.00$
	11110(14,4,0) - 14.04.00

	$Time(10, -1, 1) \rightarrow #ARG! (conversion error)$
TimeStamp(Arg1, Arg2)	Creates a TimeStamp. The arguments are a Date and a Time. See also conversion functions.
	Example: TimeStamp([Date col], [Time col])
Year(Arg1)	Extracts the year from a Date or TimeStamp. The result is of type Integer.
	Example: Year(2002-03-04) -> 2002

7.4.4.4.6 Conversion Functions

Function	Description
Date(Arg1)	Converts Arg1 to a date. If the conversion fails, an error is returned. Arg1 can be of type String or TimeStamp and the result is of type Date. If a TimeStamp is specified, the time part is removed. See also date & time functions. Example: Date("2003-03-21") -> 2003-03-21 Date("10") -> #ARG! (conversion error) Date(null) -> #NULL! Date(2003-03-21 11:37:00) -> 2003-03-21
Integer(Arg1)	Converts <i>Arg1</i> to an integer number. If the conversion fails, an error is returned. <i>Arg1</i> can be of types integer, real or string, and the result is of type integer. Real numbers are truncated, i.e., only the integer part is used. Example: Integer("-123") -> -123 Integer("-2.99") -> -2 Integer("0%") -> #ARG! (syntax error) Integer(1e20) -> #ARG! (overflow) Integer(null) -> #NULL!
Real(Arg1)	Converts <i>Arg1</i> to a real number. If the conversion fails, an error is returned. <i>Arg1</i> can be of types integer, real or string, and the result is of type real. Example: Real("1.23") -> 1.23 Real(2) -> 2.0 Real("0%") -> #ARG! (syntax error) Real(null) -> #NULL!
SE(Arg1, Arg2)	Substitutes errors. Returns <i>Arg1</i> if it is not an error, <i>Arg2</i> otherwise. <i>Arg1</i> and <i>Arg2</i> can be of any type, but must both be of the same type or null. The result is of the same type as the arguments. Example: SE(1, 2) -> 1 SE(null, 2) -> $\#$ NULL! SE(0/0, 2) -> 2
SN(Arg1, Arg2)	Substitutes null values. Returns Arg1 if it is not null,

	Arg2 otherwise. Arg1 and Arg2 can be of any type, but must both be of the same type or null. The result is of the same type as the arguments. Example: $SN(1, 2) \rightarrow 1$ $SN(null, 2) \rightarrow 2$ $SN(0/0, 2) \rightarrow \#NUM!$
String(Arg1)	Converts <i>Arg1</i> to a string. This conversion never fails except if <i>Arg1</i> is null. <i>Arg1</i> can be of any type and the result is of type string. Example: String(1.23) -> "1.23" String(null) -> #NULL!
Time(Arg1)	Converts Arg1 to a time. If the conversion fails, an error is returned. Arg1 can be of type String or TimeStamp and the result is of type Time. If a TimeStamp is specified, the date part is removed. See also date & time functions. Example: Time("11:37:00") -> 11:37:00 Time("10") -> #ARG! (conversion error) Time (null) -> #NULL! Time(2003-03-21 11:37:00) -> 11:37:00
TimeStamp(Arg1)	Converts Arg1 to a time stamp. If the conversion fails, an error is returned. Arg1 can be of type String or Date and the result is of type TimeStamp. If a Date is specified, the time part is set to 00:00:00. See also date & time functions. Example: TimeStamp("2003-03-21 11:37:00") -> 2003- 03-21 11:37:00 TimeStamp("10") -> #ARG! (conversion error) TimeStamp(null) -> #NULL! TimeStamp (2003-03-21) -> 2003-03-21 00:00:00

7.4.4.5 Reserved Words

Import Result Template Type null true false

7.4.4.6 Errors and Null

An expression is considered valid if it is syntactically correct and all function, operator and column references can be resolved. If an expression is not valid, it cannot be evaluated. This will be indicated in the SXL UI as:

#EXPR!

When evaluating an expression, some operations produce errors or null values. Each function and operator can choose how to handle arguments that are errors or null. The default behavior is to propagate the first error or null value that is encountered. So, if a function takes two arguments and the first is null and the second is an error, the default behavior is to return null. Functions that handle errors and null in other ways are explained in their Descriptions.

Errors

For operations on arguments of type real, the result is sometimes not defined. This produces a **NaN** (Not a Number) error. If the result of an operation is greater than the maximum real number, an **Infinity** error (or **-Infinity** error) is produced. Many operations are well defined for +/- **Infinity** and will work as expected, e.g., 2.5 < 1/0 returns true. When generated, these errors are grouped together as numeric errors, displayed as:

#NUM!

If the argument for a function (or operator) is invalid, an error is also produced. For example, functions expecting an index might produce an error because the index is negative and conversion functions produce an error if the argument cannot be converted. When generated, these errors are grouped together as argument errors displayed as:

#ARG!

The **IsError**(Arg1) function can be used to determine if a sub-expression results in an error. The **SE**(Arg1, Arg2) function can be used to substitute errors with a certain value, e.g. null or 0. When generating a result data set from the expression, errors are converted to null. Wrap the expression with a call to the **SN**(Arg1, Arg2) function to override this behavior.

Error	Details	Example	Description
#NUM!	NaN	0/0 atan(2) sqrt(-1)	Not a Number, means that the result is undefined. All subsequent math operations on NaN produce NaN.
#NUM!	Infinity	1/0 1e200*1e200	Infinity, means that the number is too big to store in the real data type. Many math operations treat this as a "huge" number.
#NUM!	-Infinity	-1/0 -1e200*1e200	Negative infinity, means that the number is too big to store in the real data type. Many math operations treat this as a "huge" negative number.
#ARG!	Invalid Argument	Left("Hello", -1) Mid("Hello", 0, 1)	Invalid argument. In this case because length must be positive and position cannot be zero.
#ARG!	Conversion	Real("Hello")	Conversion failed.

Null

Null values are usually only generated when retrieving a column value from the data set or by explicitly writing **null** in the expression. Results that are null, are displayed as:

#NULL!

The **IsNull**(*Arg1*) function can be used to determine if a sub-expression results in null. The **SN**(*Arg1*, *Arg2*) function can be used to substitute null with a certain value, e.g., 0.

7.4.4.7 Compatibility

The old expression language in DecisionSite Client 7.1.1 and earlier, had a different syntax and a different set of functions and operators. All the functionality of the old expression language is present in the new expression language and mapping the old onto the new is described here.

Quoted column names are now bracketed instead: "Column 1" is now [Column 1]

String literals can now contain escaped characters such as quotes, backslashes, new lines etc: "22\"", '22"', "1\n2\n", 'C:\\TEMP\\file.csv'

Constants are replaced by function calls: PI is now PI(), E is now EXP(1)

Concatenating strings is now supported via the & operator instead of +

Operator ^ is replaced by function POWER

Operator precedence is now correct: 1+2*3 is now evaluated as 1+(2*3) instead of (1+2)*3Function Compatibility

The old functions and their new counterparts are listed below:

New Function	Description
SUM	Now sums any number of arguments. See also operator +
	Now only available as an operator. See operator -
PRODUCT	Now multiplies any number of arguments. See also operator *
	Now only available as an operator. See operator /
MOD	
POWER	See also operator ^
EXP	Equivalent to POWER(x, 2.718281)
SQRT	
ABS	
LOG(num, base)	Now requires a base argument as well (not 10 by default). See function LOG10 below.
LOG10	10 logarithm, replaces old LOG(x) function
LN	Natural logarithm
FLOOR	
CEILING	
SIN	
	New Function SUM SUM PRODUCT MOD POWER EXP SQRT ABS LOG(num, base) LOG(num, base) LOG10 LN FLOOR CEILING SIN

COS	COS	
TAN	TAN	
NEG		No longer supported. See unary operator -
PI (constant)	PI()	Now a function like in Excel.
E (constant)		No longer supported. Use EXP(1) instead.
MAX	MAX	
MIN	MIN	
TOUPPERCASE	UPPER	
TOLOWERCASE	LOWER	

Operator Compatibility

The old operators and their new counterparts are listed below: **Binary:**

Old Operator	New Operator	Description
+	+	Adds numeric values. See operator & for string concatenation.
-	-	Subtract numeric values.
*	*	Multiply numeric values.
/	/	Divide numeric values.
^		No longer supported. See function POWER.
+	&	Concatenate (append) strings or lists.
Unary:		

Old Operator	New Operator	Description
	-	Negates the argument.

Examples

Here are some examples of how expressions would look using both the old and the new syntax. We assume a data set with string column "S1" and numeric columns "N1", "N2" and "Binned N1".

Old Expression	New Expression
N1 + 2 / N2	(N1 + 2) / N2
SUBTRACT(N1, "Binned N1")	N1 – [Binned N1]
N1 ^ 3 + EXP(N2, 0.5)	POWER(N1, 3) + POWER(N2, 0.5)
NEG(N1)	-N1
TOUPPERCASE(S1)	UPPER(S1)
'C:\" + S1 + '\' + N1 + '.txt'	'C:\\' & S1 & '\\' & N1 & '.txt'

7.5 Column Normalization

7.5.1 Column Normalization Overview

The Column Normalization tool can be used to standardize the values in selected columns using a number of different normalization methods. For example, this can be useful if you plan to perform a clustering later on.

7.5.2 Using Column Normalization

7.5.2.1 Normalizing Values in Selected Columns

► To normalize columns:

- 1. Select **Data > Column Normalization...**.
- Response: The Column Normalization dialog is displayed.
- Select the Value columns that you want to normalize.
 Comment: For multiple selection, press Ctrl and click on the desired columns or click one column and drag to select the following ones.
- 3. Click a radio button to select whether to work on All records or Selected records.
- 4. Select a method to **Replace empty values with** from the drop-down list.
- 5. Select a Normalization method from the drop-down list.
- 6. Select the **Overwrite previously added columns** check box to overwrite columns earlier added by this tool.
- 7. Click OK.

Response: The Column Normalization dialog is closed and the normalized columns either replace the old columns or are added to the data set, depending on your selection in the Overwrite check box.

Tip: You can also use the Column Normalization tool to replace empty values in columns without performing any normalization.

7.5.2.2 Replacing Empty Values in Columns

If *No normalization* is selected as normalization method in the Column Normalization tool, you can replace empty values in a data set with either a constant, averaged or interpolated values. See Details on Interpolation for more information on how the interpolation option works for row interpolation.

► To replace empty values in existing columns:

1. Select **Data > Column Normalization...**.

Response: The Column Normalization dialog is displayed.

- Select the Value columns in which you want to replace the empty values. Comment: For multiple selection, press Ctrl and click on the desired columns or click one column and drag to select the following ones.
- 3. Click a radio button to select whether to work on All records or Selected records.
- 4. Select a method to **Replace empty values with** from the drop-down list.
- 5. Select No normalization as the Normalization method.
- 6. Select the **Overwrite previously added columns** check box to overwrite columns created by this tool.
- 7. Click OK.

Response: The Column Normalization dialog is closed and data is added to the previously empty fields of the columns in the data set according to the selected replacement method.

7.5.2.3 Details on Interpolation

Empty values in the data set can be replaced with either a constant, averaged or interpolated values. The row interpolation of the Column Normalization tool works like this:

If the first value is empty it is replaced with the first non-empty numerical value in the order the columns were entered.

If the last value is empty it is replaced with the previous non-empty numerical value in the order the columns were entered.

If an empty value is found between non-empty numerical values, the values are calculated as the linear interpolation.

If all values in a row are empty, they will be replaced by zero.

Example:

С А В D 2 3 4 null null null 3 4 1 null 3 4 1 null null 4 2 null 4 1 2 3 1 null null null null null

Becomes:

А	С	В	D
2	2	3	4
3	3	3	4
1	2	3	4
1	2	3	4
1	2	3	4
1	2	3	3
0	0	0	0

7.5.3 User Interface

7.5.3.1 Column Normalization Dialog

Column Normalization		×
Column settings		
⊻alue columns:	molecular_volume density surface_area Log_Kow_fragments HLB solubility_parameter dispersion_3D polarity_3D hydrogen_bond_3D bydrogen_bond_accentor	
<u>W</u> ork on:	All records Selected records	
<u>Replace empty values with:</u>	Constant	• 0
Calculation options		
Normalization method: Z-sc	ore (subtract mean and divide by std dev) d columns	•
(<u>H</u> elp	<u> </u>	Cancel

Option	Description
Value columns	The data columns you want to normalize. Click a column name in the list to select it. To select more than one column, press Ctrl and click on the column names in the list.
Work on: All records	All records in the value columns are included in the calculations.
Work on: Selected records	Only the selected records are included in the calculations. This lets you filter out any records that you do not want to include in the calculations, using the query devices and zooming.
Replace empty values with	Defines how empty values in the data set should be replaced. From the drop-down list, select a method. Note: Empty value leaves the value empty as before. Constant allows you to replace the empty values by any constant (type a number in the text box). Row average replaces the value by the average value of the entire row. Row interpolation sets the missing value to the interpolated value between the two neighboring values in the row (see Details on interpolation for more information). Similarly, Column average and Column interpolation return the average/interpolation of the corresponding column values.
Normalization method	The method to use for the normalization. For more information about the available methods, see the methods overview. The option No

normalization gives you the opportunity to replace empty values in a column.

Overwrite	Select this check box if you want to replace any previously added
previously added	columns from the Column Normalization tool. Clear the check box if
columns	you wish to keep the old columns.
	Normalized columns will have the same name as the ones they are based on, followed by "(normalized)". If several sets of normalized columns are saved, they will also be followed by an index number, (1), etc.

To reach the Column Normalization dialog:

Select Data > Column Normalization....

7.5.4 Theory and Methods

7.5.4.1 Column Normalization Methods Overview

The following normalization methods are available in the Column Normalization tool:

- Z-score calculation
- Divide by standard deviation
- Scale between 0 and 1

7.5.4.2 Column Normalization - Z-score

Assume that there are *n* records with seven variables, A, B, C, D, E, F and G, in the data view. We use variable E as an example in the expressions. The remaining variables are normalized in the same way.

The normalized value of e_i for variable E in the ith record is calculated as

Normalized
$$(e_i) = \frac{e_i - \overline{E}}{\operatorname{std}(E)}$$

where

$$\operatorname{std}(E) = \sqrt{\frac{1}{n-1} \sum_{j=1}^{n} (e_j - \overline{E})^2}$$

$$\overline{E} = \frac{1}{n} \sum_{j=1}^{n} e_j$$

If all values for variable E are identical — so that the standard deviation of E (std(E)) is equal to zero — then all values for variable E are set to zero.

7.5.4.3 Column Normalization - Divide by Standard Deviation

Assume that there are *n* records with seven variables, A, B, C, D, E, F and G, in the data view. We use variable E as an example in the expressions. The remaining variables are normalized in the same way.

The normalized value of e_i for variable E in the ith record is calculated as

Normalized (
$$e_i$$
) = $\frac{e_i}{\operatorname{std}(E)}$

where

$$\operatorname{std}(E) = \sqrt{\frac{1}{n-1} \sum_{j=1}^{n} (e_j - \overline{E})^2}$$

$$\overline{E} = \frac{1}{n} \sum_{i=1}^{n} e_i$$

If all values for variable E are identical — so that the standard deviation of E (std(E)) is equal to zero — then all values for variable E are left unchanged.

7.5.4.4 Column Normalization - Scale Between 0 and 1

Assume that there are *n* records with seven variables, A, B, C, D, E, F and G, in the data view. We use variable E as an example in the expressions. The remaining variables are normalized in the same way.

The normalized value of e_i for variable E in the ith record is calculated as

Normalized
$$(e_i) = \frac{e_i - E_{\min}}{E_{\max} - E_{\min}}$$

where

 E_{\min} = the minimum value for variable E

 $E_{\rm max}$ = the maximum value for variable E

If all values for variable E are identical, so that E_{\min} is equal to E_{\max} , then all values for variable E are set to zero.

7.6 Pivot Data

7.6.1 Pivot Data Overview

Pivoting, in its simplest form, means rotating a table. Mostly, though, it also includes performing some form of aggregation, so that the new table is more compact than the original. To better understand how the pivoting tool works, study one of the examples.

7.6.2 Using Pivot Data

7.6.2.1 Pivoting the Data Set

To pivot the current data set:

- Select Data > Pivot Data.... Response: The Tall/Skinny => Short/Wide dialog is opened.
- 2. In the **Identity** list, select one or more columns. Comment: Each unique value in the chosen column produces a row in the generated table. You can choose more than one column. Doing so means that the new table will have a separate row for *each unique combination* of values in the chosen columns.
- 3. In the **Category** list, select one or more columns.

Comment: Each unique value in the chosen column produces a new column in the generated table. Selecting more than one column means that the new table will have a separate column for *each unique combination* of values in the chosen columns.

4. In the Values list, select one or more columns. Comment: The column selected under Values is the column from which the data is pulled. It is possible to select more than one Value column. The values in the generated table are always computed as the average of values in the original table,

unless the original values are strings. If so, values in the generated table will consist of concatenated strings. To change the way the values are calculated, right-click on the Method and select a different method from the list, or use Ctrl+click to select multiple methods.

5. In the **Other Columns** list, select one or more columns.

Comment: This option allows you to include an overall average of a particular measurement, for each row in the generated table. For each column selected here, one new column will be created in the new table. To change the way the measurements are calculated, right-click on the Method and select a different method from the list, or use Ctrl+click to select multiple methods.

6. Click **OK**.

7.6.2.2 Example of Pivoting

Pivoting a data set means changing it from a tall/skinny format to a short/wide format. Consider the following tall/skinny table, based on a series of temperature measurements:

City	Month	Temp
London	February	4
New York	February	6
London	May	16
New York	May	19
London	August	28
New York	August	26
London	November	13
New York	November	11

As we add more observations, the table grows taller, but remains three columns wide. While useful during data collection, this format may not be appropriate for certain types of calculations or visualizations. For example, the entities that interest us are the different cities, so we may want a representation with a single record for each city.

Tall/Skinny=>Short/Wide conversion lets us pivot this table, producing the following (note that avg(Temp) is the average of a single cell):

City	avg(Temp) for February	avg(Temp) for May	avg(Temp) for August	avg(Temp) for November
London	4	16	28	13
New York	6	19	26	11

Each city is now represented by a single record, which makes this format very suitable for Spotfire DecisionSite profile charts. This example demonstrates three steps:

- Creating a row for each unique value in City.
- Creating a column for each unique value in Month.
- Entering a value from Temp for each cell in the resulting grid.

In the Tall/Skinny => Short/Wide dialog, the following settings would be made:

- Identity: City
- Category: Month
- Values: Temp
7.6.2.3 Example of Pivoting with Aggregation

Note: To understand this example, it is recommended to read Example of Pivoting first. Apart from changing format from tall/skinny to short/wide, pivoting can be used to create a more compact table. Consider the following table, based on a series of temperature measurements:

City	Month	Day	Temp
London	February	1	5
London	February	15	8
London	May	1	15
London	May	15	22
New York	February	1	9
New York	February	15	7
New York	May	1	18
New York	May	15	24

Tall/Skinny=>Short/Wide conversion lets us pivot and aggregate this table, producing the following:

City	avg(Temp) for February	avg(Temp) for May
London	6.5	18.5
New York	8	21

A smaller table has been created, summarizing the original table. In the Tall/Skinny => Short/Wide dialog, the following settings would be made:

- Identity: City
- Category: Month
- Values: Temp

7.6.3 User Interface

7.6.3.1 The Tall/Skinny => Short/Wide Dialog

This dialog allows you to configure how pivoting is performed.

Pivot (Tall/Skinny =>	Short/Wide)	
	Identify records	; by the c	olumn(s):
Identity	Name	Туре	•
	٧X	Integer	
		Integer	_
	☐ Year	Integer	
	Cadmium	Integer	
	Chrome	Integer	
	Create a new c	olumn fo	reach value in:
Category	Name	Туре	
	Π×	Integer	
		Integer	
	☐ Year	Integer	
	🗖 Cadmium	Integer	
	Chrome	Integer	
	Use values in t	he follow	ing column(s):
Values	Name	Туре	Method (right-click to change, Ctrl+click to multiselect
	Year	Integer	Average
	⊡t ©admium	Integer	Average
	Chrome	Integer	Average
		Integer	Average
			I
	Transfer the fo	llowing co	olumn(s) to the new data set:
Other Columns	Name	Туре	Method (right-click to change, Ctrl+click to multiselect 🔺
	🗹 Cadmium	Integer	Average
	🗹 Chrome	Integer	Average
	InChrome	Integer	Average
	Copper	Integer	Average
Help			OK Cancel

Option	Description
Identity	Each unique value in the chosen column produces a row in the generated table. You can choose more than one column. Doing so means that the new
	table will have a separate row for <i>each unique combination</i> of values in the chosen columns.
Category	Each unique value in the chosen column produces a new column in the generated table.
	Selecting more than one column means that the new table will have a separate column for <i>each unique combination</i> of values in the chosen columns.
Values	The column selected under Values is the column from which the data is pulled. It is possible to select more than one Value column.
	The values in the generated table are always computed as the average of values in the original table, unless the original values are strings. If so, values in the generated table will consist of concatenated strings. To change the way the values are calculated, right-click on the Method and select a different method from the list, or use Ctrl+click to select

multiple methods.

Other Columns This option allows you to include an overall average of a particular measurement, for each row in the generated table. For each column selected here, one new column will be created in the new table. To change the way the measurements are calculated, right-click on the Method and select a different method from the list, or use Ctrl+click to select multiple methods.

Method Selection List

Right-click on the Method to change the method of calculation for your column. Ctrl+click to select multiple methods.

	Use values in t	he followi	ng colun	nn(s):
	Name	Туре	Metho	d (right-click to change, Ctrl+click t
H	🗹 Year	Integer	Averag	Ctrl+click to multiselect
	🗖 Cadmium	Integer	Averag	
	Chrome	Integer	Averag	 Average
	InChrome	Integer	Avera	Count all values
	•			Count rows
	Transfer the fo	llowing co	olumn(s)	Count unique values
	Name	Tune	Metho	First value
	Cadmium	Integer	Averar	Last value
		Integer		Maximum va je
		Integer	Avera	Median
		Integer	Averar	Merge all values
	1 00pp0.	meger		Merge unique values
				Most common value
				Standard deviation
				All

To reach the Tall/Skinny => Short/Wide dialog:

Select **Data > Pivot Data...**.

7.7 Depivot Data

7.7.1 Depivot Data Overview

Pivoting, in its simplest form, means rotating a table. While the Pivot Data tool transforms a table from the tall/skinny variant to the short/wide form, the Depivot Data tool does the opposite. While most tools in DecisionSite require that data is short and wide, there may be occasions when you want to view data in a different form, such as a bar chart visualization showing different years on the x-axis.

7.7.2 Using Depivot Data

7.7.2.1 Depivoting the Data Set

To depivot the current data set:

1. Select **Data > Depivot Data...**.

Response: The Depivot (Short/Wide => Tall/Skinny) dialog is opened.

- 2. In the **Available columns** list, click to select the columns that you want to transform. Comment: For multiple selection, press **Ctrl** and click on the desired columns in the Available columns list. You can sort the columns in the list alphabetically by clicking on the Name bar.
- 3. Click on the Add >> button to send the selected columns to the Columns to transform list.

Comment: These columns should be the ones that contain the actual values and that you want to combine into a new value column. For example, "Sales 2005", "Sales 2004" and "Sales 2003".

- 4. In the **Available columns** list, click to select the columns that you want to pass through the depivoting process without any transformation.
- 5. Click on the **Add** >> button to send the selected columns to the **Columns to pass through** list.

Comment: These columns can contain other categorical information, IDs, etc. For example, "Region", "Name" or "Priority".

Type a new Category column name in the provided text field.
 Comment: For instance, "Year" could be used when sales figures for several different years are to be combined to a single column.

Select the data Type for the new column from the drop-down list.

Type a new Value column name in the provided text field.

Comment: For instance, "Sales" containing sales figures for several different years. Select the data **Type** for the new column from the drop-down list.

7. Click OK.

7.7.2.2 Example of Depivoting

Depivoting a data set means changing it from a short/wide format to a tall/skinny format. Consider the following short/wide table, containing sales data for a fictive company:

Name	Region	Sales 2003	Sales 2004	Sales 2005
Connelly	New Jersey	23	22	25
Fallon	New Jersey	34	37	38
Smiths	New York	21	30	32
Bergman	New York	35	35	35
Taylor	Texas	24	23	24
Roberts	Texas	31	30	29
Miller	Texas	29	32	33
Hanegan	Florida	24	26	25

Suzuki	Japan	45	38	39
Takahashi	Japan	47	40	45
Olsen	Europe	26	25	29
Ottosson	Europe	25	24	26
Olsson	Europe	23	22	28
James	Florida			32

If you want to view how the sales figures from the different regions vary during the years in a bar chart, the current format is not always optimal. By depivoting the data set to a tall/skinny format with all sales figures in a single column, you will be able to create a suitable bar chart with minimal effort.

Name	Region	Year	Sales
Connelly	New Jersey	Sales 2003	23
Connelly	New Jersey	Sales 2004	22
Connelly	New Jersey	Sales 2005	25
Fallon	New Jersey	Sales 2003	34
Fallon	New Jersey	Sales 2004	37
Fallon	New Jersey	Sales 2005	38
Smiths	New York	Sales 2003	21
Smiths	New York	Sales 2004	30
Smiths	New York	Sales 2005	32
Bergman	New York	Sales 2003	35
Bergman	New York	Sales 2004	35
Bergman	New York	Sales 2005	35
Taylor	Texas	Sales 2003	24
Taylor	Texas	Sales 2004	23
Taylor	Texas	Sales 2005	24
Roberts	Texas	Sales 2003	31
Roberts	Texas	Sales 2004	30
Roberts	Texas	Sales 2005	29
Miller	Texas	Sales 2003	29
Miller	Texas	Sales 2004	32
Miller	Texas	Sales 2005	33
Hanegan	Florida	Sales 2003	24
Hanegan	Florida	Sales 2004	26

Hanegan	Florida	Sales 2005	25
Suzuki	Japan	Sales 2003	45
Suzuki	Japan	Sales 2004	38
Suzuki	Japan	Sales 2005	39
Takahashi	Japan	Sales 2003	47
Takahashi	Japan	Sales 2004	40
Takahashi	Japan	Sales 2005	45
Olsen	Europe	Sales 2003	26
Olsen	Europe	Sales 2004	25
Olsen	Europe	Sales 2005	29
Ottosson	Europe	Sales 2003	25
Ottosson	Europe	Sales 2004	24
Ottosson	Europe	Sales 2005	26
Olsson	Europe	Sales 2003	23
Olsson	Europe	Sales 2004	22
Olsson	Europe	Sales 2005	28
James	Florida	Sales 2003	
James	Florida	Sales 2004	
James	Florida	Sales 2005	32

The resulting data set can easily be displayed as a bar chart showing the total sum of sales for each year, categorically colored by region:



How to do it:

- 1. Select Sales 2005, Sales 2004 and Sales 2003 as Columns to transform.
- 2. Select **Region** and **Name** as Columns to pass through.

- 3. Type **Year** as the Category column name and make sure String is the selected data type.
- 4. Type **Sales** as the Value column name and select the data type Integer.
- 5. Click **OK**.

7.7.3 User Interface

7.7.3.1 Depivot (Short/Wide => Tall/Skinny) Dialog

		Columna to transform		
aliable <u>c</u> olumns:	_	Loiumns to gransform:		7
ame nter text bere		Name Salec 2005		-
alac 2005	<u>A</u> dd >>	Sales 2003		
ales 2003		Sales 2003		
ales 2003	<< <u>R</u> emove			
egion				
ame	Re <u>m</u> ove All			
		Keep NULL values		
		Columna to pass through:		
		Name		7
		Periop		-
	A <u>d</u> d >>	Name		
	<< Remo <u>v</u> e			
	Remove All			
Resulting new columns				
Category column name (contains old column	names):			
Year			Type: String 💽	
Valu <u>e</u> column name:				
Sales			Type: Integer 💌	
1				1

Option	Description
Available columns	The columns available for use in the depivot operation. Click a column name in the list to select it. To select more than one column, press Ctrl and click the column names in the list. Use one of the Add >> buttons to send the selected column to either the Columns to transform or Columns to pass through field, see below.
Enter text here	If you have a data set with many columns, you can right-click on the header of the columns in the Available columns list box and select Show Search Field from the pop-up menu. This will display a search field where you can type a search string and limit the number of items in the list. It is possible to use the wildcard characters * and ? in the search.
Add >>	Moves selected columns from the Available columns field to the field next to the button.

Removes a column and brings it back to the Available columns field.
Removes all columns from the selected columns fields.
The selected columns containing the values that you wish to combine into a single column. The column names of these columns will be used as category values in the resulting new category column. Typically, this might be a number of columns containing the same type of data. For example, sales figures for different years.
Select this check box to transfer empty values to the depivoted data view. If the check box is cleared, all records containing empty values will be discarded.
The selected columns containing information that should be transferred to the depivoted data set without any transformation. This could be ID columns, categorical information such as Region, Priority etc.
Type a column name that summarizes the information provided in the columns that you have selected to transform. For instance, "Year" could be used when sales figures for several different years are to be combined to a single column.
Type a column name that shows what type of information is included in the new value column. For instance, "Sales" would be a good name for a column containing sales figures for several different years.
Specify the data type for the respective column. A column containing names should be set to string, whereas a column containing figures should be decimal or integer.

To reach the Depivot (Short/Wide => Tall/Skinny) dialog:

Select **Data > Depivot Data...**.

7.8 Transpose Data

7.8.1 Transpose Data Overview

The Transpose Data tool is used to rotate a data set, so that columns become records and vice versa. Transposing may be necessary if you want to be able to use your data in a certain type of visualization or if you just want to get a better overlook the data.

7.8.2 Using Transpose Data

7.8.2.1 Transposing Columns

Transposing a data set means rotating it, so that columns become records and vice versa.

► To transpose columns:

1. Select **Data > Transpose Data...**

Response: The Transpose Data wizard step 1 is opened.

- 2. Select an identifier column from the drop-down list. Comment: Each value in the selected column will become a column name in the transposed data set
- 3. Select whether to create columns from All records or just Selected records.

Comment: The transposed data set will have the same number of columns as the number of records selected. The upper limit is 5000.

- Click Next >.Response: Step 2 of the wizard is shown.
- Select the columns you want to include in the transposed data set, and click Add >> . Comment: Each selected column will become a separate record in the transposed data set.
- 6. Click Next >.

Response: Step 3 of the wizard is shown.

- If required, select annotation columns.
 Comment: Each transposed column will be annotated with the value of this column.
- 8. Click Finish.

Response: A message box appears, prompting you to save your previous data set.

Click Yes to save the previous data set.
 Response: The new, transposed data set replaces the original data set.

7.8.2.2 Example of Transposing

Transposing a data set means rotating it, so that columns become records and vice versa. Consider the following table, describing a series of meteorological observations:

Day	Temperature	Wind	Humidity
Monday	16	5	75
Tuesday	19	8	70
Wednesday	17	10	70
Thursday	24	9	65
Friday	26	2	75
Saturday	27	2	80
Sunday	25	4	80

As we add more observations, the table grows taller, but remains four columns wide. While useful during data collection, this format may not be appropriate for certain types of calculations or visualizations. By transposing this table, the following can be produced:

Transposed columns	Tuesday	Wednesday	Thursday	Friday
Temperature	19	17	24	26
Humidity	70	70	65	75

► To produce this result:

- 1. In a visualization, select (using the query devices) the records Tuesday, Wednesday, Thursday and Friday.
- 2. Launch the Transpose Data tool.
- 3. Select **Day** as identifier column.
- 4. Select Work on: Selected records.

5. Select **Temperature** and **Humidity** as value columns.

7.8.3 User Interface

7.8.3.1 Transpose Data Wizard Step 1

🛃 Transpose Data: step 1	of 3		×
Identifier column and rea	cords		
Select an identifier colum names in the transposed	n to be the column dataset	→	
	Identifier column:	Day	•
	<u>W</u> ork on:	 All records Selected records 	
Help		Next >	Cancel
Option	Description		
Identifier column	Each value in the s name in the transpo	elected identifier colum osed data set.	in will become a colui
Work on: All records	Creates a column f	For each record in the da	ta set. Note that this r

Work on: Selected Creates a column for each record selected in the data set. **records**

result in a very large number of columns.

► To reach the Transpose Data wizard:

Select **Data > Transpose Data...**.

7.8.3.2	Transpose Data Wizard Step 2
---------	------------------------------

Humidity	<u>A</u> dd >> << <u>B</u> emove	Temperature Wind	
<u>H</u> elp	< Back	Next >	Cancel

Description
The columns available for transposing. Only numerical columns are displayed.
The columns selected for transposing.
Moves a column to the Value columns field.
Removes a column from the Value columns field.

► To reach the Transpose Data wizard:

Select **Data > Transpose Data...**

7.8.3.3 Transpose Data Wizard Step 3

Transpose Data: step 3 of 3		×
Annotation columns setting Available <u>c</u> olumns: Day Temperature Wind	Agnotation columns:	
Help	< Back Finish Cancel	

Option	Description
Available columns	The columns available for annotation.
Annotation columns	The columns selected for annotation.
Add >>	Moves a column to the Annotation columns field.
<< Remove	Removes a column from the Annotation columns field.

► To reach the Transpose Data wizard:

Select Data > Transpose Data....

7.9 Hierarchical Clustering

7.9.1 Hierarchical Clustering Overview

The Hierarchical Clustering tool groups records and arranges them in a dendrogram (a tree graph) based on the similarity between them.

7.9.2 Using Hierarchical Clustering

7.9.2.1 Initiating a Hierarchical Clustering

► To start a clustering:

 Select Data > Clustering > Hierarchical Clustering.... Response: The Hierarchical Clustering dialog is displayed. 2. Select the value columns on which to base the clustering from the **Available columns** list and click **Add** >>.

Comment: For multiple selection, press **Ctrl** and click on the desired columns in the Available columns list. Then click Add >> to move the selected columns to the Selected columns list. You can sort the columns in the list alphabetically by clicking on the Name bar.

- 3. Click a radio button to select whether to work on All records or Selected records.
- 4. Select a method to **Replace empty values with** from the drop-down list.
- 5. Select which **Clustering method** to use for calculating the similarity between clusters. Comment: Click for information about available clustering methods.
- 6. Select which **Similarity measure** to use in the calculations. Comment: Click for information about available similarity measures.
- 7. Select which **Ordering function** to use for displaying the results. Comment: Click for information about available ordering functions.
- Type a new Column name in the text box or use the default name.
 Comment: Select the Overwrite check box if you want to overwrite a previously added column using the same name. Clear the check box to keep old columns.
- 9. Select the **Calculate column dendrogram** check box if you want to create a column dendrogram.
- 10. Click OK.

Response: The Hierarchical Clustering dialog is closed and the clustering is started. The result is displayed according to your settings in the dialog.

7.9.2.2 Hierarchical Clustering on Keys

A *structure key* is a string that lists the substructures which form a compound. Clustering on keys, then means grouping compounds with similar sets of substructures.

Clustering on keys is based only on the values within the key column, and not all the columns. The key column should contain comma separated string values for all or some of the records in the data set.

The procedure below only shows you how to cluster records based on a specific key column.

► To cluster on keys:

- 1. If you have not already done it, you should first import the keys that you want to cluster on into Spotfire DecisionSite.
- Select Data > Clustering > Hierarchical Clustering on Keys.... Response: The Hierarchical Clustering on Keys dialog is displayed.
- 3. Select the **Key column** on which to base the calculations. Comment: The key column could be any string column in the data set.
- 4. Click a radio button to select whether to work on All records or Selected records.
- 5. Select which **Clustering method** to use for calculating the similarity between clusters. Comment: Click for information about available clustering methods.
- 6. Select which **Similarity measure** to use in the calculations. Comment: Click for information about available similarity measures.
- 7. Select which **Ordering function** to use for displaying the results. Comment: Click for information about available ordering functions.
- 8. Type a new **Column name** in the text box or use the default name. Comment: Select the **Overwrite** check box if you want to overwrite a previously added column using the same name. Clear the check box to keep old columns.
- 9. Click OK.

Response: The *Hierarchical Clustering on Keys* dialog is closed and the clustering is started. A heat map and a row dendrogram visualization is created and information about the clustering is added to the visualization as an annotation.

7.9.2.3 Adding a Column from Hierarchical Clustering

The ordering column which is added to the data set upon performing a hierarchical clustering is used only to display the row dendrogram and to connect it to the heat map. In order to compare the hierarchical clustering results to those of a K-means clustering, you must first add a clustering column to your data set.

A clustering column contains information about which cluster each record belongs to, and can be used to create a trellis plot.

► To add a clustering column:

1. Perform a hierarchical clustering and locate the Row dendrogram which can be found to the left of the heat map.

Comment: For more information on how to create the row dendrogram, see Initiating a hierarchical clustering.

2. If the cluster line is not visible (a dotted red line in the row dendrogram), right-click and select **View > Cluster scale** from the pop-up menu to display it.

Comment: The cluster line will enable you to see how many clusters you are selecting in the dendrogram.

3. Click on the red circle on the cluster slider above the dendrogram and drag it to control how many clusters you want to include in the data column. You can also use the left and right keyboard arrow keys to step through the different number of clusters.

Response: All clusters for the current position on the cluster slider are shown as small, red circles in the dendrogram.

Comment: If you position the red circle at its rightmost position on the cluster slider, you get one cluster for each record. If you position it at its leftmost position, you get a single cluster that includes all records. The number of clusters is displayed as a ToolTip which is shown when clicking and holding the left mouse-button on the red circle on the cluster slider.

4. Select Add Cluster Column from the row dendrogram menu.

Response: A column with information about which cluster each record belongs to, is added to the data set.

Comment: Records in the data set that are not included in the row dendrogram will have empty values in the new clustering column.

Tip: You can also click on the **Add Clustering Column** button, **b**, to add a clustering column from the last row dendrogram.

7.9.2.4 Marking and Activating Nodes in the Dendrogram

Marking nodes

To mark a node, click just outside it and drag to enclose the node within the frame that appears and then release. You can also press **Ctrl** and click on the node to mark it. To mark more than one node, press **Ctrl** and click on all the nodes you want to mark. To unmark all nodes, drag to select an area outside the dendrogram.

When you mark a node or a number of nodes, the marked parts of the dendrogram are shaded in the color used for marked records, by default green as shown below. The corresponding records are also marked in the heat map and other visualizations.



Note: It is only possible to mark nodes in the row dendrogram, not in the column dendrogram.

Activating nodes

To activate a node, click on it in the dendrogram. The node gets a black ring around it. Only one node can be active at a time. The node remains active until another node is activated. It is possible to zoom in on the active node in the dendrogram by selecting **Zoom to Active** from the Hierarchical Clustering menu or from the dendrogram pop-up menu.



Highlighting nodes

Highlighting nodes in the dendrogram does not have any effect on the visualizations.

7.9.2.5 Zooming in the Dendrogram

You can zoom to a subtree in the row dendrogram, either by using the visualization zoom bar or the **Zoom to Active** command in the pop-up menu. The pop-up menu is brought up by right-clicking in the dendrogram.

Double-clicking on a node will give the same results as the Zoom to Active command. Doubleclicking a white surface in the dendrogram (no node) will take back the zooming one step, unlike the Reset Zoom command which takes you all the way back to the original zooming position.

The dendrogram can also be shown in log scale. This only affects the display of the dendrogram. The numbers in the cluster slider are not transformed into log values. Select **View** > **Log Scale** from the pop-up menu to view the dendrogram this way.

7.9.2.6 Resizing the Dendrogram

It is possible to adjust how much of the space in the visualization will be occupied by the dendrogram. This can be especially useful if the heat map contains a single column and the dendrogram structure is complex.

► To resize the dendrogram:

First click on the dendrogram to make sure it is in focus. Then, press **Ctrl** and use the left or right arrow key on the keyboard to make the dendrogram slimmer or wider. Comment: You cannot make the dendrogram or the heat map completely disappear by resizing them in the visualization.

7.9.2.7 Exporting a Dendrogram

Note: The Hierarchical Clustering tool allows the dendrograms to be saved with the Analysis. However, it is also possible to export the dendrograms separately and import them again via the Hierarchical Clustering: Dendrogram Import dialog.

► To export a dendrogram:

1. Perform a hierarchical clustering.

Comment: For more information, see Initiating a hierarchical clustering.

- 2. Locate the dendrogram(s) in the created heat map visualization.
- 3. Select **Export > Row Dendrogram** or **Column Dendrogram** from the menu in the top left of the heat map visualization.

Comment: The command **Export > Column Dendrogram** is only available if you selected to create a column dendrogram during the calculation.

Response: A Save As dialog is displayed.

4. Type a **File name** and save the file as a DND file.

Comment: The entire tree structure is saved even if only part of it is visible at the moment of saving.

Tip: To save the dendrogram and heat map as an image, use one of the Reporting tools of Spotfire DecisionSite: PowerPoint® Presentation, Word Presentation or Export as Web Page.

7.9.2.8 Importing a Dendrogram

Note: The Hierarchical Clustering tool allows the dendrograms to be saved with the Analysis. However, it is still possible to save the dendrograms separately and import them again via the Hierarchical Clustering: Dendrogram Import dialog.

To import a saved dendrogram:

- 1. Select **Data > Clustering > Hierarchical Clustering...** Response: The Hierarchical Clustering dialog is displayed.
- 2. Click **Import...**.

Response: The Hierarchical Clustering: Dendrogram Import dialog is displayed.

- 3. Click the **Browse...** button by the **Row dendrogram** field. Response: An Open File dialog is displayed.
- 4. Locate the previously exported **Row dendrogram** file (*.dnd) and click **Open**. Comment: Only dendrograms associated with the active data set can be opened. If there is a column missing in the data set, or if the names of the columns in the data set have been changed since the dendrogram was saved, an error message will appear and no dendrogram can be displayed.
- 5. Decide if you want to open a corresponding column dendrogram or not. Browse to locate the **Column dendrogram** file similarly to steps 3-4 above.
- 6. Type a **Column name** or use the default one.

Comment: Select the **Overwrite** check box to overwrite a column with the same name in the data set.

7. Click OK.

Comment: The column containing the hierarchical clustering order of the dendrogram is added to the data set. A heat map visualization is created with the dendrogram(s) displayed on the side(s).

7.9.3 User Interface

7.9.3.1 Hierarchical Clustering Dialog

🚰 Hierarchical Clustering			×
Available columns: Name Enter text here StdDev PhysicalLocation PCA t[3] PCA t[2] PCA t[1] LogRatio7 Length K records clustering Work on:	Add >> Add >> << <u>R</u> emove records	Selected columns: Name LogRatio6 LogRatio5 LogRatio4 LogRatio3 LogRatio2 LogRatio1	
Replace empty values with: Const	ant		• 0
Calculation options			
Clustering method: UPGM	1A (unweighted average)		•
Similarity measure:	ean distance		•
Ordering function:	ank		•
Column <u>n</u> ame: Hierard	chical Clustering Input		🗖 🖸 🖉 O 🖉 erwrite
Cal <u>c</u> ulate column dendrogram			
Help Import		ОК	Cancel

Option	Description
Available columns	Displays all available data columns on which you can perform a clustering. Click a column name in the list and click Add >> to move it to the Selected columns list. To select more than one column, press Ctrl and click the column names in the list, then click Add >>. You can choose from all columns that contain real numbers or integers. Note: You can right-click on the Name header to get a pop-up menu where you can select other attributes you would like to be visible.
Enter text here	If you have a data set with many columns, you can right-click on the header of the columns in the Available columns list box and select Show Search Field from the pop-up menu. This will display a search field where you can type a search string and limit the number of items in the list. It is possible to use the wildcard characters * and ? in the search.
Selected columns	Displays the currently selected data columns on which you want to perform a clustering.
Add >>	Adds the highlighted data column to the list of selected columns.
<< Remove	Removes the highlighted data column from the list of selected columns and places them back in the list of available columns.

Work on: All records	All records in the value columns are included in the calculations.
Work on: Selected records	Only the selected records are included in the calculations. This lets you filter out any records that you do not want to include in the calculations, using the query devices and zooming.
Replace empty values with	Defines how empty values in the data set should be replaced in the clustering. Constant allows you to replace the empty values by any constant (type a number in the text box). Row average replaces the value by the average value of the entire row. Row interpolation sets the missing value to the interpolated value between the two neighboring values in the row. Column average returns the average of the corresponding column values.
Clustering method	The clustering method to use for calculating the similarity between clusters. Click here for a description of the available methods.
Similarity measure	The similarity measure to use for the clustering. Click here for a description of the available similarity measures.
Ordering function	The ordering function to use for the clustering. Click here for a description of the available ordering functions.
Column name	The name of the new columns containing the results from the hierarchical clustering.
Overwrite	Select this check box if you want to replace a previously added column and plot (with the same name as the one typed in the Column name text box) when you add a new column. Clear the check box if you wish to keep the old column and plot.
Calculate column dendrogram	Select this check box to calculate a column dendrogram during the clustering.
Import	Opens the Hierarchical Clustering: Dendrogram Import dialog where you can import row and column dendrogram files.

► To reach the Hierarchical Clustering dialog:

Select Data > Clustering > Hierarchical Clustering....

7.9.3.2 Hierarchical Clustering on Keys Dialog

Hierarchical Clustering) on Keys	
Column settings		
Key column:	MOL2DKEYS	•
Work on:	 All records 	
	C Selected records	
Calculation options		
Clustering method:	UPGMA (unweighted average)	•
<u>S</u> imilarity measure:	Euclidean distance	•
Ordering function:	Average value	•
Column <u>n</u> ame:	Hierarchical Clustering	🔽 Overwrite
Help	ОК	Cancel

Option	Description				
Key column	The data column on which to base the calculations. The key column should contain comma separated string values for all or some of the records in the data set.				
Work on: All records	All records in the value columns are included in the calculations.				
Work on: Selected records	Only the selected records are included in the calculations. This lets you filter out any records that you do not want to include in the calculations, using the query devices and zooming.				
Clustering method	The clustering method to use for calculating the similarity between clusters. Click here for a description of the available methods.				
Similarity measure	The similarity measure to use for the clustering. Click here for a description of the available similarity measures.				
Ordering function	The ordering function to use for the clustering. Click here for a description of the available ordering functions.				
Column name	The name of the new columns containing the results from the hierarchical clustering.				
Overwrite Select this check box if you want to replace a previously added co and plot (with the same name as the one typed in the Column nam box) when you add a new column. Clear the check box if you wis keep the old column and plot.					
Open	Opens the Hierarchical Clustering: Dendrogram Import dialog where y can open row dendrogram files. Column dendrograms are not available when you are clustering on keys.				

► To reach the Hierarchical Clustering on Keys dialog:

Select Data > Clustering > Hierarchical Clustering....

7.9.3.3 Hierarchical Clustering Dendrogram Import Dialog

실 Hierarchical Cluste	ering: Dendrogram Import 📉 🔀				
Select files containing p	previously saved dendrograms.				
<u>R</u> ow dendrogram:					
C:\Documents and Se	ettings\RowDendrogram.dnd Browse				
<u>C</u> olumn dendrogram:					
C:\Documents and Se	ettings\ColumnDendrogram.dnd				
Column <u>n</u> ame:					
Hierarchical Clustering	Verwrite				
Help	OK Cancel				
Option	Description				
Row dendrogram	Click on the Browse button to display an Open File dialog, where you				
	can select the row dendrogram to open. Only row dendrograms directly associated with the open data set can be opened.				
Column	Click on the corresponding Provi se button to display an Open File				
dendrogram	dialog, where you can select the column dendrogram to open. The				
-	column dendrogram option is not available when you are accessing this				
	dialog from the Hierarchical Clustering on Keys dialog.				
Column name	The name of the new columns containing the results from the hierarchical clustering.				
Overwrite	Select this check box if you want to replace a previously added column				
(with the same name as the one typed in the Column name text bo					
	old column.				

► To reach the Hierarchical Clustering: Dendrogram Import dialog:

- 1. Select Data > Clustering > Hierarchical Clustering....
- 2. Click on the **Open...** button in the lower left part of the dialog to display the **Hierarchical Clustering: Dendrogram Import** dialog.

7.9.3.4 The Row Dendrogram

The row dendrogram shows the similarity between rows and shows which nodes each record belongs to as a result of the clustering. An example of part of a row dendrogram is shown below.

The vertical axis of the row dendrogram consists of the individual records, and the horizontal axis represents the clustering level.



The individual records in the clustered data set are represented by the rightmost nodes in the row dendrogram. Each remaining node in the dendrogram represents a cluster of all records that lie to the right of it in the dendrogram. The leftmost node in the dendrogram is thus a cluster that contains all records.

The row dendrogram is automatically displayed next to the heat map which is created upon clustering. It can, however, be hidden or displayed by selecting **View > Row dendrogram** from the Hierarchical Clustering menu.

7.9.3.5 The Column Dendrogram

The column dendrogram is drawn in the same way as the row dendrogram but shows the similarity between the variables (the selected value columns). The variables in the clustered data set are represented by the nodes at the lowest part of the column dendrogram.



To display the column dendrogram (if one has been calculated), select **View > Column Dendrogram** from the Hierarchical Clustering menu. The column dendrogram can only be displayed if it has been calculated (select this in the Hierarchical Clustering dialog).

Restricted functionality

The column dendrogram offers less interactivity than the row dendrogram. You cannot add the results from the column dendrogram to the data set and so you cannot create visualizations based on it. There is no cluster slider above the column dendrogram, no cluster line and no horizontal zooming.

7.9.3.6 Row Dendrogram Menu and Toolbar

Toolbar



The row dendrogram toolbar is located directly above the row dendrogram. The row dendrogram is automatically created upon clustering and it is located to the left of the heat map. Click on the buttons in the toolbar to activate the corresponding functions.



Displays the Hierarchical Clustering menu.

+8

Adds a new column to the data set with information about which cluster each record belongs to. The position of the red circle on the cluster slider above the dendrogram controls the number of clusters. The column can be used to create a trellis plot of the clusters.

Option	Description				
Zoom to Active	Zooms to the selected subtree so that the active node in the row dendrogram is displayed to the far left of the visualization.				
Reset Zoom	Resets the horizontal zooming to its original size so the full width of the row dendrogram is visible.				
View >					
> Log Scale	Displays the dendrogram in log scale. Affects only the display of the dendrogram and not the actual numbers of the calculated similarity measures.				
> Toolbar	Displays or hides the row dendrogram toolbar. If the toolbar has been hidden, right-click on the row dendrogram and select View > Toolba from the pop-up menu to display it again.				
> Cluster Scale	Displays or hides the cluster scale (and cluster line) above the row dendrogram. The cluster scale must be displayed if you want to select the number of clusters to be included in the added cluster column.				
> Column Dendrogram	Displays or hides the column dendrogram (if one has been created).				
> Row Dendrogram	Displays or hides the row dendrogram.				
> Include Empty	Relevant only when you have performed a clustering using selected records. This produces a Hierarchical Clustering (order) column with empty values for all of the remaining records. By marking or clearing the Include Empty option you can determine whether or not to display the records that were not a part of the clustering calculation in the hea map. Obviously, no dendrogram can be displayed for these rows.				
Remove Dendrograms	Removes the dendrograms permanently from the visualization.				
Add Cluster Column	Adds a new column to the data set with information about which cluster each record belongs to. The position of the red circle on the cluster slider above the dendrogram controls the number of clusters. The column can be used to create a trellis plot of the clusters.				
Overwrite	Selects whether or not to overwrite a Hierarchical Clustering (cluster) column, when using the Add cluster column function.				
Export >					
> Row Dendrogram	Opens a dialog where you can select a file name and save your row dendrogram.				
> Column dendrogram	Opens a dialog where you can select a file name and save your column dendrogram.				

Hierarchical Clustering menu

Note: The Hierarchical Clustering tool allows the dendrograms to be saved with the Analysis. However, it is still possible to export the dendrograms separately and then import them from within the Hierarchical Clustering: Dendrogram Import dialog.

7.9.3.7 Dendrogram Pop-up Menus

Right-click in the dendrogram to bring up the pop-up menu.

Row dendrogram pop-up menu:

Description				
Zooms horizontally so that the active node in the row dendrogram is displayed to the far left of the visualization.				
Resets the horizontal zooming to its original size so the full width of the row dendrogram is visible.				
Displays the dendrogram in log scale. Affects only the horizontal distances in the dendrogram and not the actual numbers of the calculated similarity measures.				
Displays or hides the row dendrogram toolbar. If the toolbar has been hidden, right-click on the row dendrogram and select View > Toolbar from the pop-up menu to display it again.				
Displays or hides the cluster scale (and cluster line) above the row dendrogram. The cluster scale must be displayed if you want to select the number of clusters to be included in the added cluster column.				
Displays or hides the column dendrogram (if one has been created).				
Displays or hides the row dendrogram.				
Relevant only when you have performed a clustering using selected records. This produces a Hierarchical Clustering (order) column with empty values for all of the remaining records. By marking or clearing the Include Empty option you can determine whether or not to display the records that were not a part of the clustering calculation in the heat map. Obviously, no dendrogram can be displayed for these rows.				
Removes the dendrograms permanently from the visualization.				
Adds a new column to the data set with information about which cluster each record belongs to. The position of the red circle on the cluster slider above the dendrogram controls the number of clusters. The column can be used to create a trellis plot of the clusters.				
Selects whether or not to overwrite a Hierarchical Clustering (cluster) column, when using the Add cluster column function.				

Column dendrogram pop-up menu:

Option	Description				
Zoom to Active	Zooms so that the active node in the column dendrogram is displayed at the top of the visualization.				
Reset Zoom	Resets the zooming to its original size so the full width of the row				

dendrogram is visible.

View >

> Log Scale	Displays the dendrogram in log scale. Affects only the horizontal
	distances in the dendrogram and not the actual numbers of the
	calculated similarity measures.

7.9.3.8 Cluster Slider in Dendrogram

The scale above the row dendrogram is the cluster slider. The numbers above the scale refer to the number of clusters at different positions in the dendrogram. The numbers below the scale refer to the calculated similarity measures. When you move the cursor over the scale, the number of clusters and the similarity measure at that position are given in a ToolTip.



Upper scale

The upper scale assists you in selecting the number of clusters before creating a new clustering column. Click on the red circle on the cluster slider and drag it to the horizontal position you want. The selected clusters are indicated as red circles in the dendrogram. The total number of clusters is shown in a ToolTip as long as you hold down the mouse button.

Lower scale

The lower scale shows the calculated similarity measure in the dendrogram. The position of a node along the scale represents the similarity measure between the two subnodes in that node (there are always exactly two subnodes in each node). In the figure below, the similarity measure between the two subnodes in the active node is indicated by the dotted orange arrow.



The vertical distance has no mathematical meaning in the dendrogram.

Note: There is no cluster slider above the column dendrogram. You cannot create clusters in a column dendrogram and you cannot export information about the column dendrogram as a new column.

Tip: The cluster slider can also be moved by using the left and right arrows on the keyboard. This increases or decreases the number of clusters in a stepwise fashion.

7.9.4 Theory and Methods

7.9.4.1 Hierarchical Clustering Method Overview

Hierarchical clustering arranges objects in a hierarchy with a treelike structure based on the similarity between them.

The graphical representation of the resulting hierarchy is called a dendrogram, or a tree graph. This figure shows a small part of a dendrogram.



In Spotfire DecisionSite, the vertical axis of the dendrogram consists of the individual records and the horizontal axis represents the clustering level. The individual records in the clustered data set are represented by the rightmost nodes in the row dendrogram. Each remaining node in the dendrogram represents a cluster of all records that lie below it to the right in the dendrogram, thus making the leftmost node in the dendrogram a cluster that contains all records.

Misapplication of clustering

Clustering is a very useful data reduction technique. However, it can easily be misapplied. The clustering results are highly affected by your choice of similarity measure and other input parameters. You should bear this in mind when you evaluate the results. If possible, you should replicate the clustering analysis using different methods. Apply cluster analysis with care and it can serve as a powerful tool for identifying patterns within a data set.

7.9.4.2 Hierarchical Clustering Algorithm

The algorithm used in the Hierarchical Clustering tool is a hierarchical agglomerative method. This means that the cluster analysis begins with each record in a separate cluster, and in subsequent steps the two clusters that are the most similar are combined to a new aggregate cluster. The number of clusters is thereby reduced by one in each iteration step. Eventually, all records are grouped into one large cluster.

This is how it works:

- 1. The similarity between all possible combinations of two records is calculated using a selected similarity measure.
- 2. Each record is placed in a separate cluster.
- 3. The two most similar clusters are grouped together and form a new cluster.
- 4. The similarity between the new cluster and all remaining clusters is recalculated using a selected clustering method.
- 5. Steps 3 and 4 are repeated until all records eventually end up in one large cluster.

7.9.4.3 Required Input for Hierarchical Clustering

When you start a clustering you need to specify a number of parameters.

The parameters are set in the Hierarchical Clustering dialog that you reach by selecting **Clustering > Hierarchical Clustering** from the **Data** menu.

You need to answer the following questions:

- Which clustering method should be used to calculate the similarity between clusters?
- Which similarity measure should be used to calculate the similarity between records?
- Which ordering function should be used for drawing the dendrogram?

7.9.4.4 Hierarchical Clustering Ordering Function

The ordering function controls in what vertical order the records (rows) are plotted in the row dendrogram. The two subclusters within a cluster (there are always exactly two subclusters) are weighted and the cluster with the lower weight is placed above the other cluster. The weight can be any one of the following:

- **Input rank** of the records. This is the order of the records during import to DecisionSite.
- Average value of the rows. For example, a record *a* with 5 dimensions would have the average $(a_1+a_2+a_3+a_4+a_5)/5$. The average for a record *a* with *k* dimensions is calculated as

$$\bar{a} = \frac{1}{k} \sum_{j=1}^{k} \bar{a}_j$$

Calculating the weight of a cluster

To calculate the weight w_3 of a new cluster C_3 formed from two subclusters C_1 and C_2 with a weight of w_1 and w_2 , and each containing n_1 and n_2 records, you use the following expression:

$$w_3 = \frac{n_1 \cdot w_1 + n_2 \cdot w_2}{\left(n_1 + n_2\right)}$$

7.9.4.5 Hierarchical Clustering References

Hierarchical clustering

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Sneath, P., Sokal, R. R. (1973) Numerical taxonomy, Second Edition, W. H. Freeman, San Francisco.

General information about clustering

Hair, J.F.Jr., Anderson, R.E., Tatham, R.L., Black, W.C. (1995) Multivariate Data Analysis, Fourth Edition, Prentice Hall, Englewood Cliffs, New Jersey.

7.9.4.6 Similarity Measures

7.9.4.6.1 Similarity Measures Overview

Spotfire DecisionSite contains several tools which calculate the similarity between different records (e.g., Hierarchical Clustering, K-means Clustering and Profile Search). Calculating similarities can be useful if you want to create lists of similar records which may possibly be treated as a group or if you want to find the record that is most similar to another record. The following similarity measures can be used to calculate the resemblance between records:

- Euclidean distance
- Correlation

- Cosine correlation
- City block distance
- Tanimoto coefficient (only available for Profile Search and Hierarchical Clustering)
- Half square Euclidean distance (only available for Hierarchical Clustering)

Note: When used in clustering, some of the similarity measures may be transformed so that they are always greater than or equal to zero (using 1 - calculated similarity value).

Dimensions

The term *dimension* is used in all similarity measures. The concept of dimension is simple if we are describing the physical position of a point in three dimensional space when the positions on the x, y and z axes refer to the different dimensions of the point. However, the data in a dimension can be of any type. If, for example, you describe a group of people by their height, their age and their nationality, then this is also a three dimensional system. For a record, the number of dimensions is equal to the number of variables in the record.

7.9.4.6.2 Euclidean Distance

The Euclidean distance between two profiles, a and b, with k dimensions is calculated as

$$\left\{\sum_{j=1}^{k} (a_j - b_j)^2\right\}$$

The Euclidean distance is always greater than or equal to zero. The measurement would be zero for identical profiles and high for profiles that show little similarity.

The figure below shows an example of two profiles called *a* and *b*. Each profile is described by five values. The dotted lines in the figure are the distances (a_1-b_1) , (a_2-b_2) , (a_3-b_3) , (a_4-b_4) and (a_5-b_5) which are entered in the equation above.



7.9.4.6.3 Correlation

The *Correlation* between two profiles, *a* and *b*, with *k* dimensions is calculated as cov(a, b)

std (a) · std (b)

where

$$\operatorname{cov}(a, b) = \frac{1}{k} \sum_{j=1}^{k} (a_j - \overline{a}) \cdot (b_j - \overline{b})$$
$$\operatorname{std}(a) = \sqrt{\frac{1}{k} \sum_{j=1}^{k} (a_j - \overline{a})^2}$$
$$\overline{a} = \frac{1}{k} \sum_{j=1}^{k} a_j$$

This correlation is called *Pearson Product Momentum Correlation*, simply referred to as *Pearson's correlation* or *Pearson's r*. It ranges from +1 to -1 where +1 is the highest correlation. Complete opposite profiles have correlation -1.



Profiles with identical shape have maximum correlation.

Perfectly mirrored profiles have the maximum negative correlation.

7.9.4.6.4 Cosine Correlation

The Cosine correlation between two profiles, a and b, with k dimensions is calculated as

$$\frac{\sum_{j=1}^{k} a_j \cdot b_j}{\operatorname{norm}(a) \cdot \operatorname{norm}(b)}$$

where

norm (a) = $\sqrt{\sum_{j=1}^{k} a_j^2}$

The cosine correlation ranges from +1 to -1 where +1 is the highest correlation. Complete opposite profiles have correlation -1.

Comparison between Cosine correlation and Correlation

The difference between Cosine correlation and Correlation is that the average value is subtracted in Correlation. In the example below, the Cosine correlation will be +1 between any combination of profiles a, b, and c, but it will be slightly less than that between profile d and any of the other profiles (+0.974). However, the regular Correlation will be +1 between any of the profiles, including profile d.



7.9.4.6.5 City Block Distance

The City block distance between two profiles, a and b, with k dimensions is calculated as

$$\sum_{j=1}^k \left| a_j - b_j \right|$$

The City Block distance is always greater than or equal to zero. The measurement would be zero for identical profiles and high for profiles that show little similarity.

The figure below shows an example of two profiles called *a* and *b*. Each profile is described by five values. The dotted lines in the figure are the distances (a_1-b_1) , (a_2-b_2) , (a_3-b_3) , (a_4-b_4) and (a_5-b_5) which are entered in the equation above.



In most cases, this similarity measure yields results similar to the Euclidean distance. Note, however, that with City block distance, the effect of a large difference in a single dimension is dampened (since the distances are not squared).

The name *City block distance* (also referred to as *Manhattan distance*) is explained if you consider two points in the xy-plane. The shortest distance between the two points is along the hypotenuse, which is the *Euclidean distance*. The *City block distance* is instead calculated as the distance in x plus the distance in y, which is similar to the way you move in a city (like Manhattan) where you have to move around the buildings instead of going straight through.

7.9.4.6.6 Tanimoto Coefficient

The Tanimoto coefficient between two rows, a and b, with k dimensions is calculated as

$$\frac{\sum_{j=1}^{k} a_j \cdot b_j}{\left(\sum_{j=1}^{k} a_j^2 + \sum_{j=1}^{k} b_j^2 - \sum_{j=1}^{k} a_j \cdot b_j\right)}$$

The Tanimoto similarity measure is only applicable for a binary variable, and for binary variables the Tanimoto coefficient ranges from 0 to +1 (where +1 is the highest similarity).

7.9.4.6.7 Half Square Euclidean Distance

The *Half square Euclidean distance* between two profiles, *a* and *b*, with *k* dimensions is calculated as

$$\frac{1}{2}\sum_{j=1}^{k} (a_j - b_j)^2$$

The Half square Euclidean distance is always greater than or equal to zero. The measurement would be zero for identical profiles and high for profiles that show little similarity.

The figure below shows an example of two profiles called *a* and *b*. Each profile is described by five values. The dotted lines in the figure are the distances (a_1-b_1) , (a_2-b_2) , (a_3-b_3) , (a_4-b_4) and (a_5-b_5) which are entered in the equation above.



7.9.4.7 Cluster similarity methods

7.9.4.7.1 Cluster Similarity Methods

A hierarchical clustering starts by calculating the similarity between all possible combinations of two records using a selected similarity measure. These calculated similarities are then used to derive the similarity between all clusters that are formed from the records during the clustering. You select one of the following clustering methods:

- UPGMA
- WPGMA
- Single linkage
- Complete linkage
- Ward's method

7.9.4.7.2 UPGMA

UPGMA stands for Unweighted Pair-Group Method with Arithmetic mean.

Assume that there are three clusters called C_1 , C_2 and C_3 including n_1 , n_2 and n_3 number of records. Clusters C_2 and C_3 are aggregated to form a new single cluster called C_4 .

The similarity between cluster C_1 and the new cluster C_4 in the example above is calculated as $sim_{C1,C4} = a \cdot sim_{C1,C2} + b \cdot sim_{C1,C3}$

where

sim = the similarity between the two indexed clusters and

$$a = \frac{n_2}{(n_2 + n_3)}$$
$$b = \frac{n_3}{(n_2 + n_3)}$$

7.9.4.7.3 WPGMA

WPGMA stands for Weighted Pair-Group Method with Arithmetic mean.

Assume that there are three clusters called C_1 , C_2 and C_3 including n_1 , n_2 and n_3 number of records. Clusters C_2 and C_3 are aggregated to form a new single cluster called C_4 . The similarity between cluster C_1 and the new cluster C_4 in the example above is calculated as

$$sim_{C1,C4} = \frac{1}{2} (sim_{C1,C2} + sim_{C1,C3})$$

where

sim = the similarity between the two indexed clusters.

7.9.4.7.4 Single Linkage

This method is based on minimum distance. To calculate the similarity between two clusters, each possible combination of two records between the two clusters is compared. The similarity between the clusters is the same as the similarity between the two records in the clusters that are most similar.

7.9.4.7.5 Complete Linkage

This method is based on maximum distance and can be thought of as the opposite of *Single linkage*. To calculate the similarity between two clusters, each possible combination of two records between the two clusters is compared. The similarity between the two clusters is the same as the similarity between the two records in the clusters that are least similar.

7.9.4.7.6 Ward's Method

Ward's method means calculating the incremental sum of squares. The similarity measure is automatically set to *Half square Euclidean distance* when using Ward's method. This is not configurable.

Assume that there are three clusters called C_1 , C_2 and C_3 including n_1 , n_2 and n_3 number of records. Clusters C_2 and C_3 are aggregated to form a new single cluster called C_4 .

The similarity between cluster C_1 and the new cluster C_4 in the example above is calculated as

 $\operatorname{sim}_{C1,C4} = \operatorname{a} \cdot \operatorname{sim}_{C1, C2} + \operatorname{b} \cdot \operatorname{sim}_{C1,C3} - \operatorname{c} \cdot \operatorname{sim}_{C2,C3}$

where

sim = the similarity between the two indexed clusters

$$a = \frac{n_1 + n_2}{(n_1 + n_2 + n_3)}$$
$$b = \frac{n_1 + n_3}{(n_1 + n_2 + n_3)}$$
$$c = \frac{n_1}{(n_1 + n_2 + n_3)}$$

7.10 Profile Search

7.10.1 Profile Search Overview

The Profile Search tool calculates the similarity to a selected profile for all records in the data set and adds the result as a new column. The records are then ranked according to their similarity to the master profile.

You can use an existing record from your data set or create an average profile from several marked records. The built in profile editor makes it possible to edit the master profile.

7.10.2 Using Profile Search

7.10.2.1 Initiating a Profile Search

► To initiate a profile search:

- Click to activate the profile that you want to use as master profile in one of the visualizations or mark a number of profiles on which to base the master profile.
 Comment: You can always edit the active or marked profile to obtain a master profile entirely by your choice.
- 2. Select Data > Pattern Detection > Profile Search....

Response: The Profile Search dialog is opened.

3. Select the value columns on which to base the clustering from the **Available columns** list and click **Add** >>.

Comment: For multiple selection, press **Ctrl** and click on the desired columns in the Available columns list. Then click Add >> to move the columns to the Selected columns list. You can sort the columns in the list alphabetically by clicking on the Name bar.

- 4. Click a radio button to select whether to work on All records or Selected records.
- 5. Select a method to Replace empty values with from the drop-down list.
- 6. Select whether to use profile from: **Active record** or **Average from marked records**. This is only an option if you have both marked records and an active record to begin with.

Response: The selected profile is displayed in the profile editor and the name of the profile is displayed to the left above the profile in the editor.

Comment: You can edit the profile in the editor and type a new name for the edited profile, if desired.

- 7. Select which **Similarity measure** you want to use for the profile search. Comment: Click for information about the available similarity measures.
- Type a Column name for the resulting column or use the default name. Comment: Select the Overwrite check box to overwrite an old column with the same name.
- 9. Click OK.

Response: The search is performed using the master profile displayed in the editor, and the results are added to the data set as a new column. A new scatter plot is created displaying the rank vs. the similarity, and an annotation containing information about the calculation settings is added to the visualization.

7.10.2.2 Changing a Value in a Master Profile

Note: The starting profile does not restrict you in any way. You can easily change or delete existing values in the profile to create any master profile of your choice.

► To change a value in a master profile:

- 1. Select the profile that you want to edit by activating a record in a visualization.
- 2. Select Data > Pattern Detection > Profile Search....

Response: The Profile Search dialog is opened. The active profile is displayed in the profile editor.

3. Select the value columns on which to base the clustering from the **Available columns** list and click **Add** >>.

Comment: For multiple selection, press **Ctrl** and click on the desired columns in the Available columns list. Then click Add >> to move the columns to the Selected columns list. You can sort the columns in the list alphabetically by clicking on the Name bar.

4. Click Edit....

Response: The Profile Search: Edit dialog is opened.

5. Click directly in the editor to activate the variable that you want to change and drag the value to obtain a suitable look on the profile.

Response: The new value is immediately displayed in the editor.

Comment: To set a value for a variable with a missing value, select the variable from the Active column list and type a number in the Value text box.

- 6. Type a **Profile name** in the text box or use the default name.
- 7. Click OK.

Response: The Profile Search: Edit dialog is closed and the edited profile is shown in the Profile Search dialog. The **Edited** radio button has been selected by default, but you can return to the old profile by clicking Use profile from: **Active record**.

Tip: You can also use the fields below the editor to select an Active column in the profile and edit its Value.

7.10.2.3 Removing a Value from Profile Search

► To remove a value from a master profile:

- 1. Activate the profile that you want to edit in a visualization.
- 2. Select Data > Pattern Detection > Profile Search....

Response: The Profile Search dialog is opened. The active profile is displayed in the profile editor.

- 3. Click **Edit...**.
 - Response: The Profile Search: Edit dialog is opened.
- 4. Click on the value that you want to remove and press **Delete**.
 - Response: The value for the variable is removed in the display.

Tip: You can also use the fields below the editor to select an **Active column** in the profile and remove its **Value** by pressing **Delete**.

7.10.2.4 Interpreting the Results of Profile Search

When a profile search has been performed, the selected profiles or records in the data set have been ranked according to their similarity to the selected master profile. The value of the selected similarity measure is added to the data set as a new column.

A new scatter plot can be created (optionally) displaying the Similarity plotted against the Similarity rank. This means that the record that is most similar to the master profile will be displayed in the lower, left corner of the visualization.

7.10.2.5 Adjusting the Scale of the Profile Editor

► To adjust the scale of the editor:

- 1. Click on the **Fit profile to screen** button, **[1]**, in the Profile Search: Edit toolbar.
- 2. Click on the **Reset original profile scale** button, **5**, to reset the scale.

Tip: You can also select **Fit to screen** or **Reset original scale** from the pop-up menu which is displayed by right-clicking in the edit window.

7.10.3 User Interface

7.10.3.1 Profile Search Dialog

rofile Search	
Column settings	
Avaijable columns: Name Enter text here	Add >> Selected columns: Add >> Time5 C< Time4 Time3 Time3
<u>W</u> ork on: Re <u>p</u> lace empty values with:	Move Down All records Selected records Empty value 0
Calculation options Use profile from: C Active record Active record C Average from marked records C Edited Edit Similarity measure:	149 Average 95.275
Column <u>n</u> ame:	Similarity to Average Create scatter plot (similarity vs rank)
<u>H</u> elp	OK Cancel

Option	Description				
Available columns	The data columns that you can include in the search. Click a column name in the list to select it, then click Add >> to move it to the Selected columns list. To select more than one column, press Ctrl and click the column names in the list. You can choose from any column that contains decimal numbers or integers. Note: You can right-click on the Name header to get a pop-up menu where you can related at the articlute and the selected below.				
Enter text here	If you have a data set with many columns, you can right-click on the header of the columns in the Available columns list box and select Show Search Field from the pop-up menu. This will display a search field where you can type a search string and limit the number of items in the				

	list. It is possible to use the wildcard characters * and ? in the search.				
Selected columns	Displays the currently selected data columns that you want to include in the search.				
Add >>	Moves selected columns from the Available columns list to the Selected columns list.				
<< Remove	Removes the selected columns and brings them back to the Available columns field.				
Move Up	Moves the selected columns up in the Selected columns list and restructures the profile.				
Move Down	Moves the selected columns down in the Selected columns list and restructures the profile.				
Work on: All records	All records in the value columns are included in the calculations.				
Work on: Selected records	Only the selected records are included in the calculations. Is This lets you filter out any records that you do not want to include in the calculations, using the query devices and zooming.				
Replace empty values with	Defines how empty values in the data set should be replaced. Empty value calculates the similarity between the two profiles based only on the remaining part of the profile. The result is the same as if the missing value in the profile had been identical with the value for that variable in the master profile. Constant allows you to replace the empty values by any constant (type a number in the text box). Row average replaces the value by the average value of the entire profile. Row interpolation sets the missing value to the interpolated value between the two neighboring values in the profile.				
Use profile from: Active record	Click this radio button to use an active record as the master profile.				
Use profile from: Average from marked records	Click this radio button to use an average calculated from marked profiles as the master profile.				
Use profile from: Edited	Click this radio button to use an edited profile as the master profile.				
Edit	Opens the Profile Search: Edit dialog.				
Similarity measure	The similarity measure that you want to use when performing the search.				
Column name	The name of the new columns containing the results from the profile search.				
Overwrite	Select this check box if you want to replace a previously added column (with the same name as the one typed in the Column name text box) when you add a new column. Clear the check box if you wish to keep the old column.				
Add rank column	Select this check box to add a column containing the similarity rank to the data set. In this column, the profile that is most similar to the master profile is given the number 1, the second profile is given number 2, etc.				

Create scatter plot (similarity vs rank) A new scatter plot can be created (optionally) displaying the Similarity plotted against the Similarity rank. This means that the record that is most similar to the master profile will be displayed in the lower, left corner of the visualization.

► To reach the Profile Search dialog:

Select Data > Pattern Detection > Profile Search....

7.10.3.2 Profile Search Edit Dialog

🎒 Profile	Search: Edit					×
k 2/	1					
5.40 0 /	Active (Edite	d)				
4.440					_	
3.480						
2.520				~		
1.560						
0.600	۲		Time3: 3	.000		
	Time1	Time2	Time3	Time4	Time5	
Active of	olumn: Time1		-			
 ⊻alue:	1		_			
<u>P</u> rofile na	ame: Active	(Edited)	_			
						-
н	eln			пк (Cancel	
k	Edit profile. clicking the	Allows you to m value and draggin	anually edit ng to the des	a single value in ired level.	the active co	lumn by
2/	Free hand da clicking and	rawing. Allows yo dragging the val	ou to manual ues using the	lly edit the value mouse pointer	es in the maste as a free hand	er profile by drawing tool.
‡	Fit profile to screen. Automatically adjusts the scale to show the entire profile in the edit window.					
•	Reset original profile scale. Resets the scale to the original value range. Variables outside the range will no longer be visible in the editor.					
Optior	า	Description				
Active c	olumn	Displays all colu	ımns availab	le in the profile	search.	
Value	lue Displays the value of the active column. To change the value, type a new number in the box.			lue, type a		
Profile n	ofile name The name of the edited profile. The name is displayed in the top left corner of the editorial window and it is also used in the default column name for the result of the search.					he top left fault column
► To reach the Profile Search: Edit dialog:

- 1. Select Data > Pattern Detection > Profile Search....
- 2. Click **Edit...** below the displayed profile.

7.10.3.3 Profile Search Edit Pop-up Menu

The pop-up menu in the profile search editor includes the following options:

Option	Description
Delete	Deletes the value in the active column from the master profile.
Insert	Inserts a new value in the active column at the point of the right-click. This option is only available if there is a missing value in the master profile.
Fit to screen	Automatically adjusts the scale to show the entire profile in the edit window.
Reset original scale	Resets the scale to the original value range. Variables outside the range will no longer be visible in the editor.

► To reach the Profile Search Edit pop-up menu:

Right-click in the profile editor.

7.10.4 Theory and Methods

7.10.4.1 Profile Search Method Overview

In a profile search, all profiles (data points or table rows) are ranked according to their similarity to a master profile. The similarity between each of the profiles and the master profile is calculated using one of the available similarity measures. A new data column with the value of the selected similarity measure for each individual profile is added to the original data set as well as a similarity to master profile rank column.

7.10.4.2 Required Input for Profile Search

You have to specify the following before you can start a profile search:

- Which master profile do you want to use?
- Which similarity measure should be used?
- Should empty values be excluded from the search?

Master profile

You can use an existing (active) profile as master profile or construct a new master profile as the average of several marked profiles. It is possible to edit the master profile using the built in editor before you start the search.

Similarity measures

The Profile Search tool can use a variety of similarity measures. Similarity measures express the similarity between profiles as numbers, thus making it possible to rank the profiles according to their similarity. For information about the various measures, go to the section Similarity measures.

Excluding empty values

The Profile Search tool can exclude empty values from the calculations. See Excluding empty values for more information.

7.10.4.3 Excluding Empty Values in Profile Search

The Profile Search tool can exclude empty values from the calculations. When you calculate the similarity between the master profile and a profile that has a missing value, the variable with a missing value is excluded from the comparison. The calculated similarity between the two profiles is then based only on the remaining part of the profile. The result is the same as if the missing value in the profile had been identical with the value for that variable in the master profile.

Similarity measures based on the profile gradient

If you are using a similarity measure that compares the gradients of the profiles, a missing value means that two gradients are excluded from the comparison. If we take an extreme example of a profile where every other value is missing, then there would be no gradients left in the profile to base the comparison on. Since excluding a missing value has the same effect as setting the value of the profile to the same value as in the master profile, the profile in this extreme example would then have the highest possible similarity with the master profile.

Missing values in the master profile

Any missing values in the master profile are always excluded from the search. If, for example, the second variable in the master profile has no value then this variable is always excluded in the comparison with the other profiles, even if you have not specified that you want to exclude empty values.

8 Tools

8.1 Structure Analytics

8.1.1 Structure Analytics Overview



Structures are graphical representations of chemical structures, such as molecules or parts of molecules. The Structure Analytics tools help you display structures by connecting to one or more structure databases. This allows you to visually examine the compounds in your data set by highlighting or marking records of interest. The tools also allow you to manage lists of compound identifiers generated using structure search, or imported from a file.

Viewing structures:

- Structure Viewer is a separate control window which can be used to display structures of the marked, activated or highlighted compounds in the data set. It can also be used to manage and compare lists from the various searches.
- Structures in Table is a basic table visualization that includes structures from one or more structure databases.
- Structure Marker Labels can be used to display structures when the active visualization is a scatter plot or a profile chart.

Searching for structures:

- Structure Search allows you to browse for, draw, or import a structure or a part of a structure, and search for it as a substructure, similar structures, etc.
- R-group Search allows you to search for structures containing one or more R-groups.
- List Search allows you to search for various lists of compound IDs.

Administrating structure tools:

- Structure Connection is used to set up and manage your connections to structure databases.
- Add Structure Keys is used to import structure keys which can later be used to cluster compounds based on their structure using the Hierarchical Clustering tool.
- Advanced Preferences is used to specify which structure renderer and editor to use.

8.1.2 Structure Viewer

8.1.2.1 Using Structure Viewer

8.1.2.1.1 Browsing the Data Set for Structures

The Browse tab of the Structure Viewer tool can be used to display structures of compounds in the data set. Whenever a set of compounds in a visualization has been marked, activated or highlighted, the structures corresponding to these markers will appear in Structure Viewer. The reverse is also true: when structures are marked, activated or highlighted the compounds in the visualization corresponding to the structures will dynamically be marked, activated or highlighted (if this has been specified in the Properties dialog).

To browse the data set:

1. If the Structure Viewer is not already open, select **Tools > Structure Analytics > Structure Viewer**.

Response: The Structure Viewer is displayed.

Comment: If you have not previously connected to a structure database, you may be prompted to do so now. When the connection is set up, you can start browsing for structures. If you do not have a data set in DecisionSite, the Structure Viewer will be empty until you open a data set or perform a search to populate the ID list in Structure Viewer.

- 2. Go to the **Browse** tab.
- 3. Highlight, activate or mark compounds in a visualization or structures in Structure Viewer.

Response: The structures corresponding to the compounds chosen in the visualization appear in Structure Viewer, and the compounds in the visualization corresponding to the structures in Structure viewer will be highlighted, activated or marked.

Note: Activating and marking have priority over highlighting. This means that as long as a compound or a group of compounds are activated or marked, highlighting will not have any effect. If you want to use highlighting, first make sure that no records are marked or activated.

8.1.2.1.2 Example: Creating a Table of Similar Structures

The following example demonstrates how different tools in DecisionSite for Lead Discovery can be combined to perform a typical task. The goal is to produce a table visualization showing a number of similar structures and some additional data. To achieve this, we will use the Structure Viewer, Structure Search, and Structures in Table tools.

► To create a table of similar structures:

1. Open the data set SAR.sfs in DecisionSite.

Comment: The file is included in the default installation, and can be found under Data/DrugDiscovery/Structural Activity Relationship. The file contains typical compound data.

- 2. Select **Tools > Structure Analytics > Structure Connection...**. Response: The Structure Connection dialog is displayed.
- Select Connect to: ISIS Database or SDFile. Response: The ISIS Connection: Connect dialog is displayed.
- 4. Click Browse....
- 5. Locate the file Benzo.db.

Comment: The file is included in the default installation, and can be found under Data/DrugDiscovery/Structural Activity Relationship. The file contains ISIS data.

- Click Next >.
 Response: The ISIS Connection: Configure dialog appears.
- 7. Click **Finish**, without altering the default settings.
- 8. Select Tools > Structure Analytics > Structure Viewer.
- 9. Go to the **Browse** tab in Structure Viewer.
- Mark some compounds in a visualization. Response: The structures corresponding to the marked compounds appear in Structure Viewer.
- 11. Double-click one of the structures in Structure Viewer. Response: The Structure Search dialog is displayed.
- 12. If desired, click Edit Structure.

Response: Your structure editor (e.g., ISIS/Draw) is launched with the selected structure.

- 13. In ISIS/Draw (or whatever editor you use), edit the structure.
- Click the Spotfire DecisionSite button in the top left-hand corner. Response: The edited structure is sent back to the Structure Search dialog.
- 15. In the Structure Search dialog, select **Search for: Substructure** and click **OK**. Response: In Structure Viewer, a new ID list is added, containing the IDs of the structures that share the chosen substructure.
- 16. In Structure Viewer, select some IDs in the ID list.
- Click Menu > Add > New Data Set from Structure Database. Response: The Add New Data Set from Structure Database dialog is displayed.
- 18. Select All compounds.
- Select the columns that you want to include in the new data set and click OK. Response: Since the data set is changed, the DecisionSite ID Column dialog will be displayed.
- 20. In the DecisionSite ID Column dialog, select the ID column for the new data set and click **OK**.

21. Select **Tools > Structure Analytics > Structures in Table**. Response: A table visualization with structures and other ISIS data is created.

8.1.2.1.3 Working with the ID List

8.1.2.1.3.1 Working with the ID List

The ID lists in the Structure Viewer tool lets you keep track of groups of compounds. Two tabs allow you to work with two types of lists. Each time you conduct a structure search or list search or paste a set of IDs, the result is added as a new list in the Lists tab. This way, you can always go back to a previous list of IDs. The Browse tab contains a single temporary list, representing the current set of highlighted, active or marked records.

Only the 25 most recent lists are stored on the Lists tab. To save ID lists more permanently, add the list to the portfolio, or export a list file.

If the Structure Viewer is not already open, select	Tools > Structure	Analytics > Structure
Viewer.		-

Action	Instruction
Create a list	Perform a search using the Structure Search or List Search tool.
Change list	Select a list from the drop-down list on the Lists tab.
Display structure for a compound ID	Click on a compound ID, or use Ctrl+Click to select multiple identifiers.
Copy a list	In the list, select the desired identifiers. Right-click and select Copy . Note that Ctrl + C cannot be used.
Paste a list	Copy a list of identifiers (each on a separate line) from another application. In Structure Viewer, right-click in the ID list on the Lists tab and select Paste . Note that Ctrl + V cannot be used.
Sort a list	Click on a list heading. Click again to reverse the order. To reset to the

original order, right-click and select Reset Sort Order.

Select all identifiers in a list	Right-click and select Select All in ID List.
Mark a compound in the visualization	In the list, select the desired identifiers. Right-click and select Mark in Visualization . This can be set to happen automatically. See Structure Viewer Properties dialog.
Rename a list	Add a list to the Lists tab and select it. Right-click and select Rename ID List This will launch the Rename ID List dialog.

Tip: To avoid losing the list of IDs on the Browse tab as soon as you mark a new set, copy it and paste it to the Lists tab.

8.1.2.1.3.2 Adding List Information to the Data Set

You can add the contents of the ID list (and also include additional columns from the structure database) as new columns in the current data set.

To add the list as new columns:

1. If the Structure Viewer is not already open, select **Tools > Structure Analytics > Structure Viewer**.

Response: If you have not previously connected to a structure database, you will be prompted to do so now. When the structure connection is set up, the Structure Viewer tool is displayed.

2. Select Menu > Add > Columns to Data Set....

Response: The Add Columns to Data Set dialog is displayed.

- 3. Select whether to base the new columns on **All compounds** or just the **Selected compounds** in the ID list.
- 4. Select the check box for the list-based columns you want to create, and/or click to select additional columns from the structure database from the list.
- 5. In the **Column name prefix** text box, type a prefix for the new columns.
- 6. Click **OK**.

Response: The new columns are added to Spotfire DecisionSite.

Tip: You can also click on the Add Columns to Data Set button to add columns to the data set.

8.1.2.1.3.3 Adding an ID List to the Portfolio

The **Lists** tab in Structure Viewer stores a history of the 25 most recent lists (search results, imported lists, etc). This is useful for storing results temporarily, but will not save them permanently. The following procedure describes how to use the Portfolio to save your lists.

► To add the list to the Portfolio:

1. If the Structure Viewer is not already open, select **Tools > Structure Analytics > Structure Viewer**.

Response: If you have not previously connected to a structure database, you will be prompted to do so now. When the connection is set up, the Structure Viewer tool is displayed.

- 2. Select an ID list from the drop-down list on the Lists tab, or go to the Browse tab if you want to export the highlighted, active or marked records.
- 3. In the ID list, select the compounds you want to include in the new Portfolio list. Comment: If you intend to add all the IDs in the list, it is not necessary to select them.
- 4. Select Menu > Add > List to Portfolio....

Response: The Add List to Portfolio dialog is displayed.

- 5. Select whether to add **Selected compounds** or **All compounds**.
- 6. Enter a **List name** and click **OK**.
 - Response: The list is added to the Portfolio.

Tip: You can also save lists as SDFiles, SAR tables or text files.

8.1.2.1.3.4 Importing Structure Database Data to DecisionSite

Note: If you are already working with a data set in DecisionSite, this will be closed before data from the structure database are imported.

► To import a new data set from ISIS:

1. If the Structure Viewer is not already open, select **Tools > Structure Analytics > Structure Viewer**.

Response: If you have not previously connected to a structure database, you will be prompted to do so now. When the connection is set up, the Structure Viewer tool is displayed.

2. Perform a search against the structure database to fill the **ID list** with the compounds that you wish to import.

Comment: Use the Structure Search or List Search tools.

- 3. Select Menu > Add > New Data Set from Structure Database....
- Response: The Add New Data Set from Structure Database dialog is displayed.
- 4. Click to select and include the desired **Structure Database columns**.

Comment: You can press **Shift** or **Ctrl** and click to mark multiple compounds.

5. Click **Add** >>.

Response: The selected structure database columns are moved to the Import to Spotfire list on the right.

Comment: To remove a structure database column from the selection, select it in the **Import to Spotfire** list and click **<< Remove**.

6. Click OK.

Response: A new data set, based on the current ID list, is imported into DecisionSite. **Tip:** You can double-click on the columns to move them back and forth between the lists in the dialog instead of using the **Add** >> and << **Remove** buttons.

8.1.2.1.4 Working with Structures

8.1.2.1.4.1 Copying Structures in Structure Viewer

You can copy a structure from Structure Viewer to the clipboard and paste it into other applications.

► To copy a structure:

1. If the Structure Viewer is not already open, select **Tools > Structure Analytics > Structure Viewer**.

Response: If you have not previously connected to an ISIS database, you will be prompted to do so now. When the ISIS connection is set up, the Structure Viewer tool is displayed.

- 2. Right-click on the structure you want to copy in the **Structures** pane.
- Select Copy from the pop-up menu.
 Comment: The contents of this pop-up menu is controlled by ISIS. Please refer to the ISIS documentation for more information about the available menu options.
- 4. Paste the structure in another application.

Tip: You can also export a structure as a MOL file.

8.1.2.1.4.2 Displaying Many Structures in Structure Viewer

You can view up to 6 x 6 structures at the same time in Structure Viewer.

► To display many structures:

1. If the Structure Viewer is not already open, select **Tools > Structure Analytics > Structure Viewer**.

Response: If you have not previously connected to a structure database, you will be prompted to do so now. When the connection is set up, the Structure Viewer tool is displayed.

2. Select Menu > Properties.

Response: The Structure Viewer Properties dialog is displayed.

- 3. Click in the lower right corner of the cell layout that you want to display in the Structures pane.
- 4. Click OK.

Response: The Structures pane displays the configured number of compounds (if more than one compound is marked in the ID list).

8.1.2.1.4.3 Spawning Structure Viewer Windows

If you want to keep the structures visible while hiding the Structure Viewer tool, it is possible to display structures in floating structure windows. The floating viewers always remain on top of all other windows.

► To display structures in floating structure viewers:

1. If the Structure Viewer is not already open, select **Tools > Structure Analytics > Structure Viewer**.

Response: If you have not previously connected to a structure database, you will be prompted to do so now. When the connection is set up, the Structure Viewer tool is displayed.

2. In the ID List, mark the compounds that you want to display.

Comment: Remember that marking more than a handful of compounds may obscure your view of the visualizations.

3. Select Spawn Structures from the menu, Menu -

Response: The selected structures are displayed in tiled windows, starting with the first window at the upper left corner of the screen.

Tip: Right-click on a structure window and select **Close all structure windows** or select **Close Spawned Structures** from the Structure Viewer menu to close all of the spawned viewers at once.

8.1.2.1.5 Exporting Results

8.1.2.1.5.1 Exporting a Structure from Structure Viewer

A structure can be exported from Structure Viewer as a MOL file or as a sketch file. A MOL file describes a single molecular structure which can contain disjoint fragments. Both formats can be imported in, e.g., ISIS/Draw.

► To export a structure:

1. If the Structure Viewer is not already open, select **Tools > Structure Analytics > Structure Viewer**.

Response: If you have not previously connected to a structure database, you will be prompted to do so now. When the connection is set up, the Structure Viewer tool is displayed.

- 2. Click on a structure in the structures pane to select it for export.
- 3. Select Menu > Export > Structure....

Response: The Export Structure to File dialog is displayed.

- 4. Select a location from the **Save in** drop-down list.
- 5. Enter a File name and click Save.

Tip: You can also copy a structure to the clipboard and paste it into other applications.

8.1.2.1.5.2 Exporting a SAR Table from Structure Viewer

A Structure-Activity Relationship (SAR) Table combines chemical and biological data in a spreadsheet.

Note: Microsoft® Excel must be installed on your PC to use this function.

► To export a SAR table:

1. If the Structure Viewer is not already open, select **Tools > Structure Analytics > Structure Viewer**.

Response: If you have not previously connected to a structure database, you will be prompted to do so now. When the connection is set up, the Structure Viewer tool is displayed.

- 2. Perform searches to populate the ID list.
- 3. Select an ID list.
- 4. In the ID list, select the compounds you want to include in the SAR table.
- Comment: If you intend to add all the IDs in the list, it is not necessary to select them.
 Select Menu > Export > SAR Table...
 - Response: The Export SAR Table dialog is displayed.
- 6. Select whether to export All compounds or Selected compounds.
- 7. Select the **Structure database columns** and **Spotfire columns** to include in the table. Comment: You can press **Shift** or **Ctrl** and click to select multiple compounds.
- 8. Click **Add** >>.

Response: The selected structure database columns and Spotfire columns are moved to the list on the right called Include in SAR table.

Comment: To remove an item from the SAR table, select it in the list **Include in SAR table** and click **<< Remove**.

- 9. Use the **Move up** and **Move down** buttons to change the order of the columns in the SAR table.
- 10. Click **OK**.

Response: Microsoft® Excel is launched, displaying the exported SAR table.

Tip: You can also click on the **Export SAR Table** button to bring up the dialog where the SAR table export is configured.

Note: Once the SAR table has been exported to Microsoft® Excel, make sure the cells that contain structures are not resized, or else sorting the table may not work properly.

8.1.2.1.5.3 Exporting an SDFile from Structure Viewer

Structure-data files (SDFiles) contain structures and data for any number of molecules. SDFiles can be imported into ISIS for Excel or opened directly in Spotfire DecisionSite.

► To export an SDFile:

1. If the Structure Viewer is not already open, select **Tools > Structure Analytics > Structure Viewer**.

Response: If you have not previously connected to a structure database, you will be prompted to do so now. When the connection is set up, the Structure Viewer tool is displayed.

- 2. Perform searches to populate the ID list.
- 3. Select an ID list.
- In the ID list, select the compounds you want to include in the SDFile. Comment: If you intend to include all the IDs in the list, it is not necessary to select them.
- 5. Select Menu > Export > SDFile....

Response: The Export SDFile dialog is displayed.

- 6. Select whether to export **All compounds** or **Selected compounds**.
- 7. Select the **Structure database columns** and **Spotfire columns** to include in the table. Comment: You can press **Shift** or **Ctrl** and click to select multiple compounds.

8. Click Add >>.

Response: The selected structure database columns and Spotfire columns are moved to the list on the right called Include in SDFile.

Comment: To remove an item from the SDFile, select it in the **Include in SDFile** list and click **<< Remove**.

- 9. Use the **Move up** and **Move down** buttons to change the order of the columns in the SDFile.
- 10. Click OK.

Response: The Save File dialog is displayed.

- 11. Select a location from the Save in drop-down list box.
- 12. Enter a File name and click Save.

Tip: You can double-click on columns to move them back and forth between the lists in the dialog instead of using the Add >> and << Remove buttons.

8.1.2.1.5.4 Exporting a List File from Structure Viewer

To export a list:

1. If the Structure Viewer is not already open, select **Tools > Structure Analytics > Structure Viewer**.

Response: If you have not previously connected to a structure database, you will be prompted to do so now. When the connection is set up, the Structure Viewer tool is displayed.

- 2. Select an ID list.
- In the ID list, select the compounds you want to include in the list. Comment: If you intend to include all the IDs in the list, it is not necessary to select them.

4. Select Menu > Export > List File...

Response: The Export List File dialog is displayed.

- 5. Select whether to export All compounds or Selected compounds.
- 6. Click OK.
 - Response: The Save As dialog is displayed.
- 7. Select a location from the **Save As** dialog.
- 8. Enter a File name and click Save.

Tip: You can also copy the selected compounds in the ID list to the clipboard by selecting **Menu > Edit > Copy IDs**.

8.1.2.2 User Interface

8.1.2.2.1 Structure Viewer User Interface



1. Structure Viewer toolbar

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Includes shortcuts for some of the most common commands in the Structure Viewer menu.

2. Structure Viewer menu

Menu
The menu provides all commands required to work with Structure Viewer.

3. List selector

The list selector (on the Lists tab) lets you select an ID list to work with.

4. ID list

Lists the compounds that are found in searches against the structure database (Lists tab) or the compounds that are highlighted, active or marked in the visualization (Browse tab). Click on an ID to display its structure in the Structures pane.

5. Structures pane

Displays the structures for the selected compounds in the ID list. Double-click a structure to launch Structure Search.

6. Connection

Displays the name of the database that you are currently connected to (Browse tab), or, the name of the database against which the currently selected search was performed (Lists tab).

8.1.2.2.2 Structure Viewer Menu

The Structure Viewer menu is displayed by clicking Menu - and contains all commands necessary for working with Structure Viewer.

Option	Description
Edit >	
> Copy IDs	Copies the compounds currently selected in the ID list to the clipboard.
> Copy to List	Copies the compounds currently selected in the active ID list to the Lists tab for temporary storage.
> Paste	Pastes a list of identifiers, creating a new list in Structure Viewer. The copied list can be separated with commas or line break. Note that Ctrl + V cannot be used.
> Select All in ID List	Selects all records in the current ID list.
> Invert selection in ID List	Inverts the selection so that all unselected records become selected and vice versa.
> Mark in Visualization	Marks the records in the visualizations corresponding to the selected IDs in the list.
> Rename ID List	Brings up the Structure Viewer: Rename ID List dialog, which allows you to change the default list name to a name of your choice.
> Reset Sort Order	Resets the list to the order it had before being sorted.
Add >	
> List to Portfolio	Adds the selected compounds in the ID list to the Portfolio as a new list. The Add to Portfolio dialog will prompt you to enter a list name. The list is placed as the last item on the root level.
> New Data Set from Structure Database	Creates a new data set in Spotfire DecisionSite based on the compounds in the current list. The data are imported from the currently active structure database.
> Columns to Data Set	Adds new columns to the data set. Brings up the Add New Columns dialog where you can configure what information you

	want to add from the ID list. Records that are not included in the ID list get empty values in the new columns.
Export >	
> Structure	Exports the structure selected in the Structures pane as a file (e.g., a MOL file).
> SAR Table	Exports the compounds in the ID list as a Structure-Activity Table in Microsoft® Excel. The SAR Table Export dialog will let you select which structure database columns and Spotfire columns to include. You must have Microsoft® Excel installed on your PC to use this function.
> SDFile	Exports the compounds in the ID list as an SDFile. The Export SDFile dialog will let you select which structure database columns and Spotfire columns to include.
> List File	Exports the compound IDs for compounds in the ID list as an LST file.
Spawn Structures	Opens floating structure viewer windows for the compounds selected in the ID list, with each structure in a separate window.
Close Spawned Structures	Closes all floating structure viewers.
Properties	Brings up the Structure Viewer Properties dialog where you can control how many structures to display at a time in the Structures pane.

8.1.2.2.3 Structure Viewer Pop-up Menus

ID List

Right-click in the ID list to bring up the following pop-up menu.

Option	Description
Copy IDs	Copies the compounds currently selected in the ID list to the clipboard. Note that $Ctrl + C$ cannot be used.
Copy to List	Copies the compounds currently selected in the active ID list to the Lists tab for temporary storage.
Paste	Pastes the contents of the clipboard into the ID list. Note that $Ctrl + V$ cannot be used. (This command is only available in the pop-up menu of the Lists tab.)
Select All in ID List	Selects all compounds in the current ID list.
Invert Selection in ID List	Inverts the selection in the ID list.
Mark in Visualization	Marks the records selected in the ID list in the visualizations. Note: You can set Structure Viewer to automatically mark selected records in the Structure Viewer Properties dialog.
Rename ID List	Allows you to change the default list name to a name of your choice. Note: Appears only in the Lists tab.

Reset Sort Order Resets the rows in the ID list to the original sort order.

Show All Columns If selected, all columns available in the structure database will be shown in the ID list. Otherwise, only the IDs are shown.

Structures pane

There is another pop-up menu in the Structures pane. It contains the following commands:

Option	Description
Renderer >	The renderer is the 3rd-party program that is responsible for showing structures in DecisionSite. For example, ISIS/Draw, MDL Draw, etc.
> Settings	Brings up the renderer settings dialog for the currently selected structure renderer. The renderer settings is different for different renderers. For example, if ISIS/Draw is used to render the structures you will be able to change the settings for hydrogens and atom numbers in the ISIS/Draw Settings dialog.
> Use Smooth Drawing	If selected, the structures are rendered using anti-aliasing to soften the edges. If you experience blurriness or difficulty of seeing details in your structures, clear this setting to turn off the smooth drawing.
> [list of available renderers]	The renderer currently selected is indicated by a dot. If you have access to more than one renderer you can change which one to use to display the structures in Structure Viewer by clicking on the desired renderer in this list.
Structure >	
> Structure Search	Starts the Structure Search tool with the currently selected structure as the search structure.
> R-group Search	Starts the R-group Search tool with the currently selected structure as the search structure.
	Note: This tool is only available if you have access to an ISIS/Host database.
> Export to File	Exports the selected structure as a file (e.g., a MOL file).
Properties	Brings up the Structure Viewer Properties dialog where you can control how many structures to display at a time in the Structures pane.

Connection

The pop-up menu on the connection at the bottom of Structure Viewer (Browse tab) contains commands to handle multiple connections for advanced users:

Option	Description
[list of available connections]	If you have more than one structure database connection available you will see a list of the ones currently open and be able to switch to another connection here. The connection currently selected is marked with a dot.
DecisionSite ID Column	Opens the DecisionSite ID Column dialog, where you can select which column in your data set to use as ID column in the connection to a structure database.
Connection	Displays detailed information about the currently active connection,

Details	e.g., the name of the ID columns in the database and in your data set. This information is set up by your administrator for most types of connections.
Open New Connection	Opens the Structure Connection dialog where you can select the database or type of database from which structural information is to be retrieved

8.1.2.2.4 Structure Viewer Toolbar

Menu 👻	Displays the Structure Viewer menu.
	Searches the ISIS database for structures using substructure search or similarity search.
Ø	Brings up the List Logic dialog where you can compare lists using Boolean operators (OR, AND or ONLY).
<u>_</u>	Adds the compounds in the ID list to the Portfolio as a new list. The list is placed as the last item on root level.
•8	Brings up the Add Columns to Data Set dialog where you can specify which columns you want to add from the ID list.
SAR	Exports the selected compounds in the ID list as a SAR table in Microsoft® Excel.

8.1.2.2.5 Dialogs

8.1.2.2.5.1 Add List to Portfolio Dialog

O Add List to Portfo	olio 🔀
Base the portfolio list	on the following records from the list in Structure Viewer: ounds (1 of 3)
List name: New port	ifolio list
<u>H</u> elp	OK Cancel
Option	Description
Selected compounds	Add only identifiers that have been selected in the list.
All compounds	Add all identifiers.
List name	Allows you to give the resulting portfolio list a name of your choice.
 To reach the Add List to Portfolio dialog: Select Menu > Add > List to Portfolio, or 	

• click on the Add List to Portfolio button

8.1.2.2.5.2 Add New Data Set from Structure Database Dialog

Add New Data Set from 9	Structure Database
Import data for the following re	cords from the list in Structure Viewer:
 Selected compounds (1 	of 37)
O A <u>l</u> l compounds	
Structure data <u>b</u> ase columns: corpid creation_date cas	Import to Spotfire: CDBREGNO MOLZDKEYS MOLFORMULA MOLWEIGHT
Help	Move Up Move Down OK Cancel
Option	Description
Selected compounds	Import data for the selected compounds in the current list only.
All compounds	Import data for all compounds in the current list.
Structure database columns	Displays the available fields in the structure database that you ar currently connected to.
Import to Spotfire	Displays the columns that you have selected to import to Spotfir DecisionSite as a new data set.
Add >>	Adds the selected structure database columns to the list of what a Import to Spotfire.
<< Remove	Moves selected columns from the list of what to Import to Spotf to the list of structure database columns.
Move Up	Moves the selected rows in the Import to Spotfire list up one step order of the columns in this list will determine the order of the co in the new data set.
Move Down	Moves the selected rows in the Import to Spotfire list down one

► To reach the Add New Data Set from Structure Database dialog: Select Menu > Add > New Data Set from Structure Database....

8.1.2.2.5.3 Add Columns to Data Set Dialog

Add Columns to Data Set	×
Base the columns added to the data set on the following records from the list in Structure Viewer: Selected compounds (1 of 3) All compounds	
Columns to add	_
Records included or not included in list	
Sort order	
Columns from structure database (click to select): MOL2DKEYS MOLFORMULA corpid creation_date cas MOLWEIGHT MOLSIMILARITY	
Column name prefix: ID List	-
<u>H</u> elp OK Cancel	

Option	Description
Selected compounds	Add data for the selected compounds in the current list only.
All compounds	Add data for all compounds in the current list.
Records included or not included in list	Adds a new column with the value "Yes" for records included in the ID list and "No" for remaining records in the data set.
Sort order	Adds a new column with the sort order of the records in the ID list. The first record in the list gets the value "1", the second gets "2" and so on. Records that are not included in the list get an empty value in the new column.
Columns from structure database	Click on the column names of those columns you wish to add to the data set. For instance, a similarity column might be included with the similarity score from a previously performed similarity search. Records not included in the list get an empty value in the new columns.
Column name prefix	Allows you to give the resulting columns a name template of your choice.
NT 4 T C 4' 'I	1 1 1 11 1/2 1 1/2 1 1 1 1 1 1 1/2 /

Note: Information will only be added to compounds that are already included in the data set. New records will not be added.

► To reach the Add Columns to Data Set dialog:

- Select Menu > Add > Columns to Data Set..., or
- Click on the Add Columns to Data Set button +

8.1.2.2.5.4 Rename ID List Dialog

🧿 Rename	ID List			×
List name:	Interesting Structure	98		
		OK	Cancel	

Option Description

List name Allows you to give the resulting ID list a name of your choice.

► To reach the Rename ID List dialog:

- Select Menu > Edit > Rename ID List..., or
- right-click in the ID List and select **Rename ID List...**.

8.1.2.2.5.5 Export SAR Table Dialog

• Export SAR Table		-
Base the SAR table on the for Selected compounds (All compounds	ollowing records from the list in Structure Viewer: 1 of 3)	
Structure data <u>b</u> ase columns MOL2DKEYS corpid creation_date cas MOLWEIGHT MOLSIMILARITY	: Include in <u>S</u> AR table: CDBREGND - Database ID - Spotfire MOLSTRUCTURE - Database MOLFORMULA - Database Bioavailability - Spotfire	
Spotfire <u>columns:</u> Mol Wt. Plate # Row Column LC/MS LD(50) In-vivo Activity Assay #1(IC50)	<< <u>R</u> emove	
	Move Up Move Down	
<u>H</u> elp	OK Cancel	
Option	Description	
Selected compounds	Export data for the selected compounds in the current list only.	

All compounds	Export data for all compounds in the current list.
Structure database columns	Displays the available fields in the structure database that you are currently connected to.
Spotfire columns	Displays the available columns in the current data set in Spotfire DecisionSite.
Include in SAR table	Displays the structure database columns and the Spotfire columns that you have selected to export as a SAR table.
Add >>	Adds the selected structure database columns and/or Spotfire columns to the list of what to Include in SAR table.
<< Remove	Moves selected columns from the list of what to Include in SAR table back to the list of structure database columns and/or Spotfire columns.
Move up	Moves the selected rows in the Include in SAR table list up one step. The order of the columns in this list determines the order of the columns in the resulting SAR table.
Move down	Moves the selected rows in the Include in SAR table list down one step.

► To reach the Export SAR Table dialog:

- Select Menu > Export > SAR Table..., or
- click on the Export SAR Table button

8.1.2.2.5.6 Export SDFile Dialog

Note: SDFile export is supported only from structure databases that work with the MOL-file structure format.

All compounds		
Structure database columns: MOLZDKEYS MOLFORMULA corpid creation_date cas Spotfire_columns: Mol Wt. Plate # Row Column LC/MS LD(50) In-vivo Activity Assay #11(C50)	Add >> Add >>	-
	Move <u>Up</u> Move <u>D</u> own	

Option	Description
Selected compounds	Export data for the selected compounds in the current list only.
All compounds	Export data for all compounds in the current list.
Structure database columns	Displays the available columns in the structure database that you are currently connected to.
Spotfire columns	Displays the available columns in the current data set in Spotfire DecisionSite.
Include in SDFile	Displays the structure database columns and Spotfire columns that you have selected to export as an SDFile.
Add >>	Adds the selected structure database columns and/or Spotfire columns to the list of what to Include in SDFile.
<< Remove	Moves selected fields from the list of what to Include in SDFile back to the list of structure database and/or Spotfire columns.
Move Up	Moves the selected rows in the Include in SDFile list up one step. The order of the columns in this list determines the order of the columns in the resulting SDFile.
Move Down	Moves the selected rows in the Include in SDFile list down one step.

► To reach the Export SDFile dialog:

Select Menu > Export > SDFile....

8.1.2.2.5.7 Export List File Dialog



Selected Include the selected compounds/structures in the saved list only.

All compounds Include the entire current list in the saved list.

► To reach the Export List File dialog:

Select Menu > Export > List File....

8.1.2.2.5.8 Renderer Settings Dialog

The renderer is the program that is responsible for the display of structures in Structure Viewer, Structure Search and Structures in Table. Prior to DecisionSite 8.2, MDL ISIS/Draw was used as the renderer for all tools, but in later versions of DecisionSite you may use other renderers as well.

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

ISIS/Draw Settings:

🧿 ISIS/Draw Setting	J 5		×
<u>H</u> ydrogens:			
Hetero		•	
Atom numbers:			
Off		-	
Help	ок (Cancel	
P			

Option	Description
Hydrogens	Determines whether or not hydrogens should be shown in the Structures display. Choose between Off (no hydrogens are shown), Hetero (only hydrogens on heteroatoms shown), Hetero/Terminal (only hydrogens on heteroatoms or terminal atoms are shown), and All (all hydrogens are shown).
Atom numbers	Determines whether or not atom numbers should be shown in the Structures display. Choose between Off , On , and Atom-Atom Mapped (only relevant in reactions where the query specifies exactly which atoms in the reactants correspond to the atoms in the products).

MDL Draw Settings:

hydrogens on heteroatoms shown), **Hetero/Terminal** (only hydrogens on heteroatoms or terminal atoms are shown), and **All** (all hydrogens are shown).

► To reach the Renderer Settings dialog:

- 1. In Structure Viewer, Structure Search or Structures in Table, right-click on a structure.
- 2. Select **Renderer > Settings** from the pop-up menu.

8.1.2.2.5.9 Structure Viewer Properties Dialog

This dialog is used to set the maximum number of structures to be shown in Structure Viewer at the same time. Here, it is also possible to control how the ID list interacts with the visualizations, by using the "auto-mark" function.



Option	Description
Auto-mark list selection	
Yes	Changes the set of marked records (in the visualizations) to reflect the set of selected IDs in the ID list.
No	Does not change the set of marked records.
Structures grid layout	Click the cell at the bottom-right corner of the desired cell configuration. The blue area represents the chosen configuration.

To reach the Structure Viewer Properties dialog:

Select Menu > Properties.

8.1.3 Structures in Table

8.1.3.1 Displaying Structures in a Table Visualization

The Structures in Table tool allows you to incorporate structure images from one or more structure databases into a table visualization. This makes it possible to create an interactive SAR (Structure-Activity Relationship) table.

► To launch the Structures in Table tool:

1. Select Tools > Structure Analytics > Structures in Table.

Response: If you have not previously connected to a structure database, you will be prompted to do so now. A new table visualization is created, showing a structure for each compound in the data set. The structure column appears to the far left of the table, and it will always be visible even if you scroll right in the visualization.

► To add structure columns to a Table:

- 1. Right-click on the table visualization.
- 2. Response: A pop-up menu is displayed.
- 3. Select Add Structure Column > [desired connection] from the pop-up menu.
- 4. Comment: If one or more structure database connections have been set up in the current session, you will see the available connections in the submenu after Add Structure Column. You can directly select one of them to use in the new structure column. If you want to open a new connection, click Add Structure Column > With New Connection... and select the desired connection from the drop-down list.
- 5. If desired, you can change the renderer used to display the structures from the pop-up menu, and also change the connection (which database to run against).

Note: The new structure column does not provide a query device.

Tip: To freeze one or more table columns, select **Edit > Properties**, and in the **Table** tab set the number of **Frozen columns** to 1 (or more).

8.1.3.2 Pop-up Menu

When you right-click in a table visualization you will see the table visualization pop-up menu, and also some options that are specific to DecisionSite for Lead Discovery and the Structures in Table tool. The following commands are used by Structures in Table (some of the commands are available only if you right-click on a structure column):

Option	Description
Add Structure Column >	Use this option to open another structure column in the current table visualization. It is possible to display more than one structure column and to use different connections and/or renderers.
> [list of available connections]	All live structure database connections that you have opened during the current DecisionSite session are shown in this list. Click to select the connection that you want to use for the new structure column.
> With New Connection	Opens the Structure Connection dialog, where you can connect to a different database. A new structure column will be opened with the connection you specified in the Structure Connection dialog.
Connection >	Shows which database connection the structure column you have clicked upon is using, and allows you to change the connection to a different structure database.
> [list of available	All live structure database connections that you have opened during the

connections]	current DecisionSite session are shown in this list. The active connection used by the structure column you have clicked upon is marked with a dot.
> Details	Displays detailed information about the currently active connection, e.g., the name of the ID columns in the database and in your data set. This information is set up by your administrator for most types of connections.
> Open New	Opens the Structure Connection dialog, where you can connect to a different database.
Renderer >	The renderer is the 3rd-party program that is responsible for showing structures in DecisionSite. For example, ISIS/Draw, MDL Draw, etc.
> Settings	Brings up the renderer settings dialog for the currently selected structure renderer. The renderer settings is different for different renderers. For example, if ISIS/Draw is used to render the structures you will be able to change the settings for hydrogens and atom numbers in the ISIS/Draw Settings dialog.
> Use Smooth Drawing	If selected, the structures are rendered using anti-aliasing to soften the edges. If you experience blurriness or difficulty of seeing details in your structures, clear this setting to turn off the smooth drawing.
> [list of available renderers]	The renderer currently selected is marked with a dot. If you have access to more than one renderer you can change which one to use to display the structures in Structure Viewer by clicking on the desired renderer in this list.
Structure >	
> Structure Search	Starts the Structure Search tool with the currently selected structure as the search structure.
> R-group Search	Starts the R-group Search tool with the currently selected structure as the search structure. Note: This tool is only available if you have access to an ISIS/Host database.
> Export to File	Exports the structure you click upon in the table as a file (e.g., a MOL file).

8.1.4 Structure Search

8.1.4.1 Searching for Compounds Using Structure Search

The Structure Search tool provides several search algorithms which retrieve molecules with similarities to the master structure based on things such as substructure, isomers, bonds, exact matches, etc. See the Structure Search dialog for more information regarding the individual searches that can be performed. These search methods return a list of identifiers that can be used in the Structure Viewer tool.

Note: What search methods are available depends on what type of structure connection you are using. Searches for similarity, isomer, tautomer, parent, and flexmatch are possible only with remote databases when you connect to ISIS databases.

► To search for compounds in the structure database:

- 1. In Structure Viewer or in a table visualization with structures, click to activate the compound on which you want to base the search.
- 2. Right-click on the structure and select **Structure > Structure Search...** from the popup menu.
- 3. Comment: You can also click on the Structure Search button in Structure Viewer, Response: The Structure Search dialog is displayed.
- 4. Select one of the alternatives under **Search for**.
- 5. If the **Parameters...** button becomes available, click on it to edit the parameters available for the selected search method.

Comment: Only a few of the search methods have additional parameters available. For example, if you select Similarity search, you must enter a threshold value in the Similarity Search Parameters dialog. The higher the threshold, the shorter the hit list.

 If required, click Edit Structure. Response: Your selected structure editor is launched. Edit the structure and click the

button (for ISIS/Draw) or the button (for MDL Draw). Please refer to the documentation of your current structure editor for more details.

7. Select a **Search domain**.

Comment: See Search Domains in Structure Search for more information.

8. Click OK.

Response: Structures in the database that match the search criteria are displayed in Structure Viewer. A new ID list is added.

Tip: You can also start the Structure Search tool by selecting **Tools** > **Structure Analytics** > **Structure Search...** Click **Import Structure...** to base the search on a previously saved structure or click **Edit Structure** to draw a new search molecule to use in the search.

8.1.4.2 Search Domains in Structure Search

The Structure Search and the R-group Search allows you to specify a search domain. Compounds outside the search domain will be ignored during a search. The following options are available.

Option	Description
Entire database	Searches the entire structure database that you are currently connected to. This is the default setting.
All data in the data set	Searches among the compounds included in the data set currently open in Spotfire DecisionSite only.
Selected data in the data set	Searches among the compounds included in the data set and selected using the query devices and zooming only.
Current selection in Structure Viewer	Searches among the compounds selected in the current ID list only. This is the currently displayed list on the Lists tab, or the current list on the Browse tab, depending on which is visible.

8.1.4.3 Examples of Search Molecules

Substructure

A substructure search will retrieve all structures where the substructure is wholly included. Hence, it does not have to be a chemically stable structure to produce results. This is the most common type of structure search.

Similarity

Performs a search for structures similar to the master structure. Enter a threshold value between 1 and 100. A high value means that only very similar records will be included in the resulting list.

Exact Match

Performs a search for only those structures identical to the master structure.

Isomer

Isomers are different compounds having the same molecular formula. An isomer search retrieves all molecules that are geometric isomers and stereoisomers of the master structure. Examples are cis/trans isomers or chiral molecules.



Tautomer

Tautomers are isomers that are rapidly interconverted. A tautomer search retrieves molecules that include the same atoms, but have double bonds and hydrogen atoms at different positions. Examples are Keto/Enol forms of a molecule (RCHOH-CHO <----> RCO-CH2OH), tautomers that contain metal bonds and molecules that contain charges and radicals.

Parent

Retrieves molecules that are parent molecules of a salt query.



Example:

R-group

Retrieves molecules that contain structural fragments at specific sites within a molecule. Additional settings can be changed in the R-group Search dialog. Example of an R-group query in ISIS/Draw:



Flexmatch

Retrieves molecules that exactly match the master structure, except in the ways specified in the Structure Search: Edit Flexmatch Parameters dialog.

8.1.4.4 User Interface

8.1.4.4.1 Structure Search Dialog

Note: Searches for similarity, isomer, tautomer, parent, and flexmatch are possible only with remote databases. R-group searches are available for ISIS remote databases via the R-group Search tool.

Structure Search				×
Search for:				
Substructure		•	Parameters	
			<u>E</u> dit Structure Import Structure	
				-
Search d <u>o</u> main: [Enti	re database		<u>-</u>	
List <u>n</u> ame: Subs	structure			
Connected to: ISIS:	0.3k.db			
<u>H</u> elp		OK	Cancel	
Option	Description			
Search for: Substructure	Performs a search for structure	es containin	g the substructure.	
Search for: Similarity	Performs a search for structure the Similarity Search Parameter between 1 and 100. A high val	es similar to ers dialog a lue means tl	the master structund type a threshold type a threshold that only very simil	re. Open l value ar records

will be included in the resulting list.

Search for: Exact Match	Performs a search for only those structures identical to the master structure.
Search for: Isomer	Retrieves molecules that are geometric isomers and stereoisomers of the master structure.
Search for: Tautomer	Retrieves molecules that include the same atoms, but have double bonds and hydrogen atoms at different positions.
Search for: Parent	Retrieves molecules that are parent molecules of a salt query.
Search for: Flexmatch	Retrieves molecules that exactly match the master structure, except in the ways specified in the Flexmatch Search Parameters dialog.
Parameters	Launches the Parameters dialogs where you can provide search parameters for some of the search types.
Edit Structure	Launches your current structure editor, where you can edit the structure before performing the search. The same thing is achieved by double- clicking the structure. After editing the structure and sending it back to DecisionSite, the Structure Search dialog is updated with the edited structure.
Import Structure	Launches the Open dialog where you can select a structure file for use in the search.
Search domain	Allows you to limit the search to a specified subset of the ISIS database. See Search domains in Structure Search for more information.
List name	Allows you to give the resulting structure search list a name of your choice.
Connected to	Displays the database you are currently running against. By right-clicking on the database name you can display a pop-up menu where it is possible to change to another database.

► To reach the Structure Search dialog:

Select Tools > Structure Analytics > Structure Search....

8.1.4.4.2	Flexmatch Search Parameters Dialog

Plexmatch Search Parameters	s X
Type of <u>C</u> harge Match C Atom charges C Ion charges Soth off	Type of <u>B</u> ond Match C Bond Type C Tautomer O Both off
Match on:	
🗹 Eragments	🗖 <u>R</u> adicals
🗹 Hydrogen count	🗖 <u>S</u> alt
Isotopes	✓ Stereo bonds
Metal bonds	✓ Valences
	OK Cancel

Option Description

Type of Charge Match	Allows you to specify the type of charge you want to match, or you can turn them both off so as not to match any specific charge.
Type of Bond Match	Allows you to specify the type of bond you want to match, or you can turn them both off so as not to match any specific bond.
Match on	Allows you to select the item or substance on which you want to match.

► To reach the Flexmatch Search Parameters dialog:

- 1. Select Tools > Structure Analytics > Structure Search....
- 2. Select Search for: Flexmatch and click on the Parameters... button.

8.1.4.4.3 Similarity Search Parameters Dialog

Similarity Searc	h Parameters	×
<u>T</u> hreshold value:	90	
<u>H</u> elp	OK	Cancel

Option Description

Threshold value Type a threshold value between 1 and 100. A high value means that only very similar records will be included in the resulting list.

► To reach the Similarity Search Parameters dialog:

- 1. Select Tools > Structure Analytics > Structure Search....
- 2. Select Search for: Similarity Search.
- 3. Click on **Parameters...**.

8.1.4.4.4 Pop-up Menus

Structures pane

If you right-click on the structure in Structure Search or R-group Search you will see a pop-up menu with the following commands:

Option	Description
Edit	Opens the selected structure in your current structure editor.
Renderer >	The renderer is the 3rd-party program that is responsible for showing structures in DecisionSite. For example, ISIS/Draw, MDL Draw, etc.
> Settings	Brings up the renderer settings dialog for the currently selected structure renderer. The renderer settings is different for different renderers. For example, if ISIS/Draw is used to render the structures you will be able to change the settings for hydrogens and atom numbers in the ISIS/Draw Settings dialog.
> Use Smooth Drawing	If selected, the structures are rendered using anti-aliasing to soften the edges. If you experience blurriness or difficulty of seeing details in your structures, clear this setting to turn off the smooth drawing.
> [list of available renderers]	The renderer currently selected is indicated by a dot. If you have access to more than one renderer you can change which one to use to display the structures in Structure Viewer by clicking on the desired renderer in this list. R-group search supports ISIS/Draw as renderer only.
Structure >	
> Export to File	Exports the selected structure as a file (e.g., a MOL file).
> Import from File	Launches the Open dialog where you can select a structure file for use in the search.

Connection

The pop-up menu on the connection at the bottom of the dialog contains commands to handle multiple connections for advanced users:

Option	Description
[list of available connections]	If you have more than one structure database connection available you will see a list of the ones currently open and be able to switch to another connection here. The connection currently selected is marked with a dot.
DecisionSite ID Column	Opens the DecisionSite ID Column dialog, where you can select which column in your data set to use as ID column in the connection to a structure database.
Connection Details	Displays detailed information for the currently active connection. This information is set up by your administrator for most types of connections.

Open New	Opens the Structure Connection dialog where you can select the
Connection	database or type of database from which structural information is to be
	retrieved.

8.1.5 R-group Search

8.1.5.1 Performing an R-group Search

An R-group search is conducted using the R-group Search tool. The R-group search requires that you define a root structure and preferably one or more R-group substituents in ISIS/Draw. Below is a short example of how this is done. Please refer to the ISIS/Draw documentation for more detailed information.

Note: R-group search is possible only with remote databases.

To search for a structural fragment at a specific site in a molecule:

- 1. In the visualization, mark the compound on which you want to base the search. Comment: If desired, you can also draw the entire search molecule.
- 2. Select **Tools > Structure Analytics > R-Group Search...**. Response: The R-group Search dialog is displayed.
- 3. Click Edit....

Response: ISIS/Draw is launched.

4. Edit the structure by adding R-group labels to specific sites, or create a new root structure.



Example:

Comment: To add an R-group: Select the **Atom** tool, A. Click on the atom or bond where you wish to add the R-group. Select **More...** from the drop-down list (unless R1 is already visible in the list). Select the **Query Atom** tab. Select **Rgroup...** from the Symbol list. Select **R1** (or another symbol). Click **OK** twice.

- 5. Create the R-group substituents that you wish to allow on the R-group site. Comment: Draw structural fragments that would fit on the root structure. Select Chemistry > R-Query > Attachment. Enter the number of attachment points that you require. (If an R-group is attached to two bonds on the root structure, you must designate two attachment points.) Click on your substituent structure to specify the attachment point where you want it to attach to the root structure.
- 6. Specify the R-group that the substituents belong to.

Example:

Comment: Select all the desired members. Click **Chemistry** > **R-Query** > **Rgroup**. Click the name of the R-group to create (such as R1 or R2) and click **OK**.

7. If desired, specify R-group conditions by clicking **Chemistry** > **R-Query** > **R-Logic** and making your selections in the dialog.

Example: R1 >0

Comment: R1 > 0 means that there must be at least one substituent on the root structure.

8. Click the button.

Comment: If Chem Inspector pops up to say that there are problems with transferring the structure to Spotfire DecisionSite, change the **Intended use** drop-down list option from Local mol query to **Host Database > Molecule Query**, close Chem Inspector and try again.

- 9. Response: The edited structure is brought back to the R-group Search dialog.
- 10. If desired, select either of the check boxes to modify the search.
- 11. Comment: Only allow substitution at R-groups modifies your search by setting a flag which says that you do not wish substitutions to occur anywhere but at R-groups. Allow H substituents in R-groups modifies your search by setting a flag which says that if an R-group is undefined, it can be substituted by a hydrogen. When the flag is not set, the R-group can only be substituted by anything else other than hydrogen.
- 12. Select a Search domain.

Comment: See Search Domains in Structure Search for more information.

- 13. Type a List name for the resulting list in Structure Viewer.
- 14. Click OK.

Response: Structures in the database that match the search criteria are displayed in Structure Viewer. A new ID list is added.

A complete R-group query might look something like this:



Tip: You can also perform R-group searches using the Structure Search tool, but in that case you need to draw any flags for whether or not other positions on the molecule may be substituted yourself.

8.1.5.2 R-group Search Dialog

R-group search is used to retrieve molecules that contain structural fragments at specific sites within a molecule.

R-Group Search	×		
Original query structure:	Modified query structure:		
R1 >0	C(\$*) C(\$*) R1 >0 U(\$*) C(\$*) U C(\$*) R1		
R1= F ~ CI ~ Br ~ Br	R1= F * CI * Br *		
Edit Import Import			
·			
Search d <u>o</u> main: Entire database	•		
List name: R-Group Search			
Connected to: ISIS: 0.3k.db			
Help	OK Cancel		

Option	Description	
Original query structure	Displays the original query structure before any modification has taken place.	
Modified query structure	Displays the modified structure on which the query will be performed.	
Edit	Launches ISIS/Draw, where you can edit the structure before performing the search. The same thing is achieved by double-clicking the structure. Note: You cannot use MDL Draw to edit R-group searches. Even if you have specified that you want to use MDL Draw as editor in all tools, ISIS/Draw will be launched for the R-group search, if it is available. If you do not have ISIS/Draw installed on your computer, you will not be able to reach the R-group Search tool.	
Import	Launches the Open dialog where you can select a structure file for use in the search.	
Only allow substitution at R-	Modifies your search by setting a flag which says that you do not wish substitutions to occur anywhere but at R-groups.	

groups		
Allow H substituents in R- groups	Modifies your search by setting a flag which says that if an R-group is undefined, it can be substituted by a hydrogen. When the flag is not set, the R-group can only be substituted by anything else other than hydrogen.	
The original query has been modified	Displays the various modifications which have taken place, and the reasons for doing so.	
Search domain	Allows you to limit the search to a specified subset of the structure database. See Search domains in Structure Search for more information.	
List name	Allows you to give the resulting structure search list a name of your choice.	
Connected to	Displays the structure database you are currently running against. By right-clicking on the database name you can display a pop-up menu where it is possible to change to another database.	

► To reach the R-group Search dialog:

Select Tools > Structure Analytics > R-group Search....

8.1.6 List Search

8.1.6.1 Using List Search

► To search for structures using a list or compound identifiers:

- 1. Select Tools > Structure Analytics > List Search....
- Response: The List Search dialog is displayed.
- 2. Do one of the following:

Retrieve structures for	Instruction	
A list of compound IDs	Select the Compound IDs radio button. Enter a list of IDs, separated with carriage return, and click OK .	
Compounds in a list file	Select the Compounds in file radio button. Enter the name of a list file, or click Browse to locate one. Click OK .	
Selected data	Before launching the tool, use the query devices to select a group of compounds. In the List Search dialog, click Compounds selected in the data set , then click OK .	
All compounds	Click the All compounds in the structure database radio button. Click OK .	
Pasponsa: T	he structures that are found annear in the ID list and in the Structures name	

Response: The structures that are found appear in the ID list and in the Structures pane of Structure Viewer.

8.1.6.2 List Search Dialog

List Search				
■ Retrieve structure	es for Ds: 45 168 173			
Compounds in <u>file</u> : <u>Browse</u> Compounds <u>s</u> elected in the data set <u>All compounds in the structure database (retrieve all) </u>				
List <u>n</u> ame: Connected to:	Compound IDs ISIS: 0.3k.db			
<u>H</u> elp	OK Cancel			

Option	Description	
Compound IDs	Searches for your specified Compound IDs. Enter a list of compound IDs, separated with carriage return.	
Compounds in file	Searches for compounds in a previously saved list file. Enter the name of a list file, or click Browse	
Compounds selected in the data set	Searches for the compounds selected in the visualizations.	
All compounds in the structure database	Retrieves all structures in the current structure database. Note that this may be a very large number of structures. (This option is not available for all connections.)	
List name	Allows you to give the list search result a name of your choice.	
Connected to	Shows the currently active connection against which the list search will be performed. If you are using multiple structure connections it is possible to switch to another connection using the pop-up menu.	

► To reach the List Search dialog:

Select Tools > Structure Analytics > List Search....

8.1.6.3 Details on List Search vs Item Search

Searching and comparing lists using List Search may result in different outcomes for lists, depending on whether the list is saved in a list file (LST) or pasted/entered manually. This is due to the fact that the two searches are performed a bit differently.

In ISIS Base, there are several different types of searches. Two of these are list search and item search (ID search).

For list searches, the search is controlled by the content in the list. If there are incorrect IDs in the list, that is, if the list contains IDs that are not a part of the ID column in the database, the incorrect IDs will still be included in the resulting list. However, no structures will be available for these IDs since they do not exist in the database.

For ID searches, each ID is searched for in the database, and only the records that actually exist in the database will be included in the resulting list.

Spotfire's List Search works similarly to ISIS, so if, in the List Search dialog, you paste the contents of a list in "Compound IDs" you may get a different result from when you open the list via "Compounds in list file".

This can also affect you when you are using the List Logic tool together with Structure Viewer. The List Logic tool always performs an item search, but if you save the list to an external file and then import it into Structure Viewer via the "Compounds in list file" option in List Search, you will also perform a list search. This means that the resulting list in Structure Viewer may look different than it would if you exported the results from List Logic to Structure Viewer directly.

Example:

Consider that you have an ISIS database containing the IDs 1, 5, 6, 7, etc. (i.e., the IDs 2, 3 and 4 are missing) and you perform any List Logic operation that will result in a list with the IDs 1, 2, 3 and 4. Selecting different outputs from your List Logic operation will produce the following results after displaying the list in Structure Viewer:

Save new list in	Intermediate operation	Result in Structure Viewer
Structure Viewer	(none)	A list with the ID 1 is displayed, together with the structure for this molecule.
External list file	Use List Search, select the Compounds in list file radio button, and browse to open the external list file.	A list with the IDs 1, 2, 3, 4 is displayed, but since only the ID 1 is represented in the database, this is the only ID that can display a structure.

8.1.7 Add Structure Keys

8.1.7.1 Adding Structure Keys

A *structure key* is a string that lists the substructures which form a compound. When you import keys from a structure database, this information is added to the data set as a new column. The structure keys can then be used to cluster the compounds based on their structure, using the Hierarchical Clustering on Keys tool.

► To add structure keys to the data set:

- 1. Select **Tools > Structure Analytics > Add Structure Keys...**. Response: The Add Structure Keys dialog appears.
- 2. Select a **Structure keys column**.
- 3. Comment: If you cannot find a suitable structure keys column in the drop-down list, you should contact your database administrator.
- 4. Select whether to add keys to all records or just to selected records in the data set.
- 5. Click OK.

Response: Structure keys are imported from your structure database and added to the data set. In some cases, an annotation is added to the column in DecisionSite, listing
the available keys. This is used by the Hierarchical Clustering tool to help interpret the structure keys.

Comment: The records not found in the database will have empty values in the new column.

Tip: You can now cluster your compounds based on their structures.

8.1.7.2 Add Structure Keys Dialog

5 X
MOL2DKEYS
 ⊙ <u>A</u>ll records ⊂ <u>S</u>elected records
ISIS: 0.3k.db
OK Cancel
Description
Description Select the structure database column which contains structure keys. Note: If you cannot find a suitable structure keys column in the drop- down list, you should contact your database administrator.
Description Select the structure database column which contains structure keys. Note: If you cannot find a suitable structure keys column in the drop- lown list, you should contact your database administrator. Select whether to add structure keys for all records or just for selected records.

To reach the Add Structure Keys dialog:

Select Tools > Structure Analytics > Add Structure Keys....

8.1.8 Structure Connection

8.1.8.1 Structure Connection Overview

Many tools in DecisionSite for Lead Discovery require access to structural data from a database. The Structure Connection tools are used to determine what type of database to connect to, and also to manage multiple connections. If you select to connect to a local or remote ISIS database, or to an SDFile, the ISIS Connection tool will continue to guide you through the process. For other types of connections your administrator may have set up links to specific databases that you can select directly from the Structure Connection tool. Once you have set up a connection, all the Structure Analytics tools in Lead Discovery can be used without any further database configuration.

Note: A password may be required. Contact your database administrator for more information about passwords.

8.1.8.2 Connecting to a Structure Database

► To connect to a database:

- 1. Select **Tools > Structure Analytics > Structure Connection...**. Response: The Structure Connection dialog is displayed.
- 2. Select a connection from the **Connect to:** drop-down list.

Comment: The options available in this drop-down list depend on which connections have been defined by your administrator.

3. Click OK.

Response: If you have selected **ISIS Database or SDFile** the ISIS Connection: Connect dialog is displayed, where you select which ISIS database or SDFile to connect to. See Connecting to an ISIS database for more information on how to continue. If you have selected **SDFile** you will need to specify the SDFile to use and configure it in the Configure SDFile Connection dialog. If you have selected **Embedded structure column in loaded data set** you need to configure the structure column and type in the Configure Structure Connection dialog.

If the configuration was done correctly, you can now launch any Structure Analytics tool and work with the selected structure database.

Note: You can view all previously opened connections by clicking on Connections... in the Structure Connection dialog. To close a connection, click to select the connection, then click Disconnect.

8.1.8.3 Structure Connection Dialog

Note: Multiple connections might be useful to be able to view structures from different databases simultaneously. However, when you are allowing many connections you must always remember to check on which connection a search is performed. It is therefore recommended that you not use multiple connections unless you really must.



Connections	Opens the Connections dialog, where you can manually close previously opened connections during a session.
Cancel	Allows you to close this dialog without opening a new connection. Note: The changes that you have applied in the Connections dialog will not be undone when you click Cancel in this dialog. This allows you to enter the Connections dialog and close connections without having to open a new connection.

► To reach the Structure Connection dialog:

Select Tools > Structure Analytics > Structure Connection....

8.1.8.4 Connections Dialog

Onnections		×	
Live connections: ISIS: 0.3k.db MDL/Direct on homeserver	<u>D</u> isconnect D <u>e</u> tails		
<u>Н</u> ер ОК	Cancel		

Option	Description
Disconnect	Closes the selected connection.
Details	When available, displays a window with information about the selected connection. For ISIS connections, the full path to the database file or SDFile is shown, together with information about the selected ID columns in the ISIS database and in DecisionSite.
ОК	If you have closed one or more connections using the Disconnect button, clicking OK will apply these changes. Note: Once you have applied the changes by clicking OK, the connections are closed and you must connect again if you want them to come back. Clicking Cancel in the following Structure Connection dialog will not undo the closure of connections in this dialog.

► To reach the Connections dialog:

- 1. Select Tools > Structure Analytics > Structure Connection....
- Click on the Connections... button. Comment: The Connections... button is only available if you have connected to at least one structure database.

8.1.8.5 DecisionSite ID Column Dialog

This dialog is used to specify which column in the current data set in DecisionSite to use as ID column. The information is used in the connection to a structure database.

Select ID column	in DecisionSite:	
Name V	Туре	
MOLWEIGHT	Decimal	
MOLFORMULA	String	
MOL2DKEYS	String	
creation_date	String	
corpid	String	
CDBREGNO	Integer	
Help		OK Cancel

► To reach the DecisionSite ID Column dialog:

This dialog is automatically displayed whenever an ID column needs to be specified for the current data set. For example, this will happen after you have connected to an MDL Direct database using the Structure Connection tool and try to run any of the structure analytics tools. If you need to change the ID column once a connection has been set up, you can **right-click** on the Connection at the bottom of either of the structure analytics tools and select **DecisionSite ID Column...** from the pop-up menu.

8.1.8.6 Configure Structure Connection Dialog

This dialog is used when you have loaded a data set in DecisionSite containing a structure column, and you have selected to set up a connection to this column. For example, this could be the structure column of an opened SDFile, or a column of SMILES strings in a text file.

Configure Structure Connection		
Structure column:	Structure <molfile></molfile>	
Structure format:	MDL Molfile	
ID column:	CDBREGNO	
Help	OK Cancel	
Option	Description	

Structure column	The column in the data set that contains the structure information.
Structure format	The format of the structure column. Choose from MDL Molfile, MDL Sketch file, MDL Chime String or SMILES.
ID column	The column in the data set that identifies the compounds.

► To reach the Configure Structure Column dialog:

- 1. Select Tools > Structure Analytics > Structure Connection....
- 2. Select Embedded structure column in loaded data set.
- 3. Click **OK**.

8.1.8.7 Configure SDFile Connection Dialog

This dialog is shown when you have selected to set up a direct connection to an SDFile (not via ISIS).

Configure SDFile Connection			
Structure column:	Structure <molfile></molfile>		•
Structure format:	MDL Molfile		•
ID column (SDFile):	MOLFORMULA		•
ID column (Spotfire):	MOLFORMULA		•
Help		ОК	Cancel
Option	Description		

Structure column	The column in the SDFile that contains the structure information.
Structure format	The format of the structure column. Choose from MDL Molfile, MDL Sketch file, MDL Chime String or SMILES.

ID column The column in the SDFile that identifies compounds.

ID column (Spotfire)	The column in the data set that identifies compounds. This column must contain the same type of compound identifiers as the ID column (SDFile) field (see above).
-------------------------	---

► To reach the Connect to SDFile dialog:

- 1. Select Tools > Structure Analytics > Structure Connection....
- 2. Select **SDFile**.
- 3. Click OK.

8.1.8.8 ISIS Connection

(SDFile)

8.1.8.8.1 ISIS Connection Overview

The ISIS Connection tool establishes a connection with a local or remote ISIS database, or an SDFile. Once you have done this, all the Structure Analytics tools in Lead Discovery can be used without any further database configuration.

Note: A password may be required. Contact your ISIS database administrator for more information about passwords.

8.1.8.8.2 Connecting to an ISIS Database

To connect to an ISIS database:

- Select Tools > Structure Analytics > Structure Connection.... Response: If you have the possibility to connect to multiple structure connection providers, the Structure Connection dialog is displayed.
- 2. Select Connect to: ISIS Database or SDFile.
- 3. Click OK.
 - Response: The ISIS Connection: Connect dialog is displayed.
- 4. Select an ISIS database from the drop-down list, or click **Browse...** to locate a new one.

Comment: Your installation includes a local sample database, usually located under: \Program Files\Spotfire\DecisionSite\Data\DrugDiscovery\Structural Activity Relationship\Benzo.db.

5. Click Next >.

Response: The ISIS Connection: Configure dialog is displayed. You may also be prompted for a database password. Please contact your ISIS database administrator for more information.

6. Select a Structure field (ISIS).

Comment: This is the ISIS database field that contains structural information.

7. Select an **ID field (ISIS)**.

Comment: This is the ISIS database field that uniquely identifies compounds. The column recommended by Spotfire DecisionSite is selected by default and marked with [Recommended] in the drop-down list.

8. Select an **ID column (Spotfire)** (only available if you have data in Spotfire DecisionSite).

Comment: This is the column in your current data set that uniquely identifies compounds. It should contain the same compound identifiers as the ISIS ID field.

9. Click Finish.

Response: If the configuration was done correctly, you can now launch any Structure Analytics tool and work with the ISIS database.

8.1.8.8.3 Connecting to SDFiles

With DecisionSite 9.1 and forward it is possible to open or connect to an SDFile directly. However, the connection though ISIS Connection is also available to support old workflows.

► To connect to an SDFile via ISIS Connection:

- Select Tools > Structure Analytics > Structure Connection.... Response: If you have the possibility to connect to multiple structure connection providers, the Structure Connection dialog is displayed.
- Select Connect to: ISIS Database or SDFile. Response: The ISIS Connection: Connect dialog is displayed.
- 3. Select an SDFile from the drop-down list, or click **Browse...** to locate a new one.
- 4. Click Next >.

Response: The ISIS Connection: SDFile Settings dialog is displayed, containing the guessed field type for each field.

- 5. If you wish to change the field type of one or more fields, select those rows you wish to change and click **Change Type**.
- 6. Select a field **type**. **Note:** The guessed type for date is ftext.

Comment: This drop-down list contains several types you can choose from: **ftext**, **vtext**, **long**, **real**, and **range**. To restore the changed types to the originally guessed types, click **Restore Types**. See Field Types for definitions of the various field types.

7. Click OK.

Response: The ISIS Connection: Configure dialog is displayed.

 Click Finish. Response: If the configuration was done correctly, the file can now be used as any database file.

Tip: An SDFile that has been used in a connection is actually converted to a database (db) file. This file can be found in the temporary directory on your computer (e.g., C:\Documents and Settings\USER NAME\Local Settings\Temp\). It can be saved as an ordinary db file for future use. This is especially useful if the conversion of the SDFile takes long time. You can also save data that have been imported to DecisionSite in an Spotfire Analysis File (File > Save As...) and use the ISIS Connection tool to connect the data set to the converted db file in a later session.

8.1.8.8.4 Importing an SDFile

SDFiles can be opened directly by Spotfire DecisionSite (File > Open...), but they can also be imported as a part of a longer analysis sequence.

Below is a short example of how you can combine different structure analytics tools to retrieve data from an SDFile and later also use that data as a data set in Spotfire DecisionSite.

► To import an SDFile as a data set in DecisionSite:

- 1. Follow the steps in Connecting to SDFiles to set up a connection to the desired SDFile.
- 2. Select **Tools > Structure Analytics > List Search...**. Response: The List Search dialog is displayed.
- 3. Click on All compounds in the structure database (retrieve all).
- 4. Click OK.

Response: If the Structure Viewer is not already open, it will be displayed.

- 5. From the Structure Viewer menu, select Add > New Data Set from Structure Database....
- 6. Select all columns.
- 7. Click **OK**.

8.1.8.8.5 SDFiles Field Types

Each field of an SDFile must have a field type in its definition. The field type instructs ISIS/Base what type of data to store for the field. The following table shows the ISIS/Base permitted field types with an explanation of the type of data they store. For more information about the various field types, see MDL documents *CTfile Formats* and *MDL ISIS/Base Database Maintenance*.

Field Type	Definition
Fixed text (FTEXT)	Text of a specified number of alphanumeric characters. A fixed-text field can store any number of characters up to the maximum number specified in its definition. However, no fixed-text field can contain more than 80 characters. (For example, MDL-000001 is the maximum number of characters that can be entered for a fixed-text field that has been defined to have a 10 character length.)
Variable text (VTEXT)	Alphanumeric text of an unlimited length (limited solely by computer memory).

Integer (LONG)	For PC, the value of an integer may range from -2147483647 to +2147483647.
Real (REAL)	A real number such as 1.50. The decimal-place precision of the number varies with computer systems.
Range (RANGE)	A range of real-number values such as 2.0 - 3.5. The decimal-place precision of the number varies with computer systems.

8.1.8.8.6 User Interface

8.1.8.8.6.1 ISIS Connection: Connect Dialog

ISIS Connection: Connectio:	onnect	×
<u>D</u> atabase:		
C:\\DrugDiscovery\S	tructural Activity Relationship\Benzo.db	
		_
This application was cre MDL Information System	eated with, embodies and/or executes proprietary software under license from m, Inc. © Copyright MDL Information Systems, Inc. All rights reserved.	
<u>H</u> elp	< <u>Back</u> <u>N</u> ext > <u>Finish</u> Cancel	
Option	Description	
Database	The ISIS database or SDFile from which structural informat retrieved.	ion is to be
Browse	Click here to browse for a file or database.	

► To reach the ISIS Connection: Connect dialog:

- 1. Select Tools > Structure Analytics > Structure Connection....
- 2. In the Structure Connection dialog, select ISIS database or SDFile.

8.1.8.8.6.2 ISIS Connection: Configure Dialog

ISIS Connection: (Configure	×
Fields and columns to	o use for the connection to the ISIS database	
<u>S</u> tructure field (ISIS):	structure	1
ID <u>f</u> ield (ISIS):	ID [Recommended]	[
ID <u>c</u> olumn (Spotfire):	CDBREGNO	
(The two IDs must ma	tch to browse structures for data in Spotfire)	
<u>H</u> elp	< <u>B</u> ack <u>N</u> ext> <u>Finish</u> Cancel	

Option Description

Structure field (ISIS)	The field in the ISIS database that contains the structure information.
ID field (ISIS)	The field in the ISIS database that identifies compounds. The column recommended by Spotfire DecisionSite is selected by default and marked with [Recommended] in the drop-down list.
ID column (Spotfire)	The column in the data set that identifies compounds. This column must contain the same type of compound identifiers as the ISIS ID Field (see above).

► To reach the ISIS Connection: Configure dialog:

- 1. Select Tools > Structure Analytics > Structure Connection....
- 2. In the Structure Connection dialog, select ISIS database or SDFile.
- 3. In the ISIS Connection: Connect dialog, select a database and click Next >.

8.1.8.8.6.3 ISIS Connection: SDFile Settings Dialog

◎ ISIS Connection: SDfile Settings			
Fields			
Name CDBREGNO LC/MS MOLEORMULA	Type LONG FTEXT ETEXT		<u>C</u> hange Type ▼
			Restore Types
Help		OK	Cancel
Option	Description		
Fields	Displays the guessed field types for each of the fields.		

Change Type	Allows you to change the field type of a field. You can select from
	the following types: ftext, vtext, long, real, and range. See SDFiles
	Field Types for definitions of the various field types.

Restore Types Restores all changed field types to the originally guessed types.

► To reach the ISIS Connection: SDFile Settings dialog:

- 1. Select Tools > Structure Analytics > Structure Connection....
- 2. In the Structure Connection dialog, select ISIS database or SDFile.
- 3. Select an SDFile from the drop-down list, or click **Browse...** to locate a new one.
- 4. Click Next >.

8.1.8.8.6.4 ISIS Connection: Password Dialog

Note: Contact your administrator, or consult the ISIS/Base documentation for more information on the parameters of this dialog.

ISIS Connection	: Password		×
Database: \\ISIS\R	emoteW2_50.db		
<u>U</u> sername: aisis::ais	is\MDL		_
Password:	••••		
<u>H</u> elp		0K	Cancel
Ontion	Description		
Option	Description		
Username	The predefined use	The predefined user name used to connect to the ISIS database	

Password The password to the ISIS database.

8.1.8.8.6.5 Host Request Dialog

Note: Contact your administrator, or consult the ISIS/Base documentation for more information on the parameters of this dialog.

ISIS Connection: Host Request			×		
<u>H</u> elp		0	K	Cancel	
Option	Description				

(message string) A message sent from the host. Typically a request for a password.

8.1.8.8.6.6 Database Password Dialog

Note: Contact your administrator, or consult the ISIS/Base documentation for more information on the parameters of this dialog.

🎒 ISIS Connection: Data	base Password	
The ISIS database file C:\M Database <u>p</u> assword: *****	lyl\Database\PwdProtected.db is protected.	
Help	OK Cancel	
Option	Description	
Database password	The password for this particular file. The password is probably selected by the owner of the file in order to protect the file from corruption.	

8.1.8.8.6.7 Database Info Dialog

Note: Contact your administrator, or consult the ISIS/Base documentation for more information on the parameters of this dialog.

ISIS Connection: Datab	ase Info	<u> </u>	
Database: C:\MyI\Databas	e\MissingNode.db		
Account Information			
User name: mdl			
Password:			
Connection Info			
Hos <u>t</u> :			
<u>S</u> ervice: isishost			
Help	OK Cancel		
Option	Description		
User name	The name of a registered user.		
Password	The password of the user.		
Host	The name of the remote host server.		
Service	The name of the host service.		

8.1.9 Advanced Preferences

8.1.9.1 Adding Rules for Structure Analytics Tools

Advanced users can specify which structure renderer and editor to use (in some environments other preferences may also be available), if other than the default tools for a specific type of connection are desired. For example, if you have access to both ISIS/Host and MDL Direct

connections, you can specify that you always want to use ISIS/Draw to display and edit structures and never use MDL Draw.

Note: If your administrator has already specified mandatory rules defining which renderer and editor you should use, you will not be able to change those preferences with a rule. However, it will still be possible to temporarily change the renderer for the structures shown in a specific tool.

► To add rules:

- 1. Select **Tools > Structure Analytics > Advanced Preferences**. Response: The Advanced Preferences dialog is displayed.
- 2. Click on **Add Rule...** and select the type of rule that you want to specify from the drop-down list.
- 3. Comment: You can specify which structure renderer and editor to use (in some environments other preferences may also be available).
- 4. Response: The Renderer Rule dialog or the Editor Rule dialog is displayed.
- 5. Specify the **Structure format** for which the rule should apply.
- 6. Select the desired **Renderer** or **Editor** from the drop-down list.
- 7. Select whether the rule should be valid for **All tools** or just a **Specific tool**, selected from the drop-down list.
- 8. Click OK.

Response: The rule is added to your Personal rules in the Advanced Preferences dialog.

Click **OK** to close the Advanced Preferences dialog.

Note: For information on how to specify mandatory and recommended rules, see Spotfire Developer Network.

8.1.9.2 User Interface

8.1.9.2.1 Advanced Preferences Dialog

This dialog is used by advanced users to specify which structure renderer and editor to use (in some environments other preferences may also be available), if other than the default tools for a specific type of connection are desired. For example, if you have access to both ISIS/Host and MDL Direct connections, you can specify that you always want to use ISIS/Draw to display and edit structures and never use MDL Draw.

Note: If your administrator has already specified mandatory rules defining which renderer and editor you should use, you will not be able to change those preferences here. However, it will still be possible to temporarily change the renderer for the structures shown in a specific tool.

🛃 Advanced Preferences for Structure Analytics	X
This dialog is used to view and edit rules determining the behavior of the Structure Analytics tools.	
Rules (applied in the order shown):	
- Mandatory rules (always applied) - No rules in this category	Add Rule 🔻
- Personal rules	Edit
 Use ISIS/Draw renderer for MDL Sketch File in all tools. Use ISIS/Draw renderer for MDL Molfile in all tools. 	
	Delete
L- Hecommended rules (default)	
	Move Up
	Move Down
	Import
	Export
Help	UK Cancel

Option	Description
Rules (applied in the order shown)	This list box displays all rules that have been defined on your system. There are three categories of rules: Mandatory, Personal and Recommended. The Mandatory rules (if there are any available) have been set up by your Spotfire DecisionSite administrator to ensure that you will use a predefined editor, renderer or some other rule. When mandatory rules have been specified for a certain item, you will not be able to change the preferences for that item yourself.
Add Rule	Displays a menu where you can select to add a rule for your preferred Renderer or Editor. There may also be other types of rules available, depending on your environment.
Edit	Opens the Renderer Rule or Editor Rule dialog, where you can edit the selected rule.
Delete	Deletes the selected rule.
Move Up	Moves the selected rule up within the Personal rules category. The rules are applied from the top down, so the order of the rules defined is important.
Move Down	Moves the selected rule down within the Personal rules category. The rules are applied from the top down, so the order of the rules defined is important.
Import	Opens a dialog where you can browse to a previously exported Spotfire preference file. After a file has been selected, the Import Rules dialog is displayed where you can select which of the available rules that you wish to import. Imported rules will by default be placed at the top of your Personal rules category.

Export... Opens the Export Rules dialog, where you can select to export one or all of your personal rules to a file.

To reach the Advanced Preferences dialog:

Select Tools > Structure Analytics > Advanced Preferences.

8.1.9.2.2 Editor Rule Dialog

The editor is the program that will be opened when you need to edit structures prior to a search (Structure Search and R-group Search for ISIS databases). Prior to DecisionSite 8.2, MDL ISIS/Draw was used as editor, but in later versions of DecisionSite you may use other editors as well.

The Editor Rule dialog is used to specify which editor to use in different situations.

Note: If your administrator has defined some mandatory rules, you may not be able to use your own preferences in the choice of renderer or editor, since mandatory rules have priority before personal rules.

Editor Rule	×
Structure format:	
MDL Molfile	•
E ditor:	
ISIS/Draw	▼
Valid for	
 All tools 	
C Specific tool:	
	<u></u>
Help	OK Cancel

Option	Description
Structure format	The structure format that you wish the rule to apply to.
Editor	The editor you prefer to use. Note: You cannot use MDL Draw to edit R-group searches. Even if you specify that you want to use MDL Draw as editor in all tools, ISIS/Draw will be launched for the R-group search, if it is available. If you do not have ISIS/Draw installed on your computer, you will not be able to reach the R-group Search tool.
Valid for: All tools	Select this option to apply the editor rule for all structure tools.
Valid for: Specific tool	Select this option if you just want to apply the editor rule for a specific tool (select which tool from the drop-down list).

► To reach the Editor Rule dialog:

- 1. Select Tools > Structure Analytics > Advanced Preferences.
- 2. Click on Add Rule and select Editor... from the drop-down menu.

8.1.9.2.3 Renderer Rule Dialog

The renderer is the program that is responsible for the display of structures in Structure Viewer, Structure Search and Structures in Table. Prior to DecisionSite 8.2, MDL ISIS/Draw was used as the renderer for all tools, but in later versions of DecisionSite you may use other renderers as well.

The Renderer Rule dialog is used to specify which renderer to use in different situations.

Note: If your administrator has defined some mandatory rules, you may not be able to use your own preferences in the choice of renderer or editor, since mandatory rules have priority before personal rules.

Renderer Rule		×
Structure format:		
MDL Molfile	_	
Renderer:		
ISIS/Draw)isplay Settings
,		
Valid for		
C All tools		
Specific tool:		
Structures in Table		_
Help	OK	Cancel

Option	Description
Structure format	The structure format that you wish the rule to apply to.
Renderer	The renderer you prefer to use.
Display Settings	Opens the Renderer Settings dialog for the selected renderer. The selected settings are saved with the rule, so it is possible to specify two different rules with the same renderer, but with different display settings.
Valid for: All tools	Select this option to apply the renderer rule for all structure tools.
Valid for: Specific tool	Select this option if you just want to apply the renderer rule for a specific tool (select which tool from the drop-down list).

► To reach the Renderer Rule dialog:

1. Select Tools > Structure Analytics > Advanced Preferences.

2. Click on Add Rule and select Renderer... from the drop-down menu.

8.1.9.2.4 Import Rules Dialog

Import Rules		
Select the rules to import:		
Use ISIS/Draw editor for MDL Molfile in all tools. Use ISIS/Draw editor for MDL Sketch File in all tools. Use ISIS/Draw renderer for MDL Molfile in all tools. Use ISIS/Draw renderer for MDL Sketch File in all tools.		
	[]	
Help	UK	Cancel

Click to select the rules that you wish to import.

► To reach the Import Rules dialog:

- 1. Select Tools > Structure Analytics > Advanced Preferences....
- 2. In the Advanced Preferences dialog, click Import....

8.1.9.2.5 Export Rules Dialog

kport Rules		
Select the rules to export:		
Use ISIS/Draw editor for MDL Molfile in all tools. Use ISIS/Draw editor for MDL Sketch File in all tools. Use ISIS/Draw renderer for MDL Molfile in all tools. Use ISIS/Draw renderer for MDL Sketch File in all tools.		
Help	ОК	Cancel

Click to select the rules that you wish to include in the preferences file.

► To reach the Export Rules dialog:

1. Select Tools > Structure Analytics > Advanced Preferences....

- 2. Make sure that you have added some Personal rules in the Advanced Preferences dialog.
- 3. Click **Export...**.

8.2 Portfolio

8.2.1 Portfolio Overview

The Portfolio tool allows records to be arranged into lists. You can also add annotations to both lists and records.

You work with the same portfolio all the time. It is automatically saved when you make changes to it. You can import and export contents to and from the Portfolio. Records are identified using any column in your data set. The record identifier is selected in the Portfolio: Options dialog.

8.2.2 Using Portfolio

8.2.2.1 Working with Lists

8.2.2.1.1 Working with Lists in Portfolio

This chapter shows you how to add, edit, compare and remove lists in the Portfolio.

8.2.2.1.2 Adding an Empty List to the Portfolio

To add an empty list:

- 1. If the Portfolio tool is not already open, select **Tools > Portfolio**.
- Click on the list (or the Portfolio root) beneath which you want to add the new list. Comment: A new list is always added to the end of a current collection of lists or records.
- Select New > Empty List... from the Portfolio menu. Response: The Portfolio: New List dialog is displayed.
- Type a List name of the new list and click OK. Response: The new list is added to the Portfolio below the selected list. Comment: You can use cut & paste or drag & drop to paste records and annotations into the new list.

Tip: You can also select Add New Empty List ... from the pop-up menu or click on the Add

new empty list button, , to add an empty list to the Portfolio.

8.2.2.1.3 Adding a New List of Records to the Portfolio

To add a new list from marked records:

- 1. If the Portfolio tool is not already open, select **Tools > Portfolio**.
- 2. Mark the records you want to include in the new list.
- 3. Select **New > Add New List from Marked Records** from the Portfolio menu. Response: The Portfolio: New List dialog is displayed.
- 4. Type a **List name** of the new list and click **OK**.

Response: The new list is added to the Portfolio as the last item on the root level.

Tip: You can also click on the **Add new list from marked** button, **(19)**, to add a list of records to the Portfolio.

To add a new list from search result:

- 1. If the Portfolio tool is not already open, select **Tools > Portfolio**.
- 2. Select **Search** from the Portfolio menu and enter your search string. Response: The hits from your search are shown beneath the Search pane.
- 3. Select **New > Add New List from Search Result** from the Portfolio menu. Response: The Portfolio: New List dialog is displayed.
- Type a List name of the new list and click OK. Response: The new list is added to the Portfolio as the last item on the root level. Note: The new list only contains one copy of each record, even if the search found the record in many different portfolio lists. If one of the search results is a list name, all of the records included in that list will be added to the new list.

► To add marked records to the current list:

- 1. If the Portfolio tool is not already open, select **Tools > Portfolio**.
- 2. Mark the records you want included in your current list.
- 3. Select New > Add Marked Records to List from the Portfolio menu. Response: The records are added to the end of the current Portfolio list.

8.2.2.1.4 Adding a Grouped List to the Portfolio

Categorical data can be added as a grouped list to the Portfolio. An example of such a grouped list would be one based on a column with the number of Oxygen atoms. The grouped list would include underlying lists with records for each number of oxygen atoms.

- 🗄 🗠 🗅 🛛 Oxygen

► To add a grouped list:

- 1. If the Portfolio tool is not already open, select **Tools > Portfolio**.
- 2. Mark the records you wish to include in the new list.
- Select New > Grouped List... from the Portfolio menu. Response: The Portfolio: New Grouped List dialog is displayed.
- 4. From the **Group new list by** field, select the column you wish to base the underlying lists on.
- Type a List name of the new list and click OK. Response: The new grouped list is added to the Portfolio as the last item on the root level.

8.2.2.1.5 Changing the Name of a List in the Portfolio

To change the name of a list:

- 1. If the Portfolio tool is not already open, select **Tools > Portfolio**.
- 2. Click to select the list whose name you want to change.
- 3. Select **Rename...** from the Portfolio menu.

Response: The Portfolio: Rename List dialog is displayed.

- 4. Edit the **List name**.
- 5. Click OK.
- Response: The name of the list is updated in the Portfolio.

Tip: You can also right-click and select **Rename...** from the pop-up menu or press **F2** to bring up the Portfolio: Rename List dialog for a selected list.

8.2.2.1.6 Removing a List or Record from the Portfolio

► To remove a list or a record:

- 1. If the Portfolio tool is not already open, select **Tools > Portfolio**.
- 2. Click on the list or record you want to remove.
 - Comment: Removing a list also removes all underlying lists, records and annotations.
- 3. Select **Delete** from the **Portfolio** menu.
 - Response: The list or record is removed from the Portfolio.

Tip: You can also right-click on a list or record and select **Delete** from the pop-up menu or press **Delete** on the keyboard to remove it from the *Portfolio*.

8.2.2.1.7 Adding a New Column from the Portfolio

This function can be used to express the location of records in the Portfolio. You can find out in which marked lists your records are present. The information is added to your data set as a new column showing the Portfolio Role for all records.

For each record, the names of the marked lists where the record appears are put together as strings separated by a semicolon (;). Lists are referred to by the name you have given to them, and not by the full path through the Portfolio. Records that are not present in any of the marked lists get the value "Not included" in the new column.

Note: The records that you are studying in the Portfolio must be part of your current data set in Spotfire DecisionSite. It is only the existing records that get a value in the new column. Any other records, present either in the Portfolio or Spotfire DecisionSite, get an empty value.

► To add a new column from the Portfolio:

- 1. If the Portfolio tool is not already open, select **Tools > Portfolio**.
- 2. Click on the root list if you want to base the new column on the entire Portfolio. Comment: You can restrict yourself to smaller sections of the Portfolio. Click to select only the list(s) you want to include. Records that are not present below the selected list(s) get the value "Not included" in the new column even if they are present in other unselected lists within the Portfolio.
- 3. In the Portfolio: Options dialog, select the **Overwrite old column** check box if you want to overwrite the last column added by the Portfolio tool.
- 4. Select Add New Column from the Portfolio menu.

Response: A new column is added to the data set.

Comment: Lists are referred to by the name you have given to them, and not by the full path through the Portfolio. If you have lists with identical names in your Portfolio, (which is allowed) you will have no way of separating these in the created column. If you want a unique identification of each list, you must edit the names of the lists to ensure that there are no duplicate names before the new column is added.

Tip: You can also click on the **Add new column** button, **+**, to perform this function.

8.2.2.1.8 Multiple Venn Comparison

Venn diagrams are used to visualize the various overlaps between different lists of data. Traditional Venn Diagrams are convenient ways to visualize the relationship between two or three lists. In Spotfire DecisionSite you can use the Portfolio in combination with the Pie Chart visualization to generate an alternative visualization to Venn diagrams that allows you to investigate the overlaps between any number of lists.

► To use the Portfolio for multiple Venn comparisons:

- 1. If the Portfolio tool is not already open, select **Tools > Portfolio**.
- 2. Create the lists that you want to compare in the Portfolio.
 - **Tip:** First create a main list that will contain all of the lists that you want to compare. Then add the different lists containing the desired subsets to this list. The result could be list names like "Greater than 2-fold change", "Unknown bioprocess" and "Unknown molecular function", for example.
- 3. Click on the main list containing all of the subset lists (or press **Ctrl** and click on all subset lists that you want to investigate).

Comment: Records that are not present below the selected lists get the value "Not included" in the new column even if they are present in other unselected lists within the Portfolio.

- Select Add New Column from the Portfolio menu. Response: A new column called Portfolio Role is added to the data set.
- 5. Select **Visualization > New Pie Chart** from the main DecisionSite menu bar. Response: A new pie chart is created.
- 6. Select **Portfolio Role** as the column to be mapped on both axes.
- 7. In the **Properties** dialog of the Pie Chart, select to **Color By Portfolio Role**.
- 8. Select Size By records count.
- 9. Click the Labels All records radio button.
- Select the **Pie records count** check box.
 Comment: This displays the number of records in each pie.
- 11. Make sure the Sector value and Sector percentage check boxes are cleared. Response: Now you have created a pie chart with several pies where each pie represents the number of records included in each list or combination of lists.

Examining the resulting visualization can quickly give you an overview of the size of the various overlaps between your lists:



8.2.2.2 Working with Annotations

8.2.2.2.1 Working with Annotations in Portfolio

You can add annotations to lists and records, and to the Portfolio itself. Annotations can be text strings, integers, real numbers or URLs.

8.2.2.2.2 Adding a New Annotation in the Portfolio

► To add a new annotation:

- 1. If the Portfolio tool is not already open, select **Tools > Portfolio**.
- 2. Click to select the object in the Portfolio where you want to add the annotation.
- 3. Select New > Annotation... from the Portfolio menu.
 - Response: The Portfolio: New Annotation dialog is opened.
- 4. Enter the **Annotation**.

Comment: Press Enter to get a line break in the annotation text.

5. Click Advanced >> to show optional settings.

Comment: The Advanced settings lets you enter both **Type** and **Name** for the annotation. This could be useful if you have a URL annotation, for example. A short description can be entered in the Name field to help remember the contents of the web link. Click << **Hide** to hide the optional settings.

6. Click OK.

Response: The annotation is added to the selected object in the Portfolio.

Tip: You can also click on the **Add new annotation** button, *in*, to add an annotation. You can double-click on a URL annotation in the Portfolio to open up the specified URL in a separate browser.

8.2.2.2.3 Editing an Annotation in the Portfolio

► To edit an annotation:

- 1. If the Portfolio tool is not already open, select **Tools > Portfolio**.
- 2. Click on the annotation you want to modify.
- 3. Select **Edit...** from the **Portfolio** menu.

Response: The Portfolio: Edit Annotation dialog is opened.

4. Edit the **Annotation**.

Comment: Press Enter to get a line break in the annotation text.

- Click Advanced >> to show optional settings
 Comment: The Advanced settings lets you edit both the Type and the Name of the annotation. Click << Hide to hide the optional settings.
- 6. Click **OK**.

Response: The annotation is updated in the Portfolio.

Tip: You can also right-click and select **Edit...** from the pop-up menu or press **F2** to bring up the Portfolio: Edit Annotation dialog for a selected annotation.

8.2.2.2.4 Removing an Annotation from the Portfolio

► To remove an annotation:

- 1. If the Portfolio tool is not already open, select **Tools > Portfolio**.
- 2. Click on the annotation you want to remove.
- 3. Select **Delete** from the **Portfolio** menu.

Response: The annotation is removed from the Portfolio.

Tip: You can also right-click on an annotation and select **Delete** from the pop-up menu or press **Delete** on the keyboard to remove the annotation.

8.2.2.3 Importing and Exporting

8.2.2.3.1 Importing a Portfolio

You can import other portfolios into the Portfolio. An imported portfolio will appear as a list within the Portfolio in Spotfire DecisionSite for Lead Discovery.

► To import a portfolio:

- 1. If the Portfolio tool is not already open, select **Tools > Portfolio**.
- 2. Select **Import...** from the Portfolio menu.

Response: The Open File dialog is opened.

3. From the **Files of type** drop-down list box, select the format of the portfolio you want to import.

Comment: You can import files of formats SRP or LST. You can also import XML files exported from the *Portfolio*.

- 4. Locate the portfolio you want to import and click on it.
- Click Open. Response: The imported portfolio appears as the last list on the root level in the Portfolio.

Note: If you export the entire Portfolio from Spotfire DecisionSite for Lead Discovery and import it again, it will appear as a list in the Portfolio, as will all other portfolios that are imported.

8.2.2.3.2 Exporting the Portfolio

You can export the contents of the Portfolio in order to share your lists with other users or to save an old list configuration.

► To export the Portfolio:

- 1. If the Portfolio tool is not already open, select **Tools > Portfolio**.
- Click on the root list if you want to export the entire Portfolio. Comment: You can also export parts of the Portfolio. Press Ctrl and click to select only those parts you want to export.
- 3. Select Export Marked Contents... from the Portfolio menu.

Response: The Save File dialog is displayed.

- 4. Select a location from the **Save in** drop-down list box.
- 5. Select a format from the **Save as type** drop-down list box.
- 6. Enter a **File name** and click **Save**.

Note: If you export the entire Portfolio from Spotfire DecisionSite for Lead Discovery and import it again, it will appear as a list in the Portfolio, as will all other portfolios that are imported.

8.2.2.4 Cutting, Copying and Pasting in the Portfolio

► To cut, copy or paste objects in the Portfolio:

- 1. If the Portfolio tool is not already open, select **Tools > Portfolio**.
- Click on the object you want to cut or copy. Comment: Press Ctrl and click to select multiple objects in the Portfolio.
- 3. Click the **Portfolio** menu button, **I**, to display the Portfolio menu.
- 4. Select **Cut**.

Response: The selected object is removed from the Portfolio and placed on the clipboard.

Comment: Select **Copy** to place a copy of the selected object on the clipboard.

5. Click on the list or record in the Portfolio where you want to paste the contents of the clipboard.

Comment: Lists or records can only be pasted to lists. Annotations can be pasted to lists or to records.

6. Select **Paste** from the **Portfolio** menu.

Response: The list, record or annotation that was placed on the clipboard is pasted into the Portfolio.

Comment: Lists can also be pasted into tools outside of Portfolio, such as a text editor.

Tip: You can use drag and drop to move objects in the Portfolio. The commands **Cut**, **Copy** and **Paste** are also available from the pop-up menu.

8.2.2.5 Searching the Portfolio

You can do a free text search of the Portfolio including lists, records and annotations. The search is case insensitive and uses the wildcards ? and *.

► To search the Portfolio:

- 1. If the Portfolio tool is not already open, select **Tools > Portfolio**.
- 2. If the Search pane in the Portfolio is hidden, click on the **Search** button, **(a)**, in the toolbar to display it.

Response: The Search pane is displayed.

- Enter your search string in the provided field. Comment: Enter the full element name or add a wildcard symbol to the truncated name to retrieve the search results.
- Click Search. Response: The total number of hits is shown below the Search pane. The first appearance of the search string is highlighted in the Portfolio.
- 5. Use the **Previous** (<<) and **Next** (>>) buttons to step through all matches to the search string in the Portfolio.

Response: Each found appearance of the search string is highlighted in the Portfolio, one at a time, as you step through the result of the search.

Tip: If you want all records found during the search to be automatically marked in the visualizations, select the **Mark on search** check box in the Portfolio: Options dialog.

8.2.2.6 Data Interaction in Portfolio

8.2.2.6.1 Marking in Portfolio

Do this in a visualization	and this happens in Portfolio
Mark some records in a visualization.	Nothing happens in the Portfolio.
Do this in Portfolio	and this happens in all

Click to select a list (or record) in the Portfolio. You can press **Ctrl** and click to select multiple objects in the Portfolio.

□··· □ Portfolio
 □··· □ SSS on Edited compound
 □··· □ Compounds with high MW
 □··· □ 950
 4739
 4837
 □··· □ Hierarchical Clusters
 □··· □ Marked compounds

...and this happens in all visualizations

The corresponding records are marked in the visualizations.



Note: To achieve this interaction, the records in the Portfolio must be part of the current data set in Spotfire DecisionSite. Also, the **Mark on browse** check box must be selected in the Portfolio: Options dialog. All records with the same record identifier will be marked, regardless of whether the specific record was a part of the records used to create the list or not.

Tip: If you only want to mark the records from a selected list and still want to be able to browse the other lists in the Portfolio, select the list and then choose **Mark in Visualization** from the Portfolio menu. Make sure that the **Mark on browse** check box in the Portfolio: Options dialog is cleared.

8.2.2.6.2 Activating in Portfolio

Do this in a visualization	and this happens in Portfolio
Activate a record in a visualization.	The ID of the active record is shown in the Search pane in the Portfolio. If the Search pane is hidden, click on the Search button in the toolbar to display it.
	You can now click on the Search button to search for the active record within the Portfolio.

Note: You cannot activate lists or records in the Portfolio. When you click an object, it gets marked.

8.2.3 User Interface

8.2.3.1 Portfolio User Interface Overview

This is the Portfolio user interface:



1. Portfolio menu

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The Portfolio menu contains all menu commands required to work with the Portfolio.

2. Portfolio toolbar



Includes shortcuts for some of the most common commands in the Portfolio menu. Click here for a description of the buttons.

3. Portfolio

This displays the contents of the Portfolio. You can toggle the display of subtrees in the Portfolio by clicking the plus (+) or minus (-) sign beside a list. The left and right arrow keys on the keyboard can also be used to collapse or expand a node. All subnodes can be

expanded/collapsed simultaneously by standing on the top node, e.g., Portfolio, and pressing the multiplication sign (* or x) or the minus sign (-) on the numeric keypad.

4. Search

AFFX-ThrX-3_at	Search	$\langle \rangle \rangle$
2422 item(s) found		

Via this pane, you can perform a full text search of the contents of the Portfolio. Enter a string in the search field and click on **Search**. You can use the Back (<<) and Forward (>>) buttons to browse the result from the search. The number of hits from the search are displayed right below the field. You can use the wildcards ? and * in the search string.

8.2.3.2 Portfolio Menu

The Portfolio menu is displayed by clicking and contains all commands necessary for working with the Portfolio.

Option	Description
Undo	Undoes the last delete, edit, move, cut, copy, paste or import operation in the Portfolio. You can only undo the last operation and not a series of operations.
Cut	Removes the selected objects from the Portfolio and places them on the clipboard.
Сору	Places a copy of the selected objects from the Portfolio on the clipboard.
Paste	Pastes the contents of the clipboard below the selected list in the Portfolio.
Delete	Deletes the selected objects from the Portfolio.
New >	
> Empty List	Adds a new empty list to the Portfolio below the selected list.
> List from Marked	Adds a new list with the marked records to the Portfolio. The list is placed as the last item on root level.
> Grouped List	Adds a new grouped list with the marked records to the Portfolio. This function first opens the Portfolio: New Grouped List dialog where the new list is defined. The list is placed as the last item on root level.
> Annotation	Adds a new annotation to the active object in the Portfolio. This function first opens the Portfolio: New Annotation dialog where the annotation is defined.
> Add New List from Search Result	Adds a new list containing the results from your free-text search using the Search pane to the Portfolio. The list is placed as the last item on root level. Note: The new list only contains one copy of each record, even if the search found the record in many different portfolio lists. If one of the search results is a list name, all of the records included in that list will be added to the new list.
> Add Marked Records to List	Adds the marked records from your current visualization into the Portfolio list.

	Note: You can also right-click in the visualization and add your marked records into your currently active Portfolio list.
List Logic	Brings up the List Logic dialog where you can compare the marked lists using Boolean operators (OR, AND or ONLY).
Add New Column	Adds a new column to the data set, with information about the location of the records within the marked list(s) in the Portfolio.
Rename	Lets you edit an annotation or the name of a list. This function brings up either the Portfolio: Edit Annotation dialog or the Portfolio: Rename List dialog depending on which object you have selected in the Portfolio.
Import	Imports a portfolio from a file. The imported portfolio is displayed as a list and is placed as the last item on root level in the Portfolio.
Export Marked Contents	Exports the selected parts of the Portfolio as an SRP, XML or LST file.
Mark in Visualization	Marks the records that belong to the selected Portfolio list in the DecisionSite data set and visualizations.
Search	Displays or hides the Search pane, where you can perform a free text search of the contents of the Portfolio including lists, records and annotations.
Sort Alphabetic	Lets you sort the contents of your lists alphabetically.
Sort Numeric	Lets you sort the contents of your lists numerically. Note: This sorting only applies to the leading digits.
Options	Displays the Portfolio: Options dialog.
Help	Opens this help file to the Portfolio overview page.

8.2.3.3 Portfolio Pop-up Menu

To bring up the pop-up menu, right-click in the part of the Portfolio that shows its contents.

Option	Description
Add New Empty List	Adds a new empty list to the Portfolio beneath the selected list.
Add New Annotation	Adds a new annotation to the active object in the Portfolio. This function first opens the Portfolio: New Annotation dialog where the annotation is defined.
Add New List from Search Result	Adds a new list containing the results from your free-text search using the Search pane to the Portfolio. The list is placed as the last item on root level.
Add New List from Marked Records	Adds a new list with the marked records to the Portfolio. The list is placed as the last item on root level.
Add Marked Records to List	Adds the marked records from your current visualization into the Portfolio list. Note: You can also right-click in the visualization and add your marked records into your currently active Portfolio list.

Edit	Lets you edit an annotation or the name of a list. This function brings up either the Portfolio: Edit Annotation dialog or the Portfolio: Rename List dialog depending on which object you have selected in the Portfolio.
Cut	Removes the selected objects from the Portfolio and places them on the clipboard.
Сору	Places a copy of the selected objects from the Portfolio on the clipboard.
Paste	Pastes the contents of the clipboard below the selected list in the Portfolio.
Delete	Deletes the selected objects from the Portfolio.
Undo	Undoes the last delete, edit, move, cut, copy, paste or import operation. Only the very last operation can be undone.
Sort Alphabetic	Lets you sort the contents of your lists alphabetically.
Sort Numeric	Lets you sort the contents of your lists numerically. Note: This sorting only applies to the leading digits.

8.2.3.4 Portfolio Toolbar

The Portfolio toolbar includes shortcuts for some of the most common commands in the Portfolio menu. Click on the buttons on the toolbar to activate the corresponding functions.

•	This is the Portfolio menu selector. When you click on it, a menu is displayed. Click here for a description of the available menu options.
	Adds a new empty list to the Portfolio below the selected list.
	Adds a new list with the marked records to the Portfolio. The list is placed as the last item on root level.
*	Adds a new annotation to the selected object in the Portfolio. First, the Portfolio: New Annotation dialog is opened. This is where the annotation is defined.
Ø	Brings up the List Logic dialog where you can compare the marked lists using Boolean operators (OR, AND or ONLY).
+8	Adds a new column to the data set with information about the location of the records within the selected list(s) in the Portfolio.
	Marks the records that belong to a selected list in the visualizations.
<u>à</u>	Displays or hides the Search pane, where you can perform a free text search of the contents of the Portfolio including lists, records and annotations.

8.2.3.5 Portfolio: Options Dialog

🚰 Portfolio: Options		×
Record identifier:	Analysis Name	×
Overwrite old column Help	<u> </u>	Cancel

Option	Description
Record identifier	Defines which column in the data set should be used as the identifier. You can choose the identifier from any column that contains strings or integers.
Mark on browse	Automatically marks records in the visualizations when browsing a list using the mouse or arrow keys.
Mark on search	Automatically marks records in the visualizations when they are found in a Search.
Overwrite old column	Select this check box if you want to overwrite a previously added column (from the Portfolio tool) when you add a new portfolio role column. Clear if you do not wish to overwrite.

► To reach the Portfolio: Options dialog:

Select **Options...** from the **Portfolio** menu.

8.2.3.6 Portfolio: New Annotation Dialog

🧿 Portfolio: New Anr	notation	×
Annotation: Control Pro	obe Sets - Weeks Three through Seven	
Type String -		
Name: Control		
<< Hi <u>d</u> e	Help OK Cancel	
Option	Description	
Annotation	The contents of your annotation are entered here. Press Enter line break in the annotation text.	r to force a
Туре	The type of annotation; can be String, Long, Real or URL. The set to String as default.	he type is
Name	An alias for the annotation can be entered here. If filled in, the displayed before the contents of the Annotation field in the P	e alias is ortfolio.

Advanced >>	Shows the advanced settings.
-------------	------------------------------

<< Hide Hides the advanced settings.

► To reach the Portfolio: New Annotation dialog:

- Select **New > Annotation...** from the **Portfolio** menu or
- select Add New Annotation... from the pop-up menu or
- click on the Add new annotation button,

8.2.3.7 Portfolio: New Grouped List Dialog

🚰 Portfolio: New Grou	ped List	<u>? ×</u>
Group new list by: _ID Mol Wt. Plate # Row Column LC/MS LD(50) In-vivo Activity Assay #1(IC50) Assay #2 (IC50)		
List name: In-vivo Activity Help		OK Cancel
Option	Description	

Group new list by Displays all available columns that you can choose to base your new grouped list on. The grouped list will contain an underlying list for each unique value in this column. Click on a column to select it.

List name A name for the new list is entered here.

► To reach the Portfolio: New Grouped List dialog:

Select **New > Grouped List...** from the **Portfolio** menu.

8.3 List Logic

8.3.1 Comparing Lists Using List Logic

You can compare lists using Boolean operators. This lets you determine which records are present or not in a certain combination of lists. The result is added as a new list, and you can select where you want to put it.

Note: The List Logic function only compares records in the list and its sublists. Annotations and names of sublists are not considered.

To compare lists:

 If the List Logic tool is not already open, select Tools > List Logic.... Response: The List Logic dialog is displayed. 2. Select the desired **List source**.

Comment: You can choose a list from Portfolio, Structure Viewer, from the current Data set, from an External file, or Create a new list.

3. Click to select the lists you want to compare and click **Add** >> to move them to the Lists to compare pane.

Comment: You can only compare separate lists. In other words, you cannot compare an underlying list with its parent list. When you select a list, all underlying lists are automatically included in the selection.

- 4. Select one of the three methods of logical operation: OR (All lists), AND (Any of the lists), or ONLY (This list only).
- 5. Enter a new List name.
- 6. Select where you want to save the result of the list comparison.
- 7. Click OK.

Response: In the case of Portfolio and Structure Viewer, the new list is added to the selected source as the last item on the root level. An annotation with information about how the list was created is automatically added to the new list. If External file is selected, a save dialog will appear in which you can specify where you want the file to be saved.

Tip: You can also click on the **List Logic** button in the Portfolio or Structure Viewer to start the tool.

8.3.2 List Logic Dialog

List selection List <u>source:</u> Portfolio Probe Sets Control probes grouped organism Arabidop Chips	st Add >> Add >> Selected records Marked records Marked records Selected records Marked records	s (Number) (Number)
Logical operation and exp <u>C</u> reate list from records in:	All lists Any of the lists This list only: Marked records (Number)	(AND) (OR) (ONLY)
List <u>n</u> ame: Save new list in:	List Logic	
	OK	Cancel

Option	Description
List source	Displays the sources from which you can select lists to be added. Select a source from the List Source pane. Click a list name in the pane to select it. To select more than one list, press Ctrl and click the list names in the pane.
Lists to compare	Displays the lists that are to be compared.
Add >>	Adds the lists that have been selected in the List source pane to the Lists to compare pane.
<< Remove	Removes a list from the Lists to compare pane.
All lists	Creates a new list containing only those records that are present in all of the lists.
Any of the lists	Creates a new list containing all records that are present in any of the lists. Each record will appear only once in the new list, even if that record is present in several of the selected lists.
This list only	Creates a new list containing only those records that are present in the selected list and not in any of the other lists.
List name	The name of the new list that is created.
Save new list in	Selects the location where the result of the list comparison will be saved.

► To reach the List Logic dialog:

Select **Tools > List Logic...**, or click on the **List Logic** button in Portfolio or Structure Viewer.

8.4 Web Links

8.4.1 Web Links Overview

The Web Links tool enables you to send a query to an external web site to search for information about marked records. The search results are displayed in a separate web browser. The Web Links tool is shipped with a number of predefined web sites that are ready to use. You can also set up new links to web sites of your choice.

8.4.2 Using Web Links

8.4.2.1 Sending a Query Using Web Links

Note: You need to have data in Spotfire DecisionSite to be able to send a query. The query is sent for the marked records in the visualizations. If more than one record is marked, the records are separated by the web link delimiter in the query.

To send a query using Web Links:

- 1. In a visualization, mark those records you want to search for information about.
- 2. Select **Tools > Web Links...**.
 - Response: The Web Links dialog is displayed.
 - 3. Click to select the link to the web site where you want the query to be sent.

Comment: Some web sites only allow you to search for one item at a time. If you do not get any hits from a search, mark one record at a time in the visualizations and try again.

4. Select the **Identifier column** that you want to use as input to the query. Comment: You can choose from any column in your data set.

5. Click OK.

Response: The query is sent to the web site and the results are displayed in a new web browser.

8.4.2.2 Setting Up a New Web Link

► To set up a new web link:

1. Select **Tools > Web Links...**

Response: The Web Links dialog is displayed.

2. Click Options....

Response: The Web Links Options dialog is displayed.

3. Click New.

Response: A New web link is created and selected in the list of Available web links. Comment: The Preview helps you see what the finished query will look like when it is sent.

- 4. Edit the name of the new link in the Web link name text box.
- 5. Edit the **URL** to the web link.

Comment: A dollar sign within curly brackets {\$} should be used as placeholder for the ID. Anything you enter between the left bracket and the dollar sign will be placed before each ID in the query. In the same way, anything placed between the dollar sign and the right bracket will be placed after each ID in the query.

6. Enter the **Delimiter** to use to separate the IDs in a query.

Comment: The identifiers in a query with more than one record are put together in one search string separated by the selected Delimiter. You can use AND, OR or ONLY as delimiters.

7. Click OK.

Response: The new web link is saved and is displayed together with the other available web links in the user interface.

8.4.2.3 Editing a Web Link

► To edit a web link:

- Select Tools > Web Links.... Response: The Web Links dialog is displayed.
- 2. Click **Options...**.

Response: The Web Links Options dialog is displayed.

- Click on the web link you want to edit in the list of Available web links. Response: The Web link name, URL and Delimiter for the selected web link are displayed and can be edited directly in the corresponding fields. Comment: All changes that are made are reflected in the Preview which helps you see what the finished query will look like.
- Make desired changes to the web link and click OK. Response: The web link is updated according to your changes and the Web Links Options dialog is closed.

8.4.2.4 Removing a Web Link

► To remove a web link:

1. Select Tools > Web Links....

Response: The Web Links dialog is displayed.

2. Click **Options...**.

Response: The Web Links Options dialog is displayed.

- 3. Click on the web link you want to remove in the list of **Available web links**. Response: The Web link name, URL and Delimiter for the selected web link are displayed in the corresponding fields.
- 4. Click Delete.

Response: All the fields are cleared.

Comment: You can delete many web links at a time if you select several web links in the list of **Available web links** and click **Delete**. Press **Ctrl** and click on the web links in the list to select more than one.

Tip: If you have deleted some of the default web links by mistake, you may retrieve them again by clicking the **Add defaults** button. This adds all of the default links to the Available web links list, regardless of whether or not the links already exist.

8.4.3 User Interface

8.4.3.1 Web Links Dialog

🖉 Web Links	×	
<u>₩</u> eb links:		
NIST Chemistry web NIST Chemistry web Entrez Protein Entrez Nucleotide Entrez Structure Entrez Genome Entrez PopSet OMIM Affymetrix NetAffx USPTO (US Patent	boook (Search by CAS#) boook (Search by Formula) & Trademark Office)	
Identifier column:		
Customer age	<u> </u>	
Help	Options OK Cancel	
Option	Description	
Web links	The available web links. The web links tool is shipped with a number of default links, but you can edit or add new web links to the list via the Web Links Options dialog. Click to select the link to which you want to send a query for the marked records.	
Identifier column	This is where you specify which identifier to use when you so for marked records to a web site.	end a quer
Options	Opens the Web Links Options dialog.	

f

y

► To reach the Web Links dialog:

Select Tools > Web Links....

8.4.3.2 Web Links Options Dialog

🗿 Web Links Options	<u>? ×</u>
Available web links: PubMed USPTO (US Patent & Trademark Office) NIST Chemistry webbook (Search by CAS# NIST Chemistry webbook (Search by Formu Entrez Protein Entrez Nucleotide Entrez Structure Entrez Genome Entrez PopSet OMIM New web link New web link	Web link name: Entrez Genome URL: http://www.ncbi.nlm.nih.gov/entrez/query.fcgi ?cmd=search&db=Genome&term={\$} Delimiter:
Preview: http://www.ncbi.nlm.nih.gov/entrez/query.fo OR Orange OR Pear	<u>Add defaults</u> <u>New</u> <u>Delete</u> sgi?cmd=search&db=Genome&term=Apple <u>DK</u> <u>Cancel</u>

Option	Description
Available web links	The available web links that are listed in the Web Links user interface.
Web link name	The name of the web link. Click on a web link in the list of Available web links to edit the name in this field.
URL	The URL to the web link. Click on a web link in the list of Available web links to edit the URL in this field. A dollar sign within curly brackets is used as a placeholder for the ID in the query. Anything you enter between the left bracket and the dollar sign will be placed before each ID in the query. Likewise, anything placed between the dollar sign and the right bracket will be placed after each ID in the query. The preview shows you what the query will look like.
Delimiter	The separator that should be used between the IDs in a query with more than one record. Click on a web link in the list of Available web links to edit the delimiter in this field.
Add defaults	Adds the default web links (that Spotfire DecisionSite Statistics is shipped with) to the list of Available web links. The current links are not updated, instead copies of the links are added. This allows you to have two different versions of the default links. For example, one version could contain your own personal settings.

New	Adds a New web link to the list of available web links and lets you edit its name, URL and Delimiter in the fields to the right.
Delete	Deletes the selected web link(s) in the list of Available web links.
Preview	Shows you a preview of the URL with three IDs (Apple, Orange and Pear) instead of the placeholder {\$} (dollar sign within curly brackets)

► To reach the Web Links Options dialog:

Select **Tools** > **Web Links...** to display the Web Links dialog. Then click on the **Options...** button to the lower left in the **Web Links** dialog.

8.5 Compound Details

8.5.1 IDdb3 Drug Search

8.5.1.1 Searching the IDdb3 Database

The IDdb3 Drug Search tool allows you to search the Investigational Drugs database (IDdb3) using the active record in Spotfire DecisionSite or an entered drug name as search criterion. **Note:** A subscription to IDdb3 is required in order to use this tool.

► To search IDdb3:

- 1. Activate a record by clicking on it in a visualization.
- Select Tools > Compound Details > IDdb3 Drug Search.... Response: The IDdb3 Drug Search dialog is displayed.
- 3. Select the column on which to perform your search from the drop-down list. Comment: You can also choose to perform a Search by drug name by typing any word or name in the text box.
- 4. Click OK.

Response: The IDdb3 Drug Search dialog is closed and your request is sent to IDdb3.

- If the IDdb3 web site does not recognize you from earlier, you will have to enter your User name and Password in a Log In dialog.
 Comment: Select the check box Remember the password to skip this dialog in the future.
- 6. The search results are displayed in a separate web window.
8.5.1.2 IDdb3 Drug Search Dialog

🕘 IDdb3 Drug Search			×
Select Column			
MOLNAME		-	
C Search by drug name			
Help	ОК	Cancel	

Option Description

Select Column	The columns available for searching are listed. Select the column in which the value to search by is found (e.g., the molecule name) from the drop-down list.
Search by drug name	Type any search string to search the IDdb3 for drugs of that name. No wildcards are allowed, and the search is performed as a perfect match to the entered string.

To reach the IDdb3 Drug Search dialog:

Select Tools > Compound Details > IDdb3 Drug Search....

8.6 Computation Services

8.6.1 Computation Services Overview

The Computation Services is built to allow you to add any specific type of computation or "tool" to your analysis. Different types of statistical calculations can be added to the data set or included in Guides for easy distribution to others.

The out-of-the-box version of Computation Services supports connection to R, S-PLUS and SAS servers, but other types of connectors can also be added. For more information, see Spotfire Developer Network.

Note: This help file does not contain any information regarding how to write your scripts. For specific information on how to write scripts, see literature for the respective scripting language.

8.6.2 Using Computation Services

8.6.2.1 Computation Services Quick Reference

Action	Instruction
Start Computation Services	From the main menu bar of DecisionSite, select Tools > Computation Services > SAS or R or S-PLUS or whatever type of server you want to connect to.

Create a new configuration	In Computation Services, click File > New . Write or paste a script in the Script field, add input and output parameters and result handlers. Test the configuration. See Suggested Workflow or Example Configuration for more information.
Open an earlier saved configuration	In Computation Services, click File > Open . Browse to locate the configuration of interest and click Open .
Add an input parameter	 Select the parameter in the script and click on the Add as Input Parameter button, Select the Data type of the parameter from the drop-down list. Tip: You can also start by clicking Add on the Input Parameters tab, edit the default parameter name and then write the script that includes the parameter.
Add prompts	Add at least one input parameter. Select the Data type of the parameter from the drop-down list. In the Input Parameters tab, select Prompt: [prompt type] from the Value drop-down list. Configure the prompt in the Prompt Settings dialog by adding a label and other information.
Add an output parameter	 Select the parameter in the script and click on the Add as Output Parameter button, Select the Data type of the parameter from the drop-down list. Tip: You can also start by clicking Add on the Output Parameters tab, edit the default parameter name and then write the script that includes the parameter.
Define what to do with the results	Make sure that you have defined the output parameter that you want to use as result. On the Result Handling tab , click Add . From the menu, select the type of result handler that you want to use. If applicable, configure the selected result handler to work on the desired output parameter.
Add resulting columns to the data set	Make sure that you have defined at least one output parameter as the data type Dataset. On the Result Handling tab , click Add . From the menu, select one of the following alternatives: Add to Current Data Set (Automatic Key Matching), Add to Current Data Set (Row by Row), Replace Current Data Set, or Open in Other DecisionSite Instance. Note: The result handlers for adding columns will only be visible in the Add menu if you have defined at least one output parameter of the type Dataset.

Add resulting output as a file	 Make sure that you have defined at least one output parameter as the data type File. On the Result Handling tab, click Add. From the menu, select the Launch File option. Note: The Launch File result handler will only be visible in the Add menu if you have defined at least one output parameter of the type File.
Test a configuration	In Computation Services, select Execute > Run .
Save a configuration	In Computation Services, select File > Save .
Incorporate a configuration in a Guide	Test your configuration to make sure it is fully functional. In Computation Services, select File > Send to Analysis Builder . In Analysis Builder, select the action Start Data computation - SAS (or R, S-PLUS, etc.). Click < Add Link . Complete the Guide in Analysis Builder and Save it. Tip: For more information about how to create Guides, see Analysis Builder Overview.
Minimize Computation Services	Click on the top right x-button. This will hide Computation Services, but the current configuration will be remembered when you reopen the tool.
Close Computation Services	In Computation Services, select File> Exit.

8.6.2.2 Suggested Workflow

To create a new script configuration using Computation Services:

- If Computation Services is not already open, select Tools > Computation Services > SAS or R or S-PLUS, or whatever the type of computation server you are running against.
- 2. Select File > Connector Settings... and specify the address to your Server.
- 3. Select whether to **Keep session open until manually closed** or not. See Connector Settings dialog for more information about this option.
- 4. Create the script by either typing or pasting existing script code in the Script field of Computation Services.
- 5. Add the desired input parameters to the **Input Parameters** tab and specify whether they should be prompted or not.
- 6. Add the desired output parameters to the **Output Parameters** tab.
- 7. Specify how you want to present your results on the **Result Handling** tab.
- 8. Test the configuration by selecting **Execute** > **Run**.
- 9. View the **Execution Log** to see if there were any errors during execution.
- 10. If there were any problems, go back to fix them.
- 11. Select **File > Send to Analysis Builder** and add the **Start Data computation R** action (or whatever the type of computation you have created) to a suitable Guide.

8.6.2.3 Example Configuration

Below is the creation of a very simple configuration shown in detail to exemplify how you can work with Computation Services. The workflow would be exactly the same for S-PLUS and SAS servers.

Note: For information on how to write scripts, please refer to any literature for the respective scripting language.

Creating an R configuration which adds a user specified integer to selected columns in the data set:

- 1. In DecisionSite, open the data set in which you want to modify columns. Comment: It is not necessary to have data loaded in DecisionSite when defining or running a configuration, but in this example the data is used for testing purposes further down in this step instruction.
- 2. Select Tools > Computation Services > R.

Response: Spotfire Computation Services for R is displayed.

- 3. In Computation Services, select File > Connector Settings.... Response: The Connector Settings dialog is displayed.
- Specify the address to your R Server by either typing in the text field (e.g., 4. http://myRserver:9080) or selecting a predefined server from the list shown by clicking on ...
- 5. On the Input Parameters tab, type a suitable **Prompt dialog title** in the specified field. In this example we use the text "Add Integer to Columns". Comment: According to Spotfire UI Guidelines the title should be short and concise and written using book title capitalization, without any closing punctuation.
- 6. On the Input Parameters tab, type a suitable **Prompt dialog description** in the specified field. In this example we use the text "This is an example R-script calculation which adds the integer provided below to all specified columns in the data set.". Comment: The description is not necessary in all configurations, but it can be useful to further explain what the configuration does, or to add more guidance to the end users during execution.
- 7. In the **Script** field, type **dataout** <- **x** + **datain**.

Script:

```
dataout <- x + datain
```

Comment: This is the actual script which will be computed on the R server. In this example we want a user-specified integer, x, to be added to the values of the input columns in the datain parameter, and finally the resulting columns in the dataout parameter to be returned to the current data set as new columns.

```
8. Select the input parameter x in the script:
      Script:
```

```
dataout <- 🛛 + datain
```

9. Click on the Add as Input Parameter button, Response: The parameter x is added to the Input Parameters tab.

10. On the Input Parameters tab, from the **Data type** drop-down list, select **Integer**.

Response: The Prompt Settings: Integer dialog is displayed.

Prompt Settings: Integration 1	jer	×
l abel:		
Integer to add to the selecte	ed columns:	
Default <u>v</u> alue:		
5		
Mi <u>n</u> value:	Ma <u>x</u> value:	
0	115	
<u>H</u> elp	OK	Cancel

12. In the dialog, specify the **Label** that you want the end user of the configuration to see upon execution. In this example we use the text "**Integer to add to the selected columns:**".

Comment: Try to make the label as clear as possible to ensure that the end users of the script understand what the input parameter should be. According to Spotfire UI Guidelines, the label for a text field should use sentence-style capitalization and end with a colon.

- 13. If desired, add a default value and/or min and max values to limit the allowed input values.
- 14. Click OK.
- 15. In the **Script** field, select the input parameter **datain** and click on the Add as Input Parameter button,
- 16. On the Input Parameters tab, from the **Data type** drop-down list, select **Dataset**.
- 17. From the Value drop-down list, select Prompt: Data set.
- 18. Response: The Prompt Settings: Data Set dialog is displayed.

Prompt Settings: Data Set	×
Label:	
Select a number of columns (max 7):	
Data types:	
String	
Integer Beal	
Time	1
Date	
Uptional settings	1
Minimum number of columns: 1	
Maximum number of columns: 7	
Help OK Cancel	

19. In the dialog, specify the Label that you want the end user of the configuration to see upon execution. In this example we use the text "Select a number of columns (max 7):".

- 20. Select the **Data types** of the columns that will be available for selection. In this example we will add an integer to the values of the specified columns, so Integer and Real are suitable data types.
- 21. If desired, add a Minimum number of columns (in this example we use 1) and a Maximum number of columns (in this example we use 7).
- 22. Click OK.
- 23. In the **Script** field, select the output parameter **dataout** and click on the Add as Output Parameter button,
- 24. On the Output Parameters tab, from the **Data type** drop-down list, select **Dataset**.
- 25. On the Result Handling tab click on Add.
- 26. From the Add menu select **Add to current data set (row by row)**.

Response: The Add to Current Data Set (Row by Row) dialog is displayed.

Add to Current Data Set (Row by Row)	×
Output parameter:	
dataout	-
Input parameter for matching of rows:	
datain	-
, Column name template (original name represented by *);	
Calculated *	_
✓ Overwrite <u>existing columns</u>	
<u>H</u> elp OK Cancel	

Comment: This is just one of many result handlers available. See Result Handling tab for more information about the other options.

- 27. In the dialog, make sure that dataout is selected as Output parameter and datain is selected as Input parameter for matching of rows.
- 28. If desired, modify the **Column name template** to add a custom prefix and/or suffix to the calculated columns.
- 29. Test the script by selecting **Execute > Run**.

Response: The prompt dialog is displayed with the title you provided in step 3.

	_
O Add Integer to Columns	×
This is an example R-script calculation which adds the integer provided below to all specified columns in the data set. Integer to add to the selected columns: 5 Select a number of columns (max 7): Available columns: Name Columns: Name Column1	
Column1 Column2 Column3 Column3 Column3 Column4 Column5	
Records selection: All	
OK Cancel	

Comment: What columns you see in the Available columns list depends on which data set you have opened and which data types you specified in step 18. You can also rightclick on the Name header and select the Show search field option, if you want to further limit the number of shown columns in this list.

- 30. In the dialog, type the desired integer and select the desired columns.
- 31. Click OK.

Response: The computation is performed and the resulting columns are added to the data set.

32. Save the configuration or send it to Analysis Builder (File > Send to Analysis Builder) to incorporate the action Start Data computation - R in a Guide. In the latter case you should also remember to save the Guide.

8.6.2.4 General Concepts

The handling of forbidden characters in column names differs for different computation servers. To avoid possible problems with forbidden characters in column names, Computation Services temporarily translates the column names that are sent to a server in the following manner:

- Allowed characters are a-z, A-Z, 0-9. Any other characters will be temporarily removed from the column names when the configuration is executed on the server.
- The column name cannot start with a number. If the available column name starts with a number, the number will be removed.
- The column name may be a maximum of 32 characters long. If the available column names are longer, they will be shortened and, if necessary, supplied with a suffix number to be distinguished from other columns with the same name.
- All column names will be converted to lower case, since some computation servers do not make any difference between upper and lower case characters.

The translation is initiated by each connector separately. Any columns that are sent to a server as input parameters will be translated, provided they contain any of the forbidden characters. When the columns are returned from the server as output parameters, they will receive their original names again, if applicable. The translated column names will be used during the whole computation server session.

Tip: If you are interested in seeing what the actual column name used in the computation looked like, you can retrieve this information from the Execution Log.

8.6.3 User Interface

8.6.3.1 Computation Services User Interface Overview

This is the Computation Services user interface:



1. Computation Services menus

The File, Execute and Help menus contain menu commands used to work with Computation Services.

2. Toolbar



Includes shortcuts for some of the most common commands in Computation Services. See Computation Services toolbar for a description of the different buttons.

3. Script

This pane displays the contents of your current script. This is where you create a new script or modify an existing script. Depending on what type of computation server you have selected, the scripting language should be R, SAS, S-PLUS or some other type of script. This help file does not contain any information regarding how to write your scripts.

4. Input Parameters

The Input Parameters tab contains the selected input parameters and handles any type of prompt settings for these parameters.

The prompt settings determine what the end user of the configuration will see upon execution. All defined prompts will be shown in a single prompt dialog. The title of the prompt dialog is defined on the Input Parameters tab, along with a field with room for a more thorough description of what the configuration does.

5. Output Parameters

The Output Parameters tab contains the selected output parameters.

6. Result Handling

The Result Handling tab is where you specify what kind of result you want to receive when running the configuration.

7. Execution Log

The Execution Log tab contains a read-only text field displaying the progress of execution of a configuration along with any errors.

► To reach Computation Services:

Select **Tools > Computation Services > R** or **SAS** or **S-PLUS** or whatever the type of your current computation server.

8.6.3.2 Computation Services Menus

File menu:

Option	Description
New	Empties Computation Services, so that you can start a new configuration. Any information you have currently open in the Script pane, or in any of the tabs, will be cleared.
Open	Opens an earlier saved configuration. This configuration contains the actual script along with any defined input and output parameters, as well as the specified result handlers and prompt settings.
Save	Saves the current configuration including the script, all input and output parameters, as well as the specified result handlers and prompt settings to an earlier specified file.
Save As	Saves the current configuration including the script, all input and output parameters, as well as the specified result handlers and prompt settings, after you have provided a file name in the Save dialog.
Send to Analysis Builder	Sends the current configuration to Analysis Builder as an available action, so that the calculation can be incorporated in a Guide.
Connector Settings	Displays the Connector Settings dialog, which handles the connection to the computation server.
Close All Sessions	Closes all sessions currently open on the computation server. This option may be necessary to use if you have selected the option to Keep session open until manually closed in the Connector Settings dialog and you encounter any problems due to data left on the server from earlier computations.
Exit	Closes Computation Services.

Option	Description
Run	Runs the current configuration.
Log Level >	Defines the level of details to be shown in the Execution Log tab when a configuration is run. The log level is saved in the registry per user and connector.
> Inform	Use this log level if you just want to view warnings and errors.
> Debug	Use this log level if you want to display all log information available.

Execute menu:

Help menu:

Option	Description
Computation Services Help	Launches the online help system.

8.6.3.3 Computation Services Toolbar

The Computation Services toolbar includes shortcuts for some of the most common commands in the menus. Click on the buttons on the toolbar to activate the corresponding functions.

- Empties Computation Services, so that you can start a new configuration. Any information you have currently open in the Script pane, or in any of the tabs, will be cleared.
- Opens a configuration earlier saved using Computation Services. This configuration contains the actual script along with any defined input and output parameters, as well as the specified result handlers and prompt settings.
- Saves the current configuration including the script, all input and output parameters, as well as the specified result handlers and prompt settings to an earlier specified file.
- Sends the current configuration to Analysis Builder as an available action, so that the calculation can be incorporated in a Guide.
- Adds the selected text in the script text area as an input parameter. Same functionality as the Add button on the Input Parameters tab.
- Adds the selected text in the script text area as an output parameter. Same functionality as Add button on the Output Parameters tab.
- Runs the current script configuration.
- Displays the Connector Settings dialog, which handles the connection to the computation server.

8.6.3.4 Input Parameters Tab

Input Parameters Output Parameters	Result Handling Execution	n Log	
Prompt dialog title: My Example Calculation	Prompt dialog de This is an exam	escription: ple R-script calculation which adds	an entered integer to all specifie
Parameter name	Data type	Value	
x	Integer	Prompt: Integer	• <u>A</u> dd
datain	Dataset	Prompt: Data set	<u></u> <u>R</u> emove
			Move <u>U</u> p
			Move <u>D</u> own
I			

Option	Description
Prompt dialog title	The text in this field is displayed as the title of the prompt dialog when the configuration is executed. Maximum length is 80 characters.
Prompt dialog description	The text entered here is also displayed in the prompt dialog. Typically, this would be a description of what the configuration does or a more thorough description of the parameters that the end user of the tool should provide. Maximum length is 1000 characters.
Parameter name	A string matching a parameter in the script. If you have selected a parameter in the Script field and then clicked on the Add as input
	parameter button, \blacksquare , the parameter name is already set to the selected text. If no parameter was selected before you clicked Add, a default parameter is added and you can edit the parameter name in the text box. Note: Make sure you type a correct parameter name. The allowed parameter names differ for the various scripting languages.
Data type	Select the data type of the parameter from the drop-down list. Not all data types described in this help file is available for all types of connectors.
Value	A drop-down list with the possibility to select either a constant or one of the prompt types available for the selected data type.
	Opens a dialog with the possibility to enter a constant when the constant value is selected, and a prompt setting when a prompt value is selected.
Add	Adds the text selected in the Script field as an input parameter. Same functionality as the Add as Input Parameter button on the toolbar.
Remove	Removes the selected input parameter.
Move Up	Moves the selected input parameter up one step. The position defines the order in the prompt dialog.
Move Down	Moves the selected input parameter down one step. The position defines the order in the prompt dialog.

8.6.3.5 Output Parameters Tab

Input Parameters	Output Parameters	Result Handling	Execution Log					
Parameter name dataout					Data type Dataset	×	<u>A</u> dd <u>R</u> emove	
Option	De	escriptio	n					
Parameter	name A s par Par tex par No par	string match ameter in th ameter butto t. If no paran ameter is ad te: Make su ameter nam	ing a param e Script fie on, , , the meter was s Ided and yo re you type es differ fo	neter in the ld and the parameter selected l bu can ed e a correct r the vari	he script en clicko ter name before yo it the parame tous scrip	If you ed on the is alre ou click rameter eter nar oting la	t have select he Add as (ady set to t ked Add, a r name in th me. The allo anguages.	eted a Dutput he selected default ne text box. owed
Data type	Sel	ect the data	type of the	paramet	er from t	the drog	p-down list	-

AddAdds the text selected in the Script field as an output parameter. Same
functionality as the Add as Output Parameter button on the toolbar.RemoveRemoves the selected output parameter.

8.6.3.6 Result Handling Tab

Input Parameters	Output Parameters	Result Handling	Execution Log		
Result handler					
Add to Current Da	ata Set (Row by Row) -	output.dataout by i	input.datain		<u>A</u> dd ▼
					<u>R</u> emove
					Settings
1					

Option	Description
Result Handler	Displays all result handlers currently in use.
Add	Displays a list of the available result handlers. What result handlers are available depends on the data types of your current output parameters. The current version of Computation Services allows you to present your

	results in the following manners:
	View in Result Dialog
	Add to Current Data Set (Automatic Key Matching)
	Add to Current Data Set (Row by Row)
	Replace Current Data Set
	Open in Other DecisionSite Instance
	Launch File
Remove	Removes the selected result handler.
Settings	Displays the settings for the selected result handler.

If you remove an output parameter that has been used to define a result handler, the result handler will turn red in the list. Either delete the incorrect result handler, or open the Settings... for the result handler and change it to work on another output parameter. You can also add the missing parameter again to fix the problems.

8.6.3.7 Execution Log Tab

Input Parameters	Output Parameters	Result Handling	Execution Log
Processing	output persmet	ara	
Paramete	• dataout		
Calling outro	t-handlers		
Merging outp	nut with loade	data	
Column n	ame template: Ca	alculated *	
Removing	columns to be	overwritten	
Adding c	lumns		
Connec	ting to data so	urce	
Joinin	g records from (data source	
Hand	ling extra colu	ms	
Mapp:	ing source colu	mns to view	· ·
Buil	ding join condi	tions	
Fetcl	ning records		
Sort:	ing		
Execution con	upleted success	fully.	▼

The Execution Log shows detailed information about a configuration when it is run. The level of details is set under the menu option **Execute** > **Log Level**. If desired, the resulting log can be copied using the right-click menu and saved for future reference.

8.6.3.8 Prompt Dialogs

8.6.3.8.1 Prompt Settings: Boolean Dialog

Use this type of prompt for user input of the type yes/no. The resulting prompt will be a check box which can be empty or selected.

Prompt Settings: Boolea	in	×
Label: Always overwrite columns with	h the same names	
Default value: true		
O <u>f</u> alse		
Help	ОК	Cancel

According to Spotfire UI Guidelines the label for a check box should use sentence-style capitalization and end without a full stop.

Resulting prompt for the example above:

Always overwrite columns with the same names

8.6.3.8.2 Prompt Settings: Column Name Dialog

Use this type of prompt when you want user input in the form of a column name string.

Prompt Settings: Column Name	×
Label: Column name:	_
Data types:	
String Integer Real Time Date Date and Time	
Coptional settings	
<u>R</u> egexp matching: J.*	
Help OK Cancel	

Description
The text that will be displayed above the column name selection in the prompt dialog when the configuration is executed. Try to make the label as clear as possible to ensure that the end users understand what the input parameter should be. According to Spotfire UI Guidelines the label for a drop-down list should use sentence-style capitalization and end with a colon.
Select the data types of the columns you want the end user to see upon prompting for the specific parameter.
Type any kind of regular expression to limit the available columns in the prompt. Example: If you type Exp in the Regexp matching field, only columns containing 'Exp' somewhere in the column name will be visible, e.g., Experiment1, Experimental results, Expression, MyExperiments, etc. See Introduction to Regular Expressions in the Query Devices chapter for more information.

Resulting prompt for the example above:

Column name:	
eye color	•

8.6.3.8.3 Prompt Settings: Data Set Dialog

Use this type of prompt when you want user input in the form of one or more columns from the current data set.

🥺 Prompt Settings: Data Set 🛛 🗙
Label:
Select a column containing heights:
Data types:
String
Integer Real
Time
Date and Time
Optional settings
Minimum number of columns: 1
Maximum number of columns: 1
<u>H</u> elp OK Cancel

Option	Description
Label	The text that will be displayed above the column selection in the prompt dialog when the configuration is executed. Try to make the label as clear as possible to ensure that the end users of the script understand what the input parameter should be.
Data types	Select the data types of the columns you want the end user to see upon prompting for the specific parameter.
Minimum number of columns	The minimum number of columns that you want to use as input for the selected parameter.
Maximum number of columns	The maximum number of columns that you want to use as input for the selected parameter.

Resulting prompt for the example above:

Select a column containing heights:	
Avaijable columns:	Selected columns:
Name 🛆	Add >> Name
Enter text here	
age	<< <u>R</u> emove
height (m)	
weight (kg)	Move Up
	Move Down
Records selection: All	

The end user of the configuration will be presented with a column selector with all columns of the specified data type in the Available columns field. The end user will also have the

possibility to choose whether to work on All records, Marked records or Selected records by choosing the appropriate option from the Records selection drop-down list.

Tip: If there are too many columns to choose from in the Available columns list, it is possible to right-click on the Name header and select Show search field from the pop-up menu. Then, any search string can be used to limit the number of available columns.

8.6.3.8.4 Prompt Settings: File Dialog

Use this type of prompt when you want user input in the form of a file.

Note: If the resulting file is to be processed via one of the predefined Open, Edit or Print options in the Launch File Dialog, the output parameter name used must end with the desired file extension (example: outfile.txt). See Launch File Dialog for more information.

	×
on:	
0K	Cancel
	n: OK

According to Spotfire UI Guidelines, the label for a text field should use sentence-style capitalization and end with a colon.

Resulting prompt for the example above:

Use this file in the calculation:	
myinputdataset.txt	Browse

8.6.3.8.5 Prompt Settings: Integer Dialog

Use this type of prompt when you want user input in the form of an integer.

Prompt Setting	s: Integer 🔀
<u>L</u> abel:	
Age:	
Default <u>v</u> alue:	
33	
Mi <u>n</u> value:	Ma <u>x</u> value:
0	115
Help	OK Cancel
Option	Description
Option Label	Description The text that will be displayed above the input field in the prompt dialog when the configuration is executed. Try to make the label as clear as possible to ensure that the end users of the configuration understand what the input parameter should be. According to Spotfire UI Guidelines, the label for a text field should use sentence-style capitalization and end with a colon.

Min value	If desired, type the lowest acceptable value that can be used as input. If an end user tries to provide a lower value, an error message will be displayed upon execution.
Max value	If desired, type the highest acceptable value that can be used as input. If an end user tries to provide a lower value, an error message will be displayed upon execution.
D 1.	

Resulting prompt for the example above:

Age:			
33			

8.6.3.8.6 Prompt Settings: List Dialog

Use this type of prompt when you want user input in the form of a string selected from a predefined list.

	: LISC	<u> </u>	
Label:			
Favorite color:			
Selectable <u>option</u> :	<u>⊻</u> alue:		
black	6	<u>Add</u>	
red [value: 1] (defaul green [value: 2] blue [value: 3]	lt)	<u>R</u> emove	
orange [value: 4] yellow [value: 5]		Move <u>U</u> p	
		Move <u>D</u> own	
		Set as De <u>f</u> ault	
l <u>H</u> elp	ОК	Cancel	
Dption	OK Description	Cancel	
L <u>H</u> elp Dption Label	UK Description The text that will be a dialog when the conf clear as possible to er understand what the i UI Guidelines the lab capitalization and end	displayed above the lagration is executed insure that the end use input parameter shou bel for a drop-down l d with a colon.	list selection in the prompt I. Try to make the label as ers of the configuration Id be. According to Spotfir ist should use sentence-styl
Lelp	UK Description The text that will be a dialog when the confi clear as possible to er understand what the i UI Guidelines the lab capitalization and end The list item text as y selectable option sho calculations.	displayed above the liguration is executed input parameter should be connected to a displayed above the liguration is executed input parameter should be connected to a displayed be connected be connected to displayed be connec	list selection in the prompt I. Try to make the label as ers of the configuration ild be. According to Spotfir ist should use sentence-styl played for the end users. Ea a value to be used in the act

	the selectable options shown in the drop-down list.
Add	Adds the current pair of selectable option/value to the list.
Remove	Removes the selected option from the list.
Move Up	Moves the selected option up in the list.
Move Down	Moves the selected option down in the list.
Set as Default	Sets the selected option as the default value shown to the end user upon execution.

Resulting prompt for the example above:

F	avorite color:	
	red	-

8.6.3.8.7 Prompt Settings: Real Dialog

Use this type of prompt when you want user input in the form of a decimal number.

Prompt Settings: Re	al	×
Label: Height:		
Default <u>v</u> alue: 1.65		
Mi <u>n</u> value: 0.1	Ma <u>x</u> value: 3	
<u>H</u> elp	ОК	Cancel

Option	Description
Label	The text that will be displayed above the input field in the prompt dialog when the configuration is executed. Try to make the label as clear as possible to ensure that the end users of the configuration understand what the input parameter should be. According to Spotfire UI Guidelines, the label for a text field should use sentence-style capitalization and end with a colon.
Default value	If desired, type a value for default display in the prompt dialog.
Min value	If desired, type the lowest acceptable value that can be used as input. If an end user tries to provide a lower value, an error message will be displayed upon execution.
Max value	If desired, type the highest acceptable value that can be used as input. If an end user tries to provide a lower value, an error message will be displayed upon execution.

Resulting prompt for the example above:

Height: 1.65

8.6.3.8.8 Prompt Settings: String Dialog

Use this type of prompt when you want user input in the form of a string.

Prompt Settings: String				
Label:				
Favorite color:				
Default <u>v</u> alue:				
green				
Maximum string length (1-999): 30				
Help	ОК	Cancel		

Option	Description
Label	The text that will be displayed above the text field in the prompt dialog when the configuration is executed. Try to make the label as clear as possible to ensure that the end users of the configuration understand what the input parameter should be. According to Spotfire UI Guidelines, the label for a text field should use sentence-style capitalization and end with a colon.
Default value	If desired, type a text for default display in the prompt dialog.
Maximum string length (1-999)	If desired, type the maximum length of the string to be used as input. If an end user tries to provide a longer string, an error message will be displayed upon execution.

Resulting prompt for the example above:

	vorite color:
ļ	een

8.6.3.9 Result Handling Dialogs

8.6.3.9.1 Add to Current Data Set (Automatic Key Matching)

Use this result handler when you want the resulting columns to be added to your current data set using an automatic primary key matching.

Note: This method requires that you actually have good primary keys available, that is, that there is a column on the server with exactly the same name as one in your DecisionSite data set, and that some of the values are matching. If not, you should probably use the Add to Current Data Set (Row by Row) result handler instead.



Select the output parameter that you want to add to your DecisionSite data set from the dropdown list. Only output parameters defined as the data type Dataset are available in the list.

How it works:

For all column names that are identical in DecisionSite and on the server, the contents of the columns will be compared. If the values are identical, new values are added to the rows where there was a match. If the same value occurs in more than one place in the key column, the first value will be used.

Tip: If your key columns have names that do not match, it is easy to change the names in DecisionSite.

8.6.3.9.2 Add to Current Data Set (Row by Row)

Use this result handler when you want the resulting columns to be added to your current data set using a row by row matching. This will make sure that the results are added to the correct rows, even if the calculation has been performed using marked or selected records only.

Add to Current Data Set (Row by Row)	×
Output parameter:	
Y	•
Input parameter for matching of rows:	
×	•
Column <u>n</u> ame template (original name represented by *):	
Calculated *	
Verwrite existing columns	
Help OK	Cancel

Option	Description			
Output parameter	Select the output parameter that you want to add to your DecisionSite data set from the drop-down list. Only output parameters defined as the data type Dataset are available in the list.			
Input parameter for matching ofSelect the input parameter whose settings will be used in the mat of rows to the existing data set.TownImage: Select the input parameter whose settings will be used in the mat of rows to the existing data set.				
rows	Example: If several input parameters are available, but the x prompt uses marked records only, it might be suitable to use the x input parameter for matching of rows and, hence, not add anything to those rows where the x input parameter was empty upon calculation.			
Column name	Used for adding prefix and/or suffix to all calculated columns. Type			

template	[prefix]*[suffix] in the text field, where * is the original input column names.
	Example: If 'Calculated * Result' is typed in the Column name template field, and columns with the names 'Height' and 'Weight' are used in the calculation, the resulting names added to DecisionSite will be 'Calculated Height Result' and 'Calculated Weight Result'.
Overwrite existing columns	Select the check box if you want any columns with the same names as specified in the Column name templates field to be overwritten upon execution.

8.6.3.9.3 Replace Current Data Set

Use this result handler when you want the result of the calculation to be a new data set in your current DecisionSite Client instance. Any previous data set in DecisionSite will be closed when the new data set is opened.

Replace Current Data 9	5et	×
Output parameter:		
Y		F
1		
<u>H</u> elp	ОК	Cancel

Select the desired output parameter from the drop-down list.

8.6.3.9.4 Open in Other DecisionSite Instance

Use this result handler when you want the result of the calculation to be a new data set in either a new DecisionSite instance or another, currently running DecisionSite instance. Any previous data set in the selected DecisionSite instance will be closed when the new data set is opened.

🧿 Open in Other De	cision5ite Instance 🔀		
Output parameter:			
Open in: <u>n</u> ew DecisionSitu new or <u>e</u> xisting D <u>H</u> elp	e instance DecisionSite instance OK Cancel		
Option	Description		
Output parameter	Select the output parameter that you want to send as a new data set to another DecisionSite instance from the drop-down list. Only output parameters defined as the data type Dataset are available in the drop- down list.		
Open in: new DecisionSite instance	Use this option to open the resulting data so instance.	et in a new DecisionSite	

Open in: new or	Use this option to allow the end user of the configuration to select
existing	whether to open the resulting data set in a new or in an existing
DecisionSite	DecisionSite instance. If this option is selected, the Open Resulting
instance	Data Set in DecisionSite dialog will be displayed upon execution.

8.6.3.9.5 Launch File

Use this result handler when you want the result of the calculation to be launched as a file in another program.

Note: If the resulting file is to be processed via one of the predefined Open, Edit or Print options in the Launch File Dialog, the output parameter name used must end with the desired file extension (example: outfile.txt). The extension used should also be defined on the end user's computer, see Tip below.

Launch File		2	×
Output parameter:		•	
Execute method:			
Open			
⊖ <u>E</u> dit			
C <u>P</u> rint			
C <u>C</u> ommand line:			
%1			
<u>H</u> elp	 Ж	 Cancel	

Option	Description
Output parameter	Select the output parameter that you want to launch as a file in another program from the drop-down list. Only output parameters defined as the File data type are available in the list.
Execute method: Open	Use this method to open the resulting file in its standard application. Example: An XLS file will be normally opened by Microsoft Excel. Note: To use this option, the selected output parameter name must include a file extension connected to a known program.
Execute method:	Use this method to open the resulting file for editing in its standard application. Example: An XLS file will be normally opened by Microsoft Excel.
Edit	Note: To use this option, the selected output parameter name must include a file extension connected to a known program.
Execute method:	Use this method to print the resulting file from its standard application.
Print	Note: To use this option, the selected output parameter name must include a file extension connected to a known program.
Execute method:	Use this method if you want to specify which program to send the file to
Command line	or to run other custom commands. The following syntax can be used for

the command line: "%path%\%program name%" %1. Example: "%PROGRAMFILES%\Windows NT\Accessories\wordpad.exe" %1.

Tip: You can specify what program will be associated with a certain type of action for a specific file type on your computer. See the online help for your operating system for more information. (In Windows XP this is made in Windows Explorer, Tools > Folder Options. On the File Types tab, select the file of interest and click Advanced. Add the selected actions (Open, Edit, Print, etc.) to the list.)

8.6.3.10 Other Dialogs

8.6.3.10.1 Connector Settings Dialog

This dialog may look different depending on the type of computation server you are connecting to. It is used to define what server to use and possibly also which other settings to use upon script execution.

Note: No connection is made until you actually run the script. If you want to test the connection when you set up the configuration, use the Test button (see below).

Onnector Settings: SAS	×
<u>S</u> erver:	
bridge://sasserver:8081	
Username:	
administrator	
Password:	
••••••	
Prompt user for login when executing the script	
Keep session open until manually closed	
Eorce single-quotation for string parameters	
Help Iest OK Cancel	

Option	Description
Server	Enter the address to the calculation server that you want to use. Type "(local)" in this field if you want to run against a local SAS Base client on your own computer.
	Opens the Servers dialog where you can select from a list of predefined calculation servers.
Username	Type the user name required to work against the calculation server. In some cases this field may be missing.
Password	Type the password required to work against the calculation server. In some cases this field may be missing.
Request timeout (minutes)	If your computation takes a long time, you can increase the Request timeout to prevent that the execution is interrupted before the

calculation is finished.

Prompt user for login when executing the script	This option is available in the design phase of a configuration only. Select this check box if you want the end users of the configuration to log into the server upon execution. If this option is cleared, the configuration will always use the connector settings provided during the design phase.
Keep session open until manually closed	This option is available in the design phase of a configuration only. Select this check box to use a single session on the server for all Computation Services calculations run during a DecisionSite session. This means that the data is built up and changed on the server as the various configurations are run. Note: When you use this option the different steps of a Guide with
	increase the risk of errors upon execution if links in a Guide are clicked in the wrong order or if requests times out.
Force single- quotation for string parameters	Use this option to be able to run SAS configurations created with DecisionSite 8.1.1. This option should normally be cleared.
Test	Validates the connection without closing the dialog.

To reach the Connector Settings dialog:

- If Computation Services is not already started, select Tools > Computation Services > SAS, R or S-PLUS or whatever the name of the computation server you want to connect to.
- 2. Select File > Connector Settings....

8.6.3.10.2 Servers Dialog

This dialog lists all servers currently defined as calculation servers for a specific connector. Click on the server that you want to use upon configuration execution, then click OK.

Servers		×
Defined servers:		
http://myRserver http://Rserver1:8012		
<u>H</u> elp	ОК	Cancel

8.6.3.10.3 Constant Definition Dialog

The constant definition dialog's appearance varies depending on what data type you are defining a constant for. Just enter the value that you want to use in the calculation and click OK. Example dialogs:

Constant: String		×
Value:		
<u>H</u> elp	ОК	Cancel
Constant: Roolean		× I
Constant. Doolean	_	
Value: O true		
 false 		
Hala	04	Concol

8.6.3.10.4 DecisionSite Data Set Definition Dialog

This dialog defines what data to use in the calculation when the Input: Data set option has been chosen for an input parameter.

DecisionSite Data Set		×
 <u>Records to include from Decision</u> All records Marked records Selected records 	ionSite data set:	
Help	OK	Cancel

Click the appropriate radio button to select whether the calculation shall be performed on all records, marked records or on records selected using the query devices or zooming only.

8.6.3.10.5 Computation Services Result Dialog

This is a dialog containing the results from a Computation Services calculation. It displays the input parameters and the output parameters of the executed configuration. You can copy selected results by using the pop-up menu in the dialog.

Comput	ation Services Result
Name	Value
input.x	green
input.b	eye color
input.a	1
input.k	33
input.m	1.65
input.o	True
input.q	Spotfire.ComputationServices.Dataset.FilteredDataReader
input.s	D:\Data\testfile.txt
input.u	SystemComObject
output.Y	green
output.z	eye color
output.c	1
output.j	33
output.p	Spotfire.ComputationServices.Dataset.ImportAgentWrapper
<u>H</u> elp	Dose

8.6.3.10.6 Open Resulting Data Set in DecisionSite Dialog

This dialog is presented when the creator of a Computation Services configuration has chosen to open the result of a calculation in a DecisionSite instance other than the one running the configuration.

8.7 Distance Calculator

You can calculate the distance between two markers in a 2D or 3D scatter plot by using the Distance Calculator.

Click on the marker you want to use as the origin. Then move the mouse pointer over other markers and the distance to the origin will be displayed in the Distance Calculator window. The Distance Calculator also displays the distance from one marker to another along the different axes.

More specifically the distances calculated are:

distance =
$$\sqrt{(\Delta x)^2 + (\Delta y)^2 + (\Delta z)^2}$$

 $\Delta x = |x(active) - x(highlighted)|$
 $\Delta y = |y(active) - y(highlighted)|$
 $\Delta z = |z(active) - z(highlighted)|$

Note: The Distance Calculator only handles Real, Float and Integer types. If a column contains other types, no values will be displayed in the Distance Calculator window.

► To reach the Distance Calculator:

Select Tools > Distance Calculator.

8.8 Administration Tools

8.8.1 Administration Tools Overview

The Administration section contains the tools needed to organize the DecisionSite environment. These tools are only available for users with Administrator privileges. The Library provides publishing of all analysis material for sharing with colleagues. Using the Library, you can collaborate with colleagues in a distributed environment and organize your analysis material. See the Library Help for more information.

DecisionSite Administrator	The DecisionSite Administrator can be reached by selecting Tools > Administration > DecisionSite Administrator . This will open a Microsoft® Internet Explorer window where Administrators can manage user privileges. Refer to the DecisionSite Administrator Help for more information.
DecisionSite Library	The Library can be accessed for various purposes. By selecting Tools > Administration > DecisionSite Library , the main view of the Library is opened. This will open a Microsoft® Internet Explorer window with the Library. Use this view to open Library items and to administrate it. Refer to the Library Help for more information.
DecisionSite Library Administrator	The DecisionSite Library Administrator can be reached by selecting Tools > Administration > DecisionSite Library Administrator . This will open a Microsoft® Internet Explorer window where Administrators can edit who is allowed to create new Library Sections, configure DecisionSite Library and Poster settings. See DecisionSite Analytic Server - Installation and Upgrade manual for more information.
Server Usage	Server usage statistics can be reached by selecting Tools > Administration > Server Usage . This will open the log file

dssaccess.sfs in DecisionSite, for an easy analysis and overview. This file contains information about all logins and logouts from all DecisionSite Clients to the DecisionSite Analytics Server. It shows which user logged in/out and when. The log is always enabled, and it is unaffected by Log Configuration File settings.

9 Guides

9.1 What is the Guides Pane?

The Guides pane is a web browser, fully integrated into the Spotfire DecisionSite environment. It is used to connect to the Spotfire DecisionSite Analytics Server, providing access to Guides as well as a location for a customized start page.

The Guides Pane is closed by default when you launch Spotfire DecisionSite. You can close and open it by clicking the Guides Pane button to the far left of the Guides Toolbar. The button on the right directs the page to the current start page.

The Guides Toolbar

The Guides Toolbar is used to open the Guides pane or to launch your own custom start page. This start page is configurable by right-clicking in the Guides Pane.



The toolbar can be made visible or hidden by selecting **View > Guides Toolbar**.

Guides

The Guides pane is primarily used to run Guides. It contains preconfigured Guides which can be run with a single click, but it can also show any custom made Guides for yourself or for others. See Guides below for more information.

9.2 Guides

A Guide is a convenient way to guide colleagues through a series of analysis steps in the DecisionSite environment. Using a Guide, information on how to perform frequent tasks, stepby-step instructions, and quick access to tools is assembled in a user friendly way. The Guides are easily designed in Analysis Builder.

Guides are shown in the Guides pane. In the Guides pane you will find the link Open Guide from Library... and the preconfigured Guides in your DecisionSite application.

Guides	<u> </u>
Data Analysi 🗟 Pivot result	s L data
Key-based Rule of 5	Creates visualizations suitable for High Screening data
Create SAR	Table using Information Link

The easiest way to run a Guide is to click the link of the Guide in the Guides pane. If the Guide you are interested in is not there, you can either run it from the Library or from a file:

- To run a Guide from the Library, either click on Open Guide from Library... in the Guides pane or select **Guides > Run from Library...** from the menu.
- To run a Guide from a file, select **Guides > Run from File...** from the menu.

When you have started the Guide, follow the instructions in the Guides pane. You can go back in a Guide to a previous step by clicking on them in the flight view of the Guide.

Guides 🛛 🔟
Contents > Pivot results This guide will pivot your results to facilitate analysis for multiple protocols, runs or batches. The pivot operation will replace the current data with a new pivoted data set. Select how you would like to pivot your data. Analyze average results per:
 <u>Protocol</u> <u>Run</u> <u>Batch</u> <u>Run per Batch</u> <u>Run across Protocols</u>

Example of a Guide as seen when run in the Guides pane.

Creating Guides

TIBCO Spotfire provides an application called Analysis Builder, where you can create your own Guides or edit a Guide file without having to write a single line of code. Analysis Builder is started by selecting **Guides > Create and Edit Guide** from the menu.

9.3 Guides Pane Options

If you right-click in the Guides pane a pop-up menu appears. Select **Options...** to display the Guides Pane Options dialog.

Page viewed when starting DecisionSite

By default, the Guides pane displays a list of your available guides. You can also select to show another web page as your start page.

To do this, type in the URL of the custom start page in the **Address** field (or click **Browse...**). This does not change which DecisionSite Analytic Server you are connected to, but merely provides a way to access other pages from DecisionSite.

The Custom Start Page will be displayed each time you start Spotfire DecisionSite. Finally, click **OK** to make the changes take effect.

If the new **Custom Start Page** is not on your local intranet or among the **Trusted Spotfire sites** (see below), a pop-up dialog will appear in which you are asked if you would like to add the URL to the list of trusted sites.

Trusted Spotfire Sites

Only sites on your local intranet, or present in the list of Trusted Spotfire sites, are allowed to access Spotfire DecisionSite using scripts or active content. Each time you enter a new

Custom Start Page you will be prompted whether or not you want to add that site to the list of Trusted Spotfire sites.

If you want to remove a site from the list, select it and then click on the **Remove** button. Some sites in the list may be grayed out and cannot be removed. These are sites that are predefined for your installation and needed by Spotfire DecisionSite.

9.4 Run from Library...

9.4.1 Open Guide from Library

The Library introduces convenient sharing of analysis material. The **Open Guide from Library...** link in the **Guides pane** allows you to access Guides located in the Library with a single click. Using this link, Guides located in the Library can be run in the Guides pane as any other Guide.



► To open Guides from Library

 Click Open Guide from Library... in the Guides pane or select Guides > Run from Library....

Response: The Open Guide from Library Dialog is shown.

2. In the Open Guide from Library Dialog, locate the Guide you want to open and click **Open**.

Response: The Guide is opened in the Guides pane.

9.4.2 Open Guide from Library Dialog

This dialog lets you select and open a Guide that is located in the Library. To find a Guide, either look through a Library Section's content, or search for the Guide.

Note: Only Guides created with Analysis Builder are available to be opened and edited in Analysis Builder.

🧿 Open f	rom Library				×
Library	Search				
Home >	> DecisionSite for	Functional Genomics			
Туре	Title *		Description	I	
1					
2	Advanced micro	array Guide	Example: T	his Guide uses a	a number
8	Microarray Guide	2	Example: T	his Guide shows	how visua
<u>H</u> elp Librar	y tab	Description		<u>O</u> pen	Cancel
Library	15	All Guides, folders an Note: Only Library Se	d Library S ections that	ections are lis you have acco	ted on this tab. ess to are listed.
Open		Select the Guide you want and click Open to open it in the Guides pane (or in Analysis Builder if you have reached this dialog from there). You can also double-click the Guide to open it.			
Searc optior	h tab าร	Description			
Search	tab	Use Search to search for the item you want to open.			
Search	for:	Enter the search string in the Search for: field and click Search . See Searching in the Library for information about search strings. If you click a folder in the Search result, you will be redirected to the Library View under the Library tab.			
Look in	:	Select which Library S	Section you	want to perfo	orm your search in.

► To reach the Open Guide from Library dialog:

- Click Open Guide from Library in the Guides pane, or
- select Guides > Run from Library... from the menu, or
- in Analysis Builder, click Guide > Open from Library....

Note: Opening a Guide in Analysis Builder will open the Guide for editing in Analysis Builder and not to the Guides pane as in the previous cases.

9.5 Create and Edit Guide

9.5.1 Analysis Builder Overview

With the Analysis Builder you can capture your commonly performed analysis processes into Guides. Creating your own Guides does not require your having to write a single line of code.

9.5.2 Using Analysis Builder

9.5.2.1 Guides Created with Analysis Builder

Guides created with the Analysis Builder can contain text and links. However, the Guides can also be extended with any number of complex tasks if you have programming experience or access to a person with these types of skills. An example of a Guide created with Analysis Builder is presented below:

Guides	_
<u>Contents</u> > My own guide title 1	
Some text I have added to my guide.	
Calculate standard deviation	
Set up visualizations	
<u>Google web link</u>	
3 Back	<u>Next</u>

1. Contents and Title

This is the flight view which is automatically added at the top of every Guide page. It includes the *Contents* link followed by the Guide title. The *Contents* link closes the Guide and goes back to the main page of the Guides pane. The title of your Guide can be configured via **Guide** > **Properties** in Analysis Builder.

2. Text and Links

This is the main part of the Guide, which you can design via Analysis Builder. You can add text and links to the Guide.

3. Back and Next

These are navigation links which are automatically added at the end of every Guide page. The first page of the Guide gets a *Next* link, following pages get a *Back* and a *Next*, and the last page of the Guide gets a *Back* and a *Back to Contents* link (same function as the *Contents* link in the flight view).

9.5.2.2 Suggested Workflow

► To create a new Guide using Analysis Builder:

- 1. Open a data set in Spotfire DecisionSite and start to perform your analysis the way that you want it to be done in the Guide.
- 2. If the Analysis Builder tool is not already open, click **Guides > Create and Edit Guide**.

- 3. Create the Guide in Analysis Builder by adding links and text to the Guide contents list. By adding actions (links) to your Guide simultaneously when you perform the analysis, you can make sure that you capture the settings used this very moment. This way you can also add links that update the same visualization to several places in the Guide
- 4. Test the Guide by selecting **Guide > Run**. The Guide will be displayed in the Guides pane. Note that if you are testing Guide steps that include opening a data set, you will clear the current Actions in DecisionSite list. Make sure that you have added all steps of your current analysis to the Guide before testing the parts of the Guide that involve switching data sets.
- 5. When you are finished with the Guide, select **Guide > Save As...** or publish it to the Library with **Guide > Publish to Library...**.
- 6. You can now send the Guide to a colleague or to your IT department for extended functionality or deployment.

9.5.2.3 Analysis Builder Quick Reference

Action	Instruction
Start Analysis Builder	From the main menu bar of DecisionSite, select Guides > Create and Edit Guide .
Create a new Guide	In Analysis Builder, click Guide > New . Edit the Guide by adding text and links.
Open a Guide from the Library	In Analysis Builder, click Guide > Open from Library Browse the Library to locate the Guide that you want to edit. Edit the Guide by adding or removing text and links. See Open from Library for more information.
Edit an existing Guide	In Analysis Builder, click Guide > Open . Browse to locate the Guide that you want to edit. Edit the Guide by adding or removing text and links. Tip: Run the Guide prior to editing to populate the Actions in DecisionSite list.
Add text to a Guide	In Analysis Builder, click Add > Text . Enter the text that you want to add in the Text Properties dialog. Click OK to close the dialog.
Add new actions to the Actions in DecisionSite list	Open a data set, run a tool or create a visualization in Spotfire DecisionSite. All actions that you have performed on your current data set are logged and included in the Actions in DecisionSite list.
Add links to a Guide	Make sure you have performed the action you want to add as a link in DecisionSite. Select the item or items you want to add to your Guide in the Actions in DecisionSite list. Click < Add Link. See How the Actions in DecisionSite list works for more information.

Update an existing visualization	Add a link that creates a visualization. Add the action for the specific visualization to a new link.
Add a hyperlink to a Guide	Double-click on a text item or select Add > Text to add a new text item. This will display the Text Properties dialog. Select the word that you want to create a hyperlink from. Click on the Hyperlink button,
Test a Guide	In Analysis Builder, select Guide > Run . Comment: The Guide will be displayed in the Guides pane as any other Guide.
Save a Guide	In Analysis Builder, select Guide > Save.
Publish a Guide to the Library	In Analysis Builder, select Guide > Publish to Library . See Publish to Library for more information.
Add a new page to a Guide	In Analysis Builder, select Add > New Page . Comment: A flight view linking back to Contents as well as Next [page] and Back links are automatically added to each page in the Guide.
Minimize the Analysis Builder	Click on the top right x-button. This will hide the Analysis Builder, but both the <i>Guide contents</i> list and the <i>Actions in</i> <i>DecisionSite</i> list will be remembered when you reopen the tool.
Close the Analysis Builder	In Analysis Builder, select Guide > Exit .

9.5.2.4 How the Actions in DecisionSite List Works

Adding Links to a Guide

All actions in the right list called Actions in DecisionSite can be added as a link to the Guide. Click to select an action in the list (use Ctrl to select several actions), and then click the < Add Link button to create a link in the Guide.

Adding Actions to the List

Actions are automatically logged in the Actions in DecisionSite list as you perform them in DecisionSite. First load data and perform the analysis as you would normally do. Your data, the visualizations you create, and the tools you start will appear as actions in the list.

Tip: To edit a previously created Guide, start by running the Guide in DecisionSite. This will furnish the list of actions with the data, visualizations and tools used in the Guide.

Automatic Logging

You do not have to turn on Analysis Builder in order for your actions to be logged. It is done automatically when you load data in DecisionSite Client, even if you have not started Analysis Builder. However, if you log out from the server, no actions will be logged while you are disconnected.

Clearing the List of Actions

The list of actions will be emptied if you close your data via File > Close in DecisionSite. **Note:** The Actions in DecisionSite list will be cleared if you open a new data set. Since you can only have one data set open at a time in Spotfire DecisionSite, the previous data will be closed when you open the new data set. If you log out from the server, the Analysis Builder will be closed and the Actions in DecisionSite list will be cleared.

9.5.2.5 Settings Captured in Links

All actions that you have performed on your current data set are included in the Actions in DecisionSite list. See How the Actions in DecisionSite list works for more information about the Actions in DecisionSite list.

Note: The Analysis Builder will log all actions that you perform in DecisionSite, even if it has not been started. The Actions in DecisionSite list will be cleared if you open a new data set.

Information links

If an information link is added via the Information Library or the Information Builder, the created Guide will include a reference to the information link or the actual query, respectively. If the information link is prompted, the end users of the Guide will see the prompts and be able to make their own selection. There is, however, no reference to the server that the Information Link is located on, so if you intend to distribute your Guide containing information links to users who work on a different server to your own, you must copy the Information Model to their server. For more information on copying data layers, see the chapter "Information Designer" of the Spotfire DecisionSite Analytics Server - Administrator's Guide, and contact your DecisionSite Analytics Server administrator.

If you want the end user of the Guide to be able to choose a different information link, you should instead include a link that starts the tool Information Library. To make the action **Start Information Library** appear in the Actions in DecisionSite list, start the tool once more after opening the information link that you used when creating the Guide and select Cancel in the Information Library dialog.

Open data (saved with Guide)

If a data set has been opened by some other means than by opening an information link, you will have the option to save the data with the Guide. This means that the data set that you are currently using will be a part of the Guide file. This can be useful for reference data that are never changed or if you want to create a prototype Guide where some IT personnel will later on modify your Guide to open data from a data source that is currently not supported by Analysis Builder.

The data set that is saved with the Guide is the currently available data. That means that if you have added or removed columns from the original data set prior to adding the link to your Guide, the embedded data will contain the modified data set.

If you want to save the data from an information link with the Guide, e.g., for testing purposes, you can first open the information link, save the data as an Analysis in DecisionSite, open the Analysis with the data and add the new action Open data (saved with Guide) to your Guide.

Visualizations

The visualizations appear in the Actions in DecisionSite list when they are created, but the actual settings for the visualization are retrieved when a link is added to the Guide contents list. All properties are saved with the specific visualization. For example, you can specify that a scatter plot should be created with two defined columns on the axes and with the markers colored by a third column. Query device settings (filtering), transformed columns and background images are also included in the link. It is also possible to add steps to the Guide where the end user of the Guide is prompted to specify which settings to use. See Prompting Guide users for input for more information.

Set query device filters

Adding this action in a link will set all query devices and also the selected properties of the Columns tab to the current state. This means that you can apply log scale, show or hide empty values, specify query device types and filter on specific columns without having to add a new
visualization. This way, you can create several links in the Guide that update your visualizations, thus creating a "bookmark" kind of function.

Note: If the data set that the end user of a Guide is using differs from the one that you were using while creating the Guide, there might be occasions when the query device settings will not be applicable.

Tools

In the current version of Analysis Builder, settings are not always saved with the tools. The various tool links will, in some cases, open the tool to the end users of the Guide, but they will have to make the calculation selections and click OK in the tool dialog for themselves. If you want the end users to use some specific settings in one of those tools, you should state this information as text in the Guide.

A number of tools, e.g., the New Column from Expression tool, can be run silently (without input from the end user). When a link is added to such a tool, you can set the Tool Option to specify whether you want the link to run the tool using the settings that you specified in the current analysis, or if you want to display the dialog to the end user of the Guide.

To add a tool which you have created using Computation Services you must first open the configuration in Computation Services and select File > Send to Analysis Builder. This will create the action Start Data computation in the Actions in DecisionSite list, which can be included in your Guide as any other action.

Multiple action links

It is possible and also often recommended to include several actions in a single link. For example, if you want the Guide to open an information link and also display one or more visualizations upon clicking the link, you can combine these actions to one link. Make sure you have performed all actions that you want to include. Then click to select all of the actions that should be included and click < Add Link. The actions will be performed in the order that they appear in the Actions in DecisionSite list, i.e., the order you performed them in your analysis.

9.5.2.6 Running Guides Locally

While you are developing a Guide, or if you create Guides that are for your own use only, you may want to run a Guide locally on your own computer, without giving other users access to it on the server.

► To run a Guide locally:

- In the main menu bar of DecisionSite, select Guides > Run from File.... Response: An Open dialog is displayed.
- 2. Browse to the Guide file that you want to run.
- Comment: Spotfire Guide files (SFG) or HTML files may be opened.
- 3. Click **Open**.

Response: The Guide that you have selected is opened in the Guides pane. Follow the instructions in the Guide as usual.

Tip: If you want to test the Guide during development, select **Guide** > **Run** in Analysis Builder. This will immediately display the Guide inside the Guides pane. It is not necessary to save the Guide prior to testing.

9.5.2.7 Prompting Guide Users for Input

All properties are saved with their respective visualization when you add that visualization to the Guide. However, there may be occasions when you want the end user of the Guide to be able to specify which columns to use on different axes, which column to color the markers by, etc., upon running the Guide.

► To prompt for input to visualizations:

1. In the *Actions in DecisionSite* list, click to select the visualizations that you want the new link to create.

Comment: See How the Actions in DecisionSite list works for more information on how to populate the list.

- 2. Make sure that Edit > Show Add Link Dialogs is selected with a check mark.
- 3. Click < Add Link.

Response: The Link Properties dialog is displayed

4. Click on the visualization action that you want to add prompting to in the **Actions performed when clicking the link** list.

Response: The Prompts... button is activated.

Comment: Prompting is not supported for multiple color bands in pie charts.

5. Click **Prompts...**.

Response: The Prompt for ... dialog is displayed.

Comment: This dialog varies depending on which type of visualization that you have selected.

- Select the check box for the things that you want the user to specify. Comment: Each selected object will result in the appearance of a setting selection in a dialog which is presented to the end user of the Guide.
- 7. If desired, change the **Title for input field in prompt dialog** to a different title. Comment: This is the title that the end user of the Guide will see above the selected setting.
- 8. Click OK.

Response: In the Link Properties dialog, the visualization action is updated with the information [Settings modified].

- 9. Repeat steps 4-7 if you want to create a multiple action link with several prompt steps.
- 10. Click OK.

Response: The link is added to the Guide contents list.

► To prompt for input to tools:

1. In the *Actions in DecisionSite* list, click to select the tool that you want the new link to start.

Comment: See How the Actions in DecisionSite list works for more information on how to populate the list.

- 2. Make sure that Edit > Show Add Link Dialogs is selected with a check mark.
- 3. Click < Add Link.

Response: The Link Properties dialog is displayed

4. Click on the tool action that you want to add prompting to in the **Actions performed when clicking the link** list.

Response: The Prompts... button is activated.

5. Click **Prompts...**.

Response: The Tool Option dialog is displayed.

- 6. Select the **Display the tool dialog, so the user can provide input** radio button. Comment: For many of the tools in DecisionSite, this is the only alternative available. The number of tools that can be run silently (without input from the end user of the Guide) will increase in coming releases of Analysis Builder.
- 7. Click OK.

Response: The Tool Option dialog is closed.

8. Click OK.

Response: The link is added to the Guide contents list.

9.5.2.8 Open and Publish Guides to the Library

The Library introduces convenient publishing of analysis material. Guides can be published to the Library for sharing with your colleagues. Located in the Library, the Guide can be opened by anyone with read access.

► To open Guides from Library in Analysis Builder:

- 1. In Analysis Builder, select Guide > Open from Library....
- In the Open from Library Dialog, locate the Guide you want to open and click Open. Response: The Guide is opened in Analysis Builder. Note: Only Guides created with Analysis Builder can be opened.

► To publish Guides to the Library:

- 1. In Analysis Builder, select Guide > Publish to Library....
- 2. In the Publish to Library Wizard Step 1(2), browse to the location where you want to publish the Guide.
- 3. In the Guide Title text box, enter the name of the Guide and click Next >.
- 4. Please enter properties of your Guide in Publish to Library Wizard Step 2(2).
- 5. Click **Finish**.
 - Response: Your Guide is published to the Library.
- 6. In the Publish to Library Guide Published step, decide if you want to email your colleagues about your new Library Guide. Click **Close** when done.

9.5.2.9 Deploying Guides to a Server

There are two ways of distributing a Guide to your colleagues. Simplest way is to publish your Guide to the Library via the **Guide > Publish to Library** menu alternative. See Publish to Library for more information. The other alternative is to deploy your Guide to the server. To deploy a Guide on the server, you need access to Spotfire DecisionSite Developer and you also need administrators rights on the DecisionSite Analytics Server. In Spotfire DecisionSite Developer you find the application DecisionSite Builder, where you can incorporate your Guides into custom DecisionSite applications or extensions.

See Spotfire DecisionSite Developer for more information on deployment, or contact your Spotfire DecisionSite Administrator.

9.5.3 User Interface

9.5.3.1 Analysis Builder User Interface Overview

This is the Analysis Builder user interface:

Analysis Builder		×
Guide Edit Add Format Help 🚹		
Guide contents:		Actions in DecisionSite:
This is my first guide. It will help you create different visualizations suitable for your specific company and analysis process. <u>Open data (saved with quide)</u> <u>Create Profile Chart of original data</u>	< Add Link	Open data (saved with guide) Original data (Signal for 501_Embryonic_ Scatter Plot (Probe Set Name vs. Probe S Pie Chart Set Query Device filters
Click the link to create some other useful visualizations		
Create visualizations		
To filter the data, click the link below:		
Set Query Device filters		
Page Break		
To open a browser and search the internet:		
Google - http://www.google.com/	How to add links?	6

1. Analysis Builder menus

The Guide, Edit, Add, Format and Help menus contain menu commands required to work with the Analysis Builder.

2. Toolbar



Includes shortcuts for some of the most common commands in the Analysis Builder. See Analysis Builder toolbar for a description of the different buttons.

3. Guide contents

This window contains the contents of your current Guide. This is where you create a new Guide or modify an existing Guide. Text is added by double-clicking were it says **Double-click to edit text** or by selecting **Add** > **Text** from the menu. Links to actions are added from the *Actions in DecisionSite* list, see below.

You can move text items, comments, links and page breaks in the Guide contents list to the desired position using a simple drag-and-drop operation.

4. Actions in DecisionSite

This list contains all actions that you have performed in DecisionSite during the latest session. A session is defined as the time from when you have opened your current data set until you close it. The Analysis Builder does not have to be started to log the events. Closing the data set will clear the action list.

Select one or more actions from this list and click < Add Link to include the action (or combined action) in the Guide. If you want to add an action that is currently not available in the action list, first perform the action in DecisionSite and it will immediately show up in the list.

5. < Add Link

Select one or more actions from the *Actions in DecisionSite* list and click this button to include the action (or combined action) in the Guide. The link will by default include the settings used in DecisionSite at the very moment you add the link.

6. How to add links?

This link opens this help file to a page with tips on how to add links to a Guide.

► To reach the Analysis Builder:

Select Guides > Create and Edit Guide.

9.5.3.2 Analysis Builder Toolbar

H

B).

The Analysis Builder toolbar includes shortcuts for some of the most common commands in the menus. Click on the buttons on the toolbar to activate the corresponding functions.

- Creates a new, empty Guide. This resets the *Guide contents* window but not the *Actions in DecisionSite* list.
- Opens a dialog where you can select a previously saved Guide file (SFG) that you can continue to work on or modify and save as a new Guide.
- Saves the current Guide as an SFG file.
- Launches the current Guide in the Guides pane. It is not necessary to save the Guide prior to using this command in Analysis Builder. Therefore, it is useful for iterative testing of the design of the Guide.

Note: If you are testing Guide steps that include opening a data set, you will clear the current *Actions in DecisionSite* list! Make sure that you have added all steps of your current analysis to the Guide before you test the parts of the Guide that involve switching data sets.

- Adds a new text element below the currently selected item, or, if no item is selected, at the bottom of the Guide contents list. The Text Properties dialog is displayed with the default text "Enter text here".
- Creates a new page in the Guide. The beginning of the new page is labeled -----Page Break----- in the Guide contents list.
- Adds a number before the selected text, link or comment item. Subsequently following text, link or comment items on the same Guide page get the next number (2, 3...), if this button is selected.
 - Adds a bullet before the selected text, link or comment item.

Indents the selected text, link or comment item.

9.5.3.3 Text Properties Dialog

The Text Properties dialog is used to enter and edit the text of a text element. Multiple paragraphs can be written within the same text element, bold formatting and hyperlinks can be applied to selected text.



command **Ctrl+B**.

Opens the Hyperlink Properties dialog, where you can create a hyperlink to an

external web page from the selected text. Also available using the short command **Ctrl+K**.

► To reach the Text Properties dialog:

The Text Properties dialog is displayed when a new text element is added to the Guide in Analysis Builder, e.g., via **Add** > **Text**. It can also be displayed by double-clicking on a previously entered text element.

9.5.3.4 Hyperlink Properties Dialog

6

The Hyperlink Properties dialog is used to insert hyperlinks to external web pages in the Guide. To add links that perform actions in DecisionSite (opens data, creates visualizations, etc.), see How the Actions in DecisionSite list works.

O Hyperlink Properties	×			
⊥ext to display: Spotfire.com URL to external web page http://www.spotfire.com Help	: OK Cancel			
Option	Description			
Text to display	The text that will be displayed as a hyperlink (green and underlined).			

URL to external web	The address to the external web page where you want to go when
page	clicking on the hyperlink. The address must begin with either http://
	or file://.

► To reach the Hyperlink Properties dialog:

- 1. In the Text Properties dialog, select the word that you want to create a hyperlink from.
- 2. Click on the Hyperlink button,

9.5.3.5 Link Properties Dialog

The Link Properties dialog is specific to each link in your Guide. Here, you can edit the link text and view which actions will be performed upon clicking the link. This is especially useful if you have created links performing multiple actions.

Link Properties		×
<u>T</u> ext to display:		
Create visualizations		
Actions performed when on the second	ticking the link or S01 Embryonic 1.txt; Signal for S02 Embryonic 2.t a (Embryonic (Average); Neonatal (Average); 1 Week (; ta (Embryonic (Average), Z Scores; Neonatal (Average) alizations before performing the actions in this link	
Don't show this dialog a	gain	1
Help	OK Cancel]
Option	Description	
Text to display	Edit the default text to display a link text of your choice in Guide.	1 the new
Actions performed when clicking the link	Displays the actions that are part of the current link. If mu actions are included in the link, the actions are ordered in list where the action first performed is number 1.	ltiple a numbered
Prompts	Displays the Prompt for dialog, if the selected action is visualization, or the Tool Option dialog, if the selected actool.	a tion is a
Close all previous visualizations before performing the actions in this link	Adds an action with the title <i>Close all visualizations</i> to the list of actions in this dialog. This means that all visualizat were open when the end user of the Guide clicked on this closed. This can be used to prevent the desktop from bein with visualizations.	e top of the ions that link will be g cluttered
Don't show this dialog again	Select this check box if you do not want to see this dialog automatically upon adding new links. To display it again, > Show Add Link Dialogs	select Edit

► To reach the Link Properties dialog:

The Link Properties dialog is automatically displayed when a new link is added to the Guide in Analysis Builder. If the check box *Don't show this dialog again* has been selected earlier, the dialog for a specific link can be displayed by double-clicking the link in the Guide contents list.

9.5.3.6 Prompt for... Dialog

The Prompt for... dialog is specific to each visualization in a link. If you have selected a scatter plot (as in the example below) the dialog will be called Prompt for Scatter Plot (or whatever the title of the visualization is) and the column names of the selected axes. This dialog allows you to decide for which properties the end user of the Guide should provide input.

Note: Only properties that you have used in your current version of the plot will be available. Hence, if you want the end user of the Guide to be able to select by which column to color by, you must make sure that you have selected some column in the Properties dialog of the visualization (in DecisionSite). Also note that prompting is not supported for multiple color bands in pie charts.

Prompt for Scatter Plot - Signal for S16_1year_1.txt vs. Detection p-v X				
Prompt user for:	Title for input field in prompt dialog:			
🔽 X-axis	X-axis:			
🔽 Y-axis	Y-axis:			
Color by	Color by:			
Shape by	Shape by:			
Labels by	Labels by:			
🗖 Size by	Size by:			
Drawing order by	Drawing order by:			
Rotate by	Rotate by:			
Line connection by	Line connection by:			
Connect order by	Connect order by:			
Help	OK Cancel			

Option	Description
Prompt user for	Select the check box for each of the properties that you want the end user of the Guide to be able to specify upon running the Guide. Note: If you want the end user of the Guide to use exactly the same settings as your current visualization, you should not allow any prompting at all.
Title for input field in prompt dialog	Enter a descriptive title to be shown in the Settings for dialog of the selected visualization. This is what the end user of the Guide will see above the drop-down list for each selected property.

► To reach the Prompt for... dialog:

1. Create visualizations and edit their properties in DecisionSite (**Edit** > **Properties** in main application).

- 2. Add a link that creates one or more visualizations to the Guide.
- 3. In the Link Properties dialog of the desired link, click to select the visualization that you want to add prompting for.
- 4. Click **Prompts...**.

9.5.3.7 Settings for... Dialog

The Settings for... dialog is displayed when running a Guide that includes prompted steps. It is specific to each visualization in a link. If you have selected a heat map, the dialog will be called Settings for Heat Map.

This dialog allows the end user of a Guide to select to certain properties for a specific visualization at run-time of the Guide. Only the properties specified by the creator of the Guide will be available.

Settings for Heat Map	2	<
Available Columns: Name Signal for S18_1year_3.txt Detection for S16_1year_1.t Detection for S17_1year_2.t Detection for S18_1year_3.t Detection p-value for S16_1y Detection p-value for S18_1y FileName for S16_1year_1.tb FileName for S16_1year_3.tb V M M Order By:	Columns: Name Type 5 Months (Average), Z Dec 1 Year (Average), Z Sc Dec 4 Weeks (Average), Z Sc Dec 1 Week (Average), Z Sc Dec 1 Week (Average), Z Dec Embryonic (Average), Z Dec Embryonic (Average), Z Dec	
Hierarchical Clustering (order)	•	
Help	OK Cancel	

This dialog varies depending on both the type of visualization and the selections that you have made in the Prompt for.. dialog.

Example:

A data set containing height, weight and eye color of a group of men and women is opened in DecisionSite and two visualizations are created; The first visualization is a scatter plot with height on the X-axis and weight on the Y-axis, and the markers are colored by eye color and sized by gender. The second visualization is a table showing all available columns in the data set.



A Guide created using Analysis Builder can be edited to prompt its end user to specify certain visualization settings as indicated below:

Settings in Properties dialog for visualization (in DecisionSite):

Color	Sice	
By Distant	Hn	- H.
C Bied C Contingour F Calegorical	Br gender	*
Custorigs Shog develocted	Digwing order	
Shape	By Norel	
F Foad Durlogice	- ERM	
C BK Free color	Note j	- MI
Labels	Bolate	
(F Bane	By [None]	
C Malighteoords	Line convection	
	By [None]	
By nessor	Order [None]	

The Properties dialog of a scatter plot.



Phoreph user for:	Title for input field in prompt dialog:
R X-min	Select X-mit
P Valia	Fielect Y-war
Colorby	Color makers by the values in the following column:
5 Sim by	are noted to be released with the ego true

Here, the scatter plot properties that were set to something other than [None], that is, Color and Size, together with the axisselections, are shown as possible prompts. The creator of this Guide has determined that the size should always be set by gender as she specified when she created the original scatter plot, so this check box is not selected in the Prompt for... dialog.

displayed upon running Guide:

Select X-ant: Iteict4 (m)			
Select Y-asic			
weight (kg)			1
Color markers by the val	as in the following	calumn	
tele com			-

The resulting Settings for... dialog shows the three selected prompt lists upon running the Guide. The titles of the lists are the ones entered by the Guide creator in the Prompt for ... dialog.



The Properties dialog of a table visualization.



In this case, the only setting that had been modified was the columns displayed in the table. Hence, this is the only item available for prompting in the Prompt for... dialog.

lare	Type		Name	Type
ige veight (Fg)	Integer Decinal)) (1)	erye tolor gender height (m)	String String Dedmail
		-		

If the selected prompt item is a list of columns, the resulting Settings for ... dialog will contain two list boxes where the end user of the Guide can move columns from Available Columns to Used Columns using the arrows >> and <<, and also sort the columns with the up and down arrows.

To reach the Settings for... dialog during development of a Guide:

- 1. Add one or more prompt steps to a visualization link using the Prompt for... dialog.
- 2. Select **Guide > Run** from the Analysis Builder menu.
- 3. Step through the Guide to locate the edited visualization link and click on it.

9.5.3.8 Guide Properties Dialog

The Guide Properties dialog controls important properties like the title and ToolTip of the Guide after it has been deployed to a server. It is recommended that you fill in all fields of the Guide Properties to facilitate efficient administration of Guides on the server.

🧿 Guide Properti	es	×			
		,			
<u>T</u> itle:	Create bar chart				
D <u>e</u> scription:					
This is a guide the creates a bar cha	at bins data into a user-specified number of bins and art visualization with the bins on the x-axis.				
T <u>o</u> olTip:	eates a bar chart by binning data into even intervals				
<u>K</u> eywords:	bar chart binning				
<u>A</u> uthor:	Charlie Brown				
<u>C</u> ompany:	ACME Industries				
Don't show this dialog when saving guide					
<u>H</u> elp	OK Cancel				

Option	Description
Title	The title of your Guide as it will be displayed in the Guides pane when it is published to a server. The title is also displayed in the flight view when you are running the Guide. It is important that the title is informative with regards to what the Guide really does. If the Guide will be published to a server, no characters other than a- z, A-Z, 0-9, ! $(),; _{ } $ and blank spaces should be used in this field due to restrictions in DecisionSite Builder.
Description	A description of the functions of the Guide. The description can make it easier for the server administrator to group similar Guides together and remove duplicates, etc.
ToolTip	A short description of the Guide to be displayed as a ToolTip when you hover with the mouse pointer over the Guide title in the Guides pane. Example: "Creates a bar chart by binning data into even intervals"
Keywords	Keywords specific to the contents of the Guide. Keywords are separated by semicolon, i.e., if you write "bar chart binning" it will be interpreted as a single keyword. To produce two keywords the words must be separated with semicolon. Hence, "bar chart ;binning" will result in the two keywords "bar chart" and "binning".

Author	The name of the Guide author. The default value is the user name that you used when logging in to DecisionSite Analytics Server. The author name can be especially important to your IT personnel if they want to perform any changes to your Guide and want to check with you that their changes are correct.
Company	The company for which you have created the Guide. This is commonly used in the package name of the Guide resource when the Guide is deployed to a server. If the Guide will be published to a server, no characters other than a-z, A-Z, 0-9, $! (),; _{ } { } ~ and blank spaces should be used in this field due to restrictions in DS Builder.$
Don't show this dialog when saving Guide	Select this check box if you do not want to see this dialog automatically when you are saving your Guides.

► To reach the Guide Properties dialog:

In Analysis Builder, click Guide > Properties.

9.5.3.9 Tool Option Dialog

O Tool Option	×
There are two ways to launch the selected tool: "New Column from Expression (Calculated Column)"	
What should happen when the user clicks the link? Bun the tool, using the settings from this analysis	
© Display the tool dialog, so the user can provide input	
Help OK Cancel	

Option

Description

Run the tool, using The tool will be run silently (without any input from the end user of the settings from this the Guide) using the same settings that you used in your calculation. analysis

Display the tool dialog, so the user can provide input The tool is started, but the end user of the Guide must provide input and click OK in the tool dialog for any calculation to be performed.

► To reach the Tool Option dialog:

- 1. Run a tool in DecisionSite.
- 2. Add a Run-the-tool link to the Guide.
- 3. In the Link Properties dialog of the desired link, click to select the tool that you want to add prompting for.
- 4. Click **Prompts...**.

Note: In the current version of Analysis Builder, not all tools have the possibility to be run silently.

9.5.3.10 Open Guide from Library Dialog

This dialog lets you select and open a Guide that is located in the Library. To find a Guide, either look through a Library Section's content, or search for the Guide.

Note: Only Guides created with Analysis Builder are available to be opened and edited in Analysis Builder.

🧿 Open f	rom Library	×
Library	Search	
Home >	 DecisionSite for Functional Genomics 	
Туре	Title *	Description
£.		
2	Advanced microarray Guide	Example: This Guide uses a number
2	Microarray Guide	Example: This Guide shows how visua
<u>H</u> elp		<u>O</u> pen Cancel

Library tab options	Description
Library	All Guides, folders and Library Sections are listed on this tab. Note: Only Library Sections that you have access to are listed.
Open	Select the Guide you want and click Open to open it in the Guides pane (or in Analysis Builder if you have reached this dialog from there). You can also double-click the Guide to open it.
Search tab options	Description
Search tab	Use Search to search for the item you want to open.
Search for:	Enter the search string in the Search for: field and click Search . See Searching in the Library for information about search strings. If you click a folder in the Search result, you will be redirected to the Library View under the Library tab.
Look in:	Select which Library Section you want to perform your search in. Either one or all Library Sections can be searched. Only Library Sections you have access to are listed.

► To reach the Open Guide from Library dialog:

- Click Open Guide from Library in the Guides pane, or
- select **Guides > Run from Library...** from the menu, or

• in Analysis Builder, click **Guide > Open from Library...**.

Note: Opening a Guide in Analysis Builder will open the Guide for editing in Analysis Builder and not to the Guides pane as in the previous cases.

9.5.3.11 Publish to Library Wizard

9.5.3.11.1 Publish to Library Wizard: Step 1(2)

This wizard helps you to publish a Guide in the Library. Using the Library, your colleagues can use your Guide from a Library Section.

This step lets you specify where in the Library your Guide should be published. Navigate in the Library by double-clicking on Library Sections and folders.

Note: Only Guides created with Analysis Builder are available.

🧿 Publish	n to Libra	ary - Step 1(2	2)					×
Home 3	> Genera	I DecisionSit	e					
🕂 New	Folder	🗙 Delete	Properties	👷 Me	mbers			
Туре	Title 🔺				Descriptio	n		
£1								
2	Actress	es and film p	opularity		Example:	Do a drill-down	on interesti	
	F							-1
Guide <u>t</u> itle:	: F	ootball						
<u>H</u> el	P				< <u>B</u> ack	<u>N</u> ext >	Cancel	

Options	Description
New Folder	Creates a new folder where you can publish your Guide. A dialog will prompt you for the new folder name. Note: The New Folder button is only displayed inside a Library Section.
Members	Lists all users with at least read access to the current Library Section. Each Library Section has its own set of access permissions. Note: The Members button is only displayed inside a Library Section.
Guide title	The name of the Guide as it will be displayed in the Library. This title will be displayed as a link in the Guides pane. It is important that the title is informative with regards to what the Guide actually does. Note: The title can be 50 characters at the most, and the following characters are not supported: $//: * ? " <> + $ & $+ = @ # \% : ; , { [] } ^ ' ~ '$

Next > Proceeds to Publish to Library Wizard: Step 2(2) where properties can be edited further.

► To reach the Publish to Library Wizard Step 1(2) dialog:

In Analysis Builder, click Guide > Publish to Library....

9.5.3.11.2 Publish to Library Wizard: Step 2(2)

This dialog lets you enter all properties of the Guide. By using detailed properties, the organization and search capabilities in the Library are greatly enhanced.

🧿 Publish to Lib	rary - Step 2(2) 🔀
Guide title:	Football
<u>D</u> escription:	A football Guide
<u>K</u> eywords:	premier; league For multiple keywords use semicolon '';'' as separator
T <u>o</u> oltip:	Football
<u>A</u> uthor:	demo@spotfire.com
<u>C</u> ompany:	Spotfire Inc
<u>H</u> elp	< <u>B</u> ack <u>F</u> inish Cancel

Option	Description
Guide title	The name of the Guide as it will be displayed in the Library. This is the title you provided in the previous step.
Description	A description of the functions of the Guide. The description can make it easier for the server administrator to group similar Guides together and remove duplicates, etc. Note: The description can be at most 650 characters. (Certain Unicode characters may take up 6 character spaces in this regard.)
Keywords	Keywords specific to the contents of the Guide. Keywords are separated by semicolon, i.e., if you write "bar chart binning" it will be interpreted as a single keyword. To produce two keywords the words must be separated with semicolon. Hence, "bar chart;binning" will result in the two keywords "bar chart" and "binning". Keyword are used to enhance organization and search capabilities. Use keywords for precise searches.
ToolTip	A short description of the Guide to be displayed as a ToolTip when you hover with the mouse pointer over the Guide title in the Guides pane. Example: "Creates a bar chart by binning data into even

	intervals"
Author	The name of the Guide author.
Company	Here you can specify the company that owns the Guide.
Finish	Click Finish to publish your Guide and proceed to the Publish to Library: Guide Published dialog where you can find information on notify your colleagues.

► To reach the Publish to Library Wizard: Step 2(2) dialog:

- 1. In Analysis Builder, click **Guide > Publish to Library...**.
- 2. In the Publish to Library Wizard: Step 1(2), select Library location, enter a title, and click **Next** >.

9.5.3.11.3 Publish to Library: Guide Published

As soon as you have saved your Guide in the Library, a dialog window will appear with a confirmation that your Guide is published. This dialog will also include a hyperlink to the Library folder containing the Guide you just published, which you can click on to view the final result.

🧿 Guide Published	×
My Guide has been published.	
You can access the Guide from this location in the DecisionSite Library: Documentation > My Guide	Copy <u>L</u> ink
Send an email to notify users about the Guide.	Send <u>E</u> mail
<u>H</u> elp	<u><u>C</u>lose</u>

Example of a confirmation from DecisionSite Library about a published item.

Option	Description
Link	Click on the link to open the Library folder containing your published Guide.
Close	Closes the notification dialog

► To reach the Publish to Library Guide Published dialog:

- 1. In Analysis Builder, click **Guide > Publish to Library...**.
- 2. In the Publish to Library Wizard: Step 1(2), select Library location, enter a title , and click **Next** >.
- 3. Enter properties in Publish to Library Wizard: Step 2(2) and click Finish.

9.5.3.12 Menus

9.5.3.12.1 Analysis Builder Guide Menu

The Guide menu contains commands used when working with Guide files:

Option	Description		
New	Creates a new, empty Guide. This resets the <i>Guide contents</i> window but not the <i>Actions in DecisionSite</i> list.		
Open	Opens a dialog where you can select a previously saved Guide file (SFG) that you can continue to work on or modify and save as a new Guide.		
Save	Saves the current Guide as an SFG file.		
Save As	Saves the current Guide to a name and location that you specify.		
Open from Library	Opens the Open from Library dialog. This opens a Guide from the Library.		
Publish to Library	Opens the Publish to Library Wizard. Publishes the current Guide to the Library for sharing.		
Run	Launches the current Guide in the Guides pane. It is not necessary to save the Guide prior to using this command in Analysis Builder. Therefore, it is useful for iterative testing of the design of the Guide. Note: If you are testing Guide steps that include opening a data set, you will clear the current <i>Actions in DecisionSite</i> list! Make sure that you have added all steps of your current analysis to the Guide before you test the parts of the Guide that involve switching data sets.		
Properties	Opens the Guide Properties dialog.		
Exit	Closes Analysis Builder. If the current Guide has been modified, you will be prompted to cause the Guide		

9.5.3.12.2 Analysis Builder Edit Menu

The Edit menu contains commands used when working with Guide files:

Option	Description	
Move Up	Moves the currently selected text, comment, link or Page Break in the Guide contents list up one step.	
Move Down	Moves the currently selected text, comment, link or Page Break in the Guide contents list down one step.	
Delete	Deletes the selected text, comment, link or Page Break from the Guide contents list. You can also press Delete on your keyboard to perform the same function.	
Text Properties	Displays the Text Properties dialog. Comments are directly opened for editing by double-clicking on the comment.	
Link Properties	Displays the Link Properties dialog.	
Show Add Link Dialogs	Shows or hides the Link Properties dialogs that are displayed when you add a link from the Actions in DecisionSite list.	

9.5.3.12.3 Analysis Builder Add Menu

The Add menu contains the following commands:

Option	Description	
Text	Opens the Text Properties dialog where you can enter a new text which will be inserted below the currently selected item, or, if no item is selected, at the bottom of the Guide contents list. The Text Properties dialog is displayed with the default text "Enter text here".	
New Page	Creates a new page in the Guide. The beginning of the new page is labeledPage Break in the Guide contents list.	
Comment	Adds a new text box with text in italics below the currently selected item, or, if no item is selected, at the bottom of the Guide contents list. The new comment item is displayed with the default text "Click to add comment". The purpose of comments is normally to indicate that something in this Guide should be changed or added by the IT department of the Guide creators company. Therefore, comments should normally be removed before the Guide is deployed to all users.	

9.5.3.12.4 Analysis Builder Format Menu

The Format menu contains the following commands:

Option	Description
Numbered	Adds a number before the selected text, link or comment item. Subsequently following text, link or comment items on the same Guide page get the next number (2, 3), if this button is selected.
Bulleted	Adds a bullet before the selected text, link or comment item.
Indented	Indents the selected text, link or comment item.

9.5.3.12.5 Analysis Builder Help Menu

The Help menu contains the following command:

Option	Description
Analysis Builder Help	Opens this help file to the Analysis Builder Overview topic.

9.5.3.12.6 Analysis Builder Pop-up Menu

The pop-up menu which is displayed upon right-clicking on an item in the Guide contents list contains the following commands:

Option	Description
Move Up	Moves the currently selected text, comment, link or Page Break in the Guide contents list up one step.
Move Down	Moves the currently selected text, comment, link or Page Break in the Guide contents list down one step.
Delete	Deletes the selected text, comment, link or Page Break from the Guide contents list. You can also press Delete on your keyboard to perform the same function.

Text Properties Displays the Text Properties dialog. Comments are directly opened for editing by double-clicking on the comment.

Link Displays the Link Properties dialog. Properties

9.6 Publish to Library

9.6.1 Publish to Library Overview

The Publish to Library tool allows you to publish custom Guides and Analysis Builder Guides to the Library. By publishing your Guides, colleagues can use them in a convenient way. To publish Analyses and Posters, see Publishing Analyses to Library and Publishing Posters to Library.

► To publish Guides to the Library:

- 1. Select Guides > Publish to Library.
- 2. In Publish to Library Wizard Step 1(3), select if you want to publish a custom made Guide or a Guide created with Analysis Builder. Click **Next** >.
- Select the location in the Library for your Guide in Publish to Library Wizard Step 2(3). Click Next >. Navigate in the Library by using double-click on Library Sections and folders.
- 4. Enter properties of your Guide in Publish to Library Wizard Step 3(3). Click Finish.
- 5. In the Publish to Library Wizard Guide Published dialog, select if you want to notify your colleagues. In this dialog you can send an email with a link to the Guide. Response: Your Guide is published to the Library in the specified location. Anyone with read access to that Library Section can now use the Guide.

9.6.2 Publish to Library Wizard

9.6.2.1 Publish Guide to Library Wizard: Step 1(3)

This wizard helps you to publish a Guide in the Library. Using the Library, your colleagues can use your Guide from a Library Section.

Both custom made Guides and Guides created with Analysis Builder can be published with the Publish to Library Wizard.

🧿 Publish Guide to Library -	Step1(3)	×	
Which Guide do you want to pu	blish?		
• Guide saved in file from <u>Ana</u>	lysis Builder		
<u>S</u> FG File:			
		Browse	
C Guide with <u>c</u> ustom develope	ed code		
Source code <u>f</u> older:			
		Browse	
Help	< <u>B</u> ack <u>N</u> ext >	Cancel	
Option	Description		
Guide saved in file from Analysis Builder (SFG File)	To publish a Guide created with Analysis Builder, click Browse to locate the SFG file containing the Guide. Tip: You can publish Analysis Builder Guides directly in Analysis Builder.		
Guide with custom developed code (Source code folder)	To Publish a custom made Guide, click Browse to locate the folder in which it is stored. Custom made Guides are Guides not created with Analysis Builder.		
Next >	Proceeds to Publish Guide to Library Wizard: Step 2(3).		

► To reach the Publish Guide to Library Wizard: Step 1(3) dialog:

Select **Guides > Publish to Library...** from the menu.

9.6.2.2 Publish Guide to Library Wizard: Step 2(3)

This step lets you specify where in the Library your Guide should the published. Navigate in the Library by using double-click on Library Sections and folders.

0 P	Publish Guide to Library - Step2(3)				
H	<u>ome</u> >	General De	cisionSite		
G	E New	Folder 🔀	Delete 🔊 Properties 🕵 M	embers	
Ту	pe	Title 🕈		Description	
£					
2)	Actresses ar	nd film popularity	Example: Do a drill-down on interesti	
Guide title: Football					
					1
Op	otior	าร	Description		
Nev	New FolderCreates a new folder where you can publish your Guide. A dialog will prompt you for the new folder name.Note: The New Folder button is only displayed inside a Library Section.				
Me	MembersLists all users with at least read access to the current Library Section. Each Library Section has its own set of access permissions. Note: The Members button is only displayed inside a Library Section.				
Guide title The name of the Guide as it will be displayed in the Library. This title will be displayed as a link in the Guides pane. It is important that the title is informative with regards to what the Guide actually does. Note: The title can be 50 characters at the most, and the following characters are not supported: $\langle / : * ? " <> + \$ \& + = @ \# \% : ;, \{ [] \} ^ ' ~ '$					
Nex	NextWhen you have selected a location where you want to publish your Guide, click Next to continue to Publish to Library Wizard: Step 3(3)				

► To reach the Publish Guide to Library Wizard: Step 2(3) dialog:

- 1. Select **Guides > Publish to Library...** from the menu.
- 2. Select which type of Guide you want to publish in Publish Guide to Library Wizard: Step 1(3) and click **Next** >.

9.6.2.3 Publish Guide to Library Wizard: Step 3(3)

This dialog lets you to enter all properties of the Guide. By using detailed properties, the organization and search capabilities in the Library are greatly enhanced.

🧿 Publish Guide	e to Library - Step3(3)		
Guide title:	Football		
<u>D</u> escription:	Football Guide from Premier League		
<u>K</u> eywords:	premier; league For multiple keuwords use semicolon "··· as separator		
Teoltin:			
Author:	Football Guide		
<u>A</u> umoi.	demo@spotfire.com		
<u>c</u> ompany.	Spothre Inc		
<u>H</u> elp	< <u>B</u> ack <u>F</u> inish Cancel		
Option	Description		
Guide title	The name of the Guide as it will be displayed in the Library. This is the title year provided in the provinge step		
	the title you provided in the previous step.		
Description	A description of the functions of the Guide. The description can make		
	it easier for the server administrator to group similar Guides together		
	Note: The description can be at most 650 characters. (Certain		
	Unicode characters may take up 6 character spaces in this regard.)		
Keywords	Keywords specific to the contents of the Guide. Keywords are		
	interpreted as a single keyword. To produce two keywords the words		
	must be separated with semicolon. Hence, "bar chart; binning" will		
	result in the two keywords "bar chart" and "binning". Keyword are used to enhance organization and search capabilities		
	Use keywords for precise searches.		
ToolTip	A short description of the Guide to be displayed as a ToolTip when		
	you hover with the mouse pointer over the Guide title in the Guides		
	intervals"		
Author	The name of the Guide author.		
Company	Here you can specify the company that owns the Guide.		
Start page	If you are publishing a custom made Guide you need to specify which		
	file that is the start page of the Guide.		
	Publish to Library Wizard: Step 1(3).		
Finish	Click Finish to publish your Guide and proceed to the Publish to		
	Library: Guide Published dialog where you can find information on		

notify your colleagues.

► To reach the Publish Guide to Library Wizard: Step 3(3) dialog:

- 1. Select Guides > Publish to Library... from the menu.
- 2. Select which type of Guide you want to publish in Publish Guide to Library Wizard: Step 1(3) and click **Next** >.
- 3. Specify the location in the Library in Publish Guide to Library Wizard: Step 2(3) and click **Next** >.

9.6.2.4 Publish Guide to Library: Guide Published

As soon as you have saved your Guide in the Library, a dialog window will appear with a confirmation that your Guide is published. This dialog will also include a hyperlink to the Library folder containing the Guide you just published, which you can click on to view the final result.

🧿 Guide Published	×
My Guide has been published.	
You can access the Guide from this location in the DecisionSite Library: Documentation > My Guide	Copy <u>L</u> ink
Send an email to notify users about the Guide.	Send <u>E</u> mail
<u>H</u> elp	<u>Close</u>

Example of a confirmation from DecisionSite Library about a published item.

Option	Description	
Link	Click on the link to open the Library folder containing your published Guide.	
Copy Link	Copies the link to the clipboard for later use. Using the link, the Guide can easily be referenced in email discussions or from web pages or portals. Using the links retrieved with Copy Link , Guides can be accessed from any web environment using the URL and name supplied.	
Send Email	Launches a new email with your default email client.	
Close	Closes the notification dialog	

If you want to send an email notification, click on the **Send Email** button. This opens an email dialog where you may enter:

- To: The email address of one or more recipients, separated by comma or semicolon.
- From: Your own email address, mandatory.
- **Subject:** The subject of the email.
- **Comment:** Any additional text you wish to appear in the email.

To reach the Publish Guide to Library Wizard: Guide Published dialog:

1. Select Guides > Publish to Library... from the menu.

- 2. Select which type of Guide you want to publish in Publish Guide to Library Wizard: Step 1(3) and click **Next** >.
- 3. Specify the location in the Library in Publish Guide to Library Wizard: Step 2(3) and click **Next** >.
- 4. Edit the Guide properties in Publish Guide to Library Wizard: Step 3(3) and click **Finish**.

10 Saving and Exporting Data

10.1 Saving SFS files

Save your Analysis by selecting **Save As...** in the **File** menu. Make sure that **Spotfire Analysis File** (*.sfs) is selected in the **Save as type** list box.

How the data is stored

If the data was loaded from a source other than the clipboard, you will get an option on how to save the actual data used in the Spotfire DecisionSite session. There are two options available:

- Saving a link to the data in a *dynamic* report file (Linked) no actual data is stored in the SFS file, merely a reference describing how to retrieve, and how to view the data.
- Saving the data in a *static* report file (Embedded) the actual data used in the session is saved in the SFS file. This is the only option available if the data was loaded from the clipboard.

Analysis Settings		×	
Data content:			
Create link to latest external data (Linked)			
Include all data in the analysis file (Embedded)			
Help	OK	Cancel	

For a number of reasons, saving the data as an SFS file with Linked data should be the preferred method, since it:

- Ensures data integrity avoids inconsistencies.
- Reduces the file size essential if you want to distribute the data.
- Ensures that the data is up-to-date.

However, since a link only references its data source, the dynamic SFS file is not good if the actual data is removed or damaged.

Files with column names that contain characters that could be interpreted as column separators, e.g., comma, semicolon, tab, etc., should always be saved with linked data to prevent Spotfire DecisionSite from finding the wrong column separators when reopening the file. If you must save the data embedded within the file, you can prevent the problem by saving the data as a TXT, SKV, or CSV file and opening it with the import agent. Column names should never contain characters that can be interpreted as column separators.

The saved link includes the file name if the data was imported from a text file, or the ODBC data source name and the SQL query used if the data was retrieved from a database using ODBC.

The way the data was saved has some implications on how the Analysis can be used and how it will behave:

- If the data itself is saved in the Analysis, the session becomes static. In other words, if the source for the data is updated, the Analysis will still show the old data. If only a link to the data was saved, the Analysis reflects all changes made to the data source each time the file is opened.
- If the Analysis is to be distributed, the recipients must have access to the data source to be able to link to the data. Static report files containing the actual data create no distribution problems.
- A static SFS file is considerably larger than a dynamic SFS file, since the latter only contains a link to the data.

10.2 Spotfire Files

10.2.1 SFS Files

All information and settings in a Spotfire DecisionSite session can be saved as a Spotfire Analysis File. This file has the file extension *.sfs*, and contains information such as:

- Current settings of the query devices, both selected values and the query device types
- Visualizations
- Coloring schemes
- Information on how to regenerate derived columns, i.e., those created by calculation and binning
- Attached background image files
- Data (either as a reference to a data source, or embedded in the Spotfire Analysis File)

By saving your current session as an Spotfire Analysis File, you can pick up your work later exactly where you left it off.

The handling of Spotfire Analysis Files differs depending on whether you include the data set in the Analysis (static SFS file), or reference the data with a link (dynamic SFS file).

10.2.2 SFT Files

SFT (Template) files are like Spotfire Analysis Files but are used as templates for quickly applying a whole range of visualization settings to a new data set.

► To create a template:

- 1. Open a data file.
- 2. Make the required visualization settings (query devices, coloring, multiple visualizations, etc).
- 3. Select File > Save As...
- 4. Enter a name for the template.
- 5. From Save as type, select Spotfire Template Files.
- 6. Click OK.

For a template file to work properly, it should only be applied to data with the same column names as the data set used to create the template. If applied to a data set with different column names, only those settings that are independent of column name will be used (e.g., visualization types, fixed color, fixed shape, size and jittering, but not query device settings, Color by, etc.). **Note:** Columns created from marked records cannot be saved in templates (SFT files).

► To apply a template:

- 1. Open a data file.
- 2. Select File > Apply Template.
- 3. Select an SFT file.
- 4. Click **OK**.

You can use any SFS file in the same way as a template file, applying the settings in the Spotfire Analysis File to your loaded data set. Use the procedure described above, but select an Spotfire Analysis File instead of SFT.

Note: The Spotfire Interactive Report Settings dialog allows you to save your visualization settings only in Spotfire DecisionSite version 7.x. In newer versions, all settings are always included in a template.

10.2.3 SFA Files

In their most simple form, SFA (Spotfire Application) files are identical to Spotfire Analysis Files. You can save your Analysis as an SFA file and open that file again just like an Spotfire Analysis File. The only difference is that when you open an SFA file, the resulting Analysis is not automatically associated with that same file. You can only save it by using **Save As** and enter a name. This helps you avoid accidentally over-writing the application file.

However, SFA files can also incorporate an application that is launched when opening the file. This application, implemented using scripts and possibly involving a visible user interface, could for instance establish database connections and perform preprocessing. The benefit is that you can fetch the data, preprocess it, and get exactly the initial visualization that you want—all by just double-clicking a file icon.

Please contact the Spotfire Central for more information on how to integrate code in SFA files.

10.2.4 Version 8.0 and Prior

For legacy reasons you can also save your Analysis as Spotfire DecisionSite 8.0 and version 7 files. There are two kinds of files used in older versions of Spotfire DecisionSite, SFS and XSF files.

Spotfire File, version 8.0 (*.sfs)

The 8.0 file is actually an 8.1 file with the possibility to be opened in a DecisionSite 8.0 environment. Data will always be embedded if you select this option (linked data is not supported).

Spotfire File, version 7 (*.sfs)

This format saves a binary SFS file in the same format as version 7.3 and is only recommended for files that must be backward compatible with Spotfire DecisionSite version 7. Linked data is not supported.

XSF Files, version 7 (*.xsf)

XSF files store exactly the same information as SFS files, but in an XML based format. Since the files are in text format rather than binary, they can be searched from a file system. XML also makes the structure of the content more clear.

10.2.5 Spotfire DecisionSite Mapping Files (SFM Files)

The Spotfire DecisionSite mapping file (*.sfm) format first establishes a coordinate system, which relates the data set's coordinate system to that of the polygon set being defined. After that, a number of polygons are defined. A polygon is defined by a fill color, an origin point, a border color, the number of points and the X, Y, and Z coordinates of the points. The Z coordinates are ignored, but they must be included. The format of the file as follows (with variables in italics):

```
COORDSYS xmin xmax ymin ymax zmin zmax
ADD
POLY fillcolor xorigin yorigin zorigin
!yes
numberofpoints
x1 y1 z1
x2 y2 z2
...
```

A sample file could look as follows:

```
COORDSYS 0.0 1.0 0.0 1.0 0.0 1.0
ADD
POLY LimeGreen 0.0 0.0 -0.02 0.0
!yes
5
0.677419 0.976261 0.0
0.680645 0.977745 0.0
0.680645 0.983680 0.0
0.677419 0.985163 0.0
0.677419 0.988131 0.0
```

The *env.sfm* file in the Spotfire DecisionSite distribution serves as an example of this background map format.

To map a data file to a Spotfire mapping file:

In your visualization, select the two axes from the data that serve as coordinates.

In the **Data and Background** tab in the **Properties** dialog, select an SFM file which has a coordinate system matching the coordinates in the axes file.

10.3 Publish Analysis to Library

10.3.1 Publishing Analyses to the Library

Using the Library, you and your colleagues can collaborate on the same Analysis, keeping everyone up to date. When publishing your Analysis, everything you save in a DecisionSite file (SFS) is stored in the Library.

Note: The Open from Library functionality is not available if you are working offline (without a connection to a server).

► How to publish an Analysis to the DecisionSite Library:

- 1. Start DecisionSite and open a data set.
- 2. Select File > Publish Analysis to Library....

Response: The first step of the wizard is displayed.

Comment: This step lets you specify where in the Library your Analysis should be published. Navigate in the Library by using double-click on Library Sections and folders to the location you want publish your Analysis to. Only Analyses, folders, and Library Sections are visible in this view.

3. Enter the name of your Analysis in **Analysis title** as it will be displayed in the Library. Comment: It is important that the title is informative with regards to what the Analysis actually does. The title can be 50 characters at the most, and following characters are not supported:

\/:*?"<>+|\$&+=@#%:;,{[]}^^'~'

4. Click **Next** >.

Response: The second step of the wizard is displayed.

Comment: This dialog lets you enter properties of the Analysis. By designating detailed properties, the organization and search capabilities in the Library are greatly enhanced.

- 5. Enter a **Description** of the functions of the Analysis.
- 6. Enter Keywords specific to the content of the Analysis.

Comment: Keywords are separated by a semicolon, i.e., if you write "primary screening; quality" this will be two keywords, "primary screening" and "quality".

7. Use the **Data content** radio buttons to specify how you want to include your Analysis data. The options are:

"Linked (Load data from the data source)" Use this option when your data resides in a data source always accessible to all users with read access of your published Analysis.

"Embedded (Save the current data set in the Analysis)" Use this option when your data cannot be accessed by all users.

8. Click Finish.

Response: The Analysis is published and the confirmation dialog for the wizard is displayed. This dialog also includes a hyperlink to the Library folder containing the Analysis you just published, which you can click on to view the final result.

10.3.2 Publish Analysis to Library Wizard: Step 1(2)

This wizard helps you to publish your Analysis to the Library. Using the Library, you and your colleagues can collaborate on the same Analysis, keeping everyone up to date. Everything you save in your DecisionSite file (SFS) is stored in the Library.

This step lets you specify where in the Library your Analysis should be published. Navigate in the Library by using double-click on Library Sections and folders.

Publish Analysis to Li	brary - Step 1(2)	×	
<u>Home</u> > General Deci	sionSite		
🖅 New Folder 🛛 🗙 D	elete 🛛 Properties 🕵 M	embers	
Type Title *		Description	
€			
Baseball data	а	Example: Check out baseball statistic	
Environment	data	Example: Explore the deposit of hea	
European de	mographics	Example: European demographic dat	
Caser experi	ments	Example: A laser experiment containi	
🧕 The periodic	table	Example: A reference of the periodic	
Analysis <u>t</u> itle: The perio	odic table		
Help Kext > Cancel			
Library tab options	Description		
New folder	Creates a new folder will prompt you for	r where you can publish your Analysis. A dialo the new folder name.	
Delete	Deletes a selected item permanently from the Library.		
Properties	Use Properties to ed as folders.	Use Properties to edit the properties of selected Library items such as folders.	
Members	Displays a list of all Library Section. Eac permissions.	Displays a list of all users with at least read access to the current Library Section. Each Library Section has its own set of access permissions.	
Analysis title	alysis titleThe name of the Analysis as it will be displayed in the Library. It important that the title is informative with regards to what the Analysis actually does.Note: The title can be 50 characters at the most, and the following		
	characters are not su	ipponea.	

 $\setminus /: * ? " <> + |$ & = @ # % ; , { [] } ^ ' ~ '

Next

Select the folder in which you want to publish your Analysis, and click **Next** to proceed to Publish Analysis to Library: Step 2(2). You can also select an existing Analysis if you want to overwrite it.

► To reach the Publish Analysis to Library: Step 1(2) dialog:

Click File > Publish Analysis to Library....

10.3.3 Publish Analysis to Library Wizard: Step 2(2)

This dialog lets you enter all properties of the Analysis. By using detailed properties, the organization and search capabilities in the Library are greatly enhanced.

🧿 Publish Analy	ysis to Library - Step 2(2)	
Analysis title:	The periodic table	
<u>D</u> escription:	Example: A reference of the periodic table.	
<u>K</u> eywords:	periodic; chemistry	
	For multiple keywords use semicolon ";" as separator	
Data content:	C Linked (Load data from the data source)	
	• Embedded (Save the current dataset in the Analysis)	
<u>H</u> elp	< <u>B</u> ack <u>F</u> inish Cancel	
Option	Description	
Analysis title	The name of the Analysis as it will be displayed in the Library is the title you provided in the previous step.	7. This
Description	A description of the functions of the Analysis. The description contain detailed information about the Analysis enabling quic overviews.	n could k
Keywords	Keywords specific to the content of the Analysis. Keywords a separated by a semicolon, i.e., if you write "primary screening quality" this will be two keywords, "primary screening" and "quality".	re ;;
Data carta-t	Use the Date content radio buttone to encode how we want to	nues.
Data content	include your Analysis data. The options are:)
	"Linked (Load data from the data source)" Use this option wh data resides in a data source always accessible to all users wit access of your published Analysis.	en your h read

 "Embedded (Save the current data set in the Analysis)" Use this option when your data cannot be accessed by all users. The "Linked (Load data from the data source)" option might be disabled. This happens when it is impossible to maintain a link.
 Finish Click Finish to publish your Analysis. When your Analysis is published, the Publish Analysis to Library: Analysis Published dialog is shown.

► To reach the Publish Analysis to Library: Step 2(2) dialog:

- 1. Click File > Publish Analysis to Library....
- 2. In the Publish Analysis to Library: Step 1(2), select Library location, enter a title, and click **Next** >.

10.3.4 Publish Analysis to Library: Analysis Published

As soon as you have saved your Analysis in the Library, a dialog window will appear with a confirmation that your Analysis is published. This dialog will also have a hyperlink to the Library folder containing the Analysis you just published, which you can click on to view the final result.

🧿 Analysis Publish	ed	×
Yield results has bee	en published.	
You can access the DecisionSite for Yiel	Analysis from this location in the DecisionSite Library: <u>d analysis > Yield results</u>	Copy <u>L</u> ink
🖅 Send an em	ail to notify users about the Analysis.	Send <u>E</u> mail
<u>H</u> elp		Close
Option	Description	
Link	Click on the link to open the Library f published Analysis.	older containing your
Copy Link	Copies the link to the clipboard for lat Analysis can easily be referenced in ea	er use. Using the link, mail discussions or fro

	Analyses can be accessed from any web environment using t URL and name supplied.	
Send Email	Launches a new email with your default email client.	
Close	Closes the notification dialog	

pages or portals. Using the links retrieved with **Copy Link**

If you want to send an email notification, click on the **Send Email** button. This opens an email dialog where you may enter:

- To: The email address of one or more recipients, separated by comma or semicolon.
- From: Your own email address, mandatory.
- **Subject:** The subject of the email.
- Comment: Any additional text you wish to appear in the email.

To reach the Publish to Library Wizard: Analysis Published dialog:

- 1. Click File > Publish Analysis to Library....
- 2. In the Publish Analysis to Library: Step 1(2), select Library location, enter a title and click **Next** >.
- 3. Edit the Analysis properties in Publish Analysis to Library: Step 2(2) and click Finish.

10.4 Publish Poster to Library

10.4.1 Publishing Posters to the Library

Publishing a DecisionSite Poster of your Analysis enables your colleagues to participate in your decision process from a Microsoft® Internet Explorer window.

Note: The Library functionality is not available if you are working offline (without a connection to a server).

Note: To open this tool and publish DecisionSite Posters, a license is required. Please contact your DecisionSite Administrator for more information.

▶ How to publish a Poster to the DecisionSite Library:

- 1. Start DecisionSite Client and open a data set.
- 2. Create the visualizations you want, and adjust the query devices to filter out data the way you want it in your Poster.
- 3. Select File > Publish Poster to Library....

Comment: You need a DecisionSite Poster license to see this option. Response: The first step of the wizard is displayed. A dialog about unsupported features may appear. Please see below for more information.

4. Use the dialog to specify which parts of the Analysis you want to include in the Poster. Select the **Visualizations** you want to include.

Comment: See Poster Visualizations for more information. The visualizations in the Poster can be displayed either as a vertical list of large plots, or tiled smaller plots next to each other.

5. Select whether or not you wish to Use list layout as default view mode.

Comment: If the visualizations in DecisionSite Client are tiled, the Publish Poster to Library tool will try to emulate the layout by default. The person looking at the published Poster can switch between Tiled and List layout.

6. Select the **Query Devices** you want to enable data filtering with.

Comment: See the Poster Query Devices for more information.

7. Select which type of **Details-on-Demand** you want to present; either Table or Web search.

Comment: See Poster Details-on-Demand for more information.

- When your Poster is designed, click Next >.
 Response: The second step of the wizard is displayed.
- 9. Select the Library Section and folder you want the Poster to be published in.
- Enter a Poster title as it will be displayed in the Library.
 Comment: It is important that the title is informative with regards to what the Analysis actually does. The title can be 50 characters at the most, and the following characters are not supported:

11. Click Next >.

Response: The third step of the wizard is displayed.

Comment: This dialog lets you enter properties of the Poster. By designating detailed properties, the organization and search capabilities in the Library are greatly enhanced.

- 12. Enter a **Description** of the purpose of the Poster.
- Enter Keywords specific to the content of the Poster.
 Comment: Keywords are separated by a semicolon, i.e., if you write "primary screening; quality" this will be two keywords, "primary screening" and "quality".
- 14. Use the **Data content** radio buttons to specify how you want to include your Poster data. The options are:

"Linked (Load data from the Information Link)" Use this option when your data resides in an Information Link accessible to all users with read access to your published Poster.

"Embedded (Save the current data set in the Poster)" Use this option when your data cannot be accessed by all users.

15. Click Finish.

Response: The Poster is published and the confirmation dialog for the wizard will appear, asking if you want to send an email notification to your colleagues. This dialog also includes a hyperlink to the Library folder containing the Poster you just published, which you can click on to view the final result.

10.4.2 Publish Poster to Library Wizard: Step 1(3)

Using this wizard you can publish a DecisionSite Poster of your Analysis, enabling your colleagues to participate in the decision process from a Microsoft[®] Internet Explorer window. Use Spotfire DecisionSite Client to create the visualizations you want, and adjust the query devices to filter out the data you want in your Poster. Launch the Publish Poster wizard by selecting **File > Publish Poster to Library...**

Note: Your need a license for DecisionSite Posters to use this feature.

Use the dialog to specify which parts of the Analysis you want to include in the Poster.

9 Publish Poster to Library	- Step 1(3)			×
<u>V</u> isualizations:		Query devices:		
Genre vs Income	•	Actress (Item Slid	ler)	•
<u>A</u> dd↓ Ad <u>d</u> →	<u>R</u> emove	Add	lemove	
🤔 Market	Share !	Year		
		Length		
🔀 Genre Length	🚹 Genre Popularity	Litle Subject		
		Actor		
		Details- <u>o</u> n-Demar	nd T	
Visualization default layout:	_	Table		<u>C</u> onfigure
• 💾 <u>I</u> iled • 🔲	🖞 Scrollable list			
Help			<u>N</u> ext >	Cancel
Option	Description			
Visualizations	Select the visual	izations of you	ur Analysis you	u want to include in

Visualization default layoutThe visualizations in the Poster can be displayed either as a scrollable list of large plots, or tiled smaller plots next to each other. Select which default layout you want. A exclamation mark icon means that some aspect of that visualization is not supported in DecisionSite Posters. Move the mouse cursor over the icon to display more information.Query devicesSelect the Query Devices you want to enable data filtering with. See Poster Query Devices for more information.Details-on-DemandSelect which type of Details-on-Demand that you want to present; either Table or Web search. See Poster Details-on-Demand for more information.NextWhen your Poster is designed, click Next > to proceed publishing.		your Poster. See Poster Visualizations for more information.
Query devicesSelect the Query Devices you want to enable data filtering with. See Poster Query Devices for more information.Details-on-DemandSelect which type of Details-on-Demand that you want to present; either Table or Web search. See Poster Details-on-Demand for more information.NextWhen your Poster is designed, click Next > to proceed publishing.	Visualization default layout	The visualizations in the Poster can be displayed either as a scrollable list of large plots, or tiled smaller plots next to each other. Select which default layout you want. A exclamation mark icon means that some aspect of that visualization is not supported in DecisionSite Posters. Move the mouse cursor over the icon to display more information.
Details-on-DemandSelect which type of Details-on-Demand that you want to present; either Table or Web search. See Poster Details-on-Demand for more information.NextWhen your Poster is designed, click Next > to proceed publishing.	Query devices	Select the Query Devices you want to enable data filtering with. See Poster Query Devices for more information.
Next When your Poster is designed, click Next > to proceed publishing.	Details-on-Demand	Select which type of Details-on-Demand that you want to present; either Table or Web search. See Poster Details-on-Demand for more information.
	Next	When your Poster is designed, click Next > to proceed publishing.

For information about which features can be included in a DecisionSite Poster, see Poster Supported Features.

► To reach the Publish Poster to Library – Step 1(3) dialog:

Click File > Publish Poster to Library....

10.4.3 Publish Poster to Library Wizard: Step 2(3)

In this step you specify where in the Library your DecisionSite Poster should be published. Navigate in the Library by using double-click on Library Sections and folders.

	n Poster to Library	- Step 2(3)				×
<u>Home</u>	> <u>Sales and Mark</u>	<u>etinq</u> > Entertainmen ^t	t			
🕂 Nev	Folder 🔀 Dele	te 🔊 Properties	🖳 Members			
Туре	Title 🕈	Description	Mod	ified By	Modified	
t.						
	. Martin Arrahatia					
oster <u>t</u> itle	e: [Movie Analysis					
	-					
<u>H</u> e	Þ		< <u>B</u> ack	<u>N</u> ext >	Cancel	
<u>H</u> e	p		< <u>B</u> ack	<u>N</u> ext >	Cancel	
<u>H</u> e Pptio	ns	Description	< <u>B</u> ack	<u>N</u> ext >	Cancel	
<u>H</u> e P ptio ew Fo	Þ NS Ider	Description Creates a new f will prompt you	< <u>Back</u> n older where y about the ne	<u>N</u> ext > ou can pub w folder na	Lish your Poster me.	 r. A
He Pption ew Fo elete	P ns Ider	Description Creates a new f will prompt you Deletes a select	< <u>Back</u> Colder where y about the ne ed item perma	Next > ou can pub w folder na anently fror	Lish your Poster me. n the Library.	r. A

Properties	Use Properties to edit the properties of selected Library items such as folders.
Members	Lists all users who have at least read access to the current Library Section. Each Library Section has its own set of access permissions.
Poster title	The name of the Poster as it will be displayed in the Library. It is important that the title is informative with regards to what the Poster actually does. Note: The title can be 50 characters at the most, and the following
	characters are not supported: $/: *? " <> + $ & = @ # %; , { [] } ^ ' ~ ``
Next	Select the folder in which you want to publish your Poster and click Next to proceed to Publish Poster to Library – Step 3(3). You can also select an existing Poster if you want to overwrite it.

► To reach the Publish Poster to Library – Step 2(3) dialog:

- 1. Click File > Publish Poster to Library....
- Design your DecisionSite Poster in Publish Poster to Library Step 1(3) and click Next >.

10.4.4 Publish Poster to Library Wizard: Step 3(3)

This dialog lets you enter properties of the Poster. By using detailed properties, the organization and search capabilities in the Library are greatly enhanced.

You also specify how the data should be handled here. See Poster data for more information.

Publish Poste	
Poster title:	Movie Analysis
<u>D</u> escription:	This Poster shows correlations between genres and other factors.
<u>K</u> eywords:	move;genre For multiple keywords use semicolon '';'' as separator
Data content:	 Linked (Load data from the Information Link) Embedded (Save the current data set in the Poster) Note: Marked records can only be included for embedded data
Help	< <u>B</u> ack <u>F</u> inish Cancel
<u>Help</u>	< <u>Back</u> <u>Finish</u> Cancel Description
<u>H</u> elp Dption Poster title	< Back

	contain detailed information about the Poster enabling a quick overview.
Keywords	Keywords specific to the content of the Poster. Keywords are separated by a semicolon, i.e., if you write "primary screening; quality" this will be two keywords, "primary screening" and "quality". Keywords are used to enhance organization and search capabilities.
Data content	Use the Data content radio buttons to specify how you want to include your Poster data. The options are: "Linked (Load data from the Information Link)" Use this option when your data resides in an Information Link accessible to all users with read access to your published Poster. "Embedded (Save the current data set in the Poster)" Use this option when your data cannot be accessed by all users. The "Linked (Load data from the Information Link)" option will be disabled unless an Information Link was used to open the data. See Poster Data for more information.
Finish	Click Finish to publish your Poster. When your Poster has been published, Publish Poster to Library Wizard: Poster Published is shown, in which you can send emails inviting colleagues to join your analysis.

► To reach the Publish Poster to Library – Step 2(2) dialog:

- 1. Click File > Publish Poster to Library....
- 2. Design your DecisionSite Poster in Publish Poster to Library Wizard: Step 1(3) and click **Next** >.
- 3. Edit the Poster properties in Publish Poster to Library Wizard: Step 2(3) and click **Next** >.

10.4.5 Publish Poster to Library: Poster Published

As soon as you have published your Poster in the Library, a dialog will appear asking if you want to send an email notification to your colleagues. This dialog will also have a hyperlink to the item you just published, which you can click on to view the final result.

Poster Published		×
Movie Analysis has be	een published.	
You can access the F <u>Sales and Marketing :</u>	Poster via this link: <u>> Entertainment > Movie Analysis</u>	Copy <u>L</u> ink
🖅 Send an emai	il to notify users about the Poster.	Send <u>E</u> mail
<u>H</u> elp		Close
Option	Description	

Option	Description
Link	Click the link to open your Poster and view the result.
Copy Link	Copies the link to the clipboard for later use. Using the link, the Poster can easily be referenced in email discussions or from web
pages or portals. Using the links retrieved with **Copy Link**, Posters can be accessed from any web environment using the URL and name supplied. Send Email Opens a dialog from which you can send an email with a link to the Poster. Closes the notification dialog Close

If you want to send an email notification, click on the **Send Email** button. This opens an email dialog where you may enter:

- To: The email address of one or more recipients, separated by comma or semicolon. •
- From: Your own email address, mandatory. •
- Subject: The subject of the email. •
- **Comment:** Any additional text you wish to appear in the email. •

A new DecisionSite Poster, Movie Analysis, has been published to the DecisionSite Library. Take a look and tell me what you think.

(Click here to login to the full Spotfire DecisionSite Poster)

Login information

Spotfire DecisionSite Poster

Movie Analysis

blade, 2004-12-06

This Poster shows correlations between genres and other factors.

Clippings

Length



Example of Poster notification email.

To reach the Publish Poster to Library Wizard: Poster Published dialog:

- 1. Click File > Publish Poster to Library....
- Design your DecisionSite Poster in Publish Poster to Library Wizard: Step 1(3) and 2. click Next >.
- In the Publish Poster to Library Wizard: Step 2(3), select Library location, enter a title, 3. and click Next >.

4. Edit the Poster properties in Publish Poster to Library Wizard: Step 3(3) and click **Finish**.

10.4.6 Poster Content

10.4.6.1 Poster Visualizations

You can include one or several visualizations in your Poster. The visualizations in the Poster can be displayed either as a vertical list of large plots, or tiled smaller plots next to each other. Select whether or not you wish to **Use list layout as default view mode**.

If you choose to include several visualizations and not use the list layout as default, you can create a layout for how they should be displayed: horizontally, vertically, or a combination of the two. The default layout will try to mimic the layout as seen in DecisionSite.

Note: Not all visualizations available in Spotfire DecisionSite can be used in a Poster. Please see Poster Supported Features for more information.

► How to include visualizations:

- 1. Select a visualization from the Visualizations drop-down list.
- 2. Mark a cell in the layout section (below the drop-down list) by clicking on it.
- Click on the <u>Add</u> → button to add the new visualization below the marked cell, or click on the <u>Add</u> → button to add the new visualization adjacent to the marked cell.

► How to remove visualizations:

- 1. Mark a cell in the layout section (below the drop-down list) by clicking on it.
- 2. Click on the <u>Hemove</u> button to remove the visualization from the layout section. The visualization will be placed in the **Visualizations** drop-down list, from where you can add it again later if you wish.

10.4.6.2 Poster Query Devices

You can include one or several query devices in your Poster. If you choose to include several query devices, you can sort them in any order you like. It is recommended that you include only those query devices that are needed, so as to keep the Poster simple and straightforward. A query device that has been set to specific values in DecisionSite will keep these settings when the Poster is opened. Note that the entire data set will still be transferred to the Poster, so no data will be lost.

► How to include query devices:

- 1. Select the query device you want to add from the Query devices drop-down list.
- 2. Click on the query device in the layout section, beneath which you want the new query device to be inserted.
- 3. Click on the **Add** button to include the new query device.
- 4. Repeat steps 1 to 3 for each query device you want to include.
- If you want to remove a query device, select it from the list by clicking on it, and then click on the **Remove** button (or press the **Delete** key). **Tip:** Press **Ctrl+A** to select all query devices, or use **Ctrl+Click** or **Shift+Click** to select several query devices at once.
- If you want to change the order of the included query devices, select one by clicking on it, and move it up or down by clicking on the tor button.

10.4.6.3 Poster Details-on-Demand

There are two kinds of Details-on-Demand windows that can be included in the Poster: Table or Web Search. Select the one you want from the drop-down list.

Table

This option includes a standard Details-on-Demand window in which the information about marked records in the visualization is displayed in a table.

Web Search

The Web Search Details-on-Demand can be configured to send a query to an external web site to search for information about marked records. For example, you can link to a search engine such as Google, or an MDL ISIS database in order to view molecular structures.

You can create several customized Details-on-Demand web searches, which will appear in the drop-down list. Either you select a pre-configured one from the drop-down list, or you select the **Add new...** option which lets you configure a new Web Search Details-on-Demand.

Note: The DecisionSite administrator can setup preconfigured ISIS Direct Details-on-Demand options from the Library Administrator tool. Such options will appear in the drop-down menu automatically for all Poster authors, and can easily be selected when publishing a new Poster. Please see the *DecisionSite Installation and Upgrade manual* for information on how to do this.



Details-on-Deman	d « Previous Next »
Viewing page 1/1	. (8 total) Open
France Italy	
Norwy Spain Spain United Kingdom United Kingdom	Image: State

A Web Search Details-on-Demand can be set to show the search results directly in the Poster. This is useful for molecular structures among other things.

A Web Search Details-on-Demand can also be set to show links for the selected records, which launches a separate browser search window when clicked.

Whether the search results should be displayed directly in the details-on-demand window of the Poster, or displayed in a new browser window, can be switched from within the Poster. You cannot configure this aspect from the **Publish Poster...** wizard.

► To create a new custom Web Search:

- 1. Select Add new... from the drop-down list. A dialog appears.
- Edit the URL to the web link. Comment: For example, open www.google.com and make a search for "replaceme". Then copy the entire URL "http://www.google.com/search?hl=en&ie=UTF-8&oe=UTF-8&q=replaceme" and paste it into the Web Search field.
- 3. Enter a dollar sign within curly brackets {\$} as a placeholder for the ID variable that will be inserted from the Poster.

Comment: For example, replace the "replaceme" variable above with {\$} so that the URL reads "http://www.google.com/search?hl=en&ie=UTF-8&oe=UTF-8&q={\$}".

Comment: Anything you enter between the left bracket and the dollar sign will be placed before each ID in the query. Similarly, anything placed between the dollar sign and the right bracket will be placed after each ID in the query.

- 4. Select the **ID column** which contains the information you want to use as input to the web search.
 - Note: If you intend to link to an ISIS database, use the column with the Compound ID.
- 5. Enter a Name for the custom Details-on-Demand you have just configured. This is the name which will appear in the drop-down list.
- 6. Click OK.

► To configure a previously created Web Search:

- 1. Select the Web Search you want from the drop-down list.
- 2. Click on the **Configure...** button.
- 3. The dialog opens and you can configure the web search.
- 4. Click **OK** when you are done.

10.4.6.4 Poster Supported Features

Not all functionality available in Spotfire DecisionSite Client can be used in a Poster. When you create a Poster and your Analysis contains unsupported features, a notification dialog will be displayed with information about unsupported features.

Note: Only unsupported features used in your Analysis are shown.

itle	Details Dick have each arrested (Gusters Dick)	
i able Foottox Diot	Plot type not supported (Custom Plot) Plot type pot supported (2D Scotter Plot)	
	Flot type not supported (30 Statler Plot)	
1		
olumns that con	itain unsupported features:	
Vame	Details	
Binned Length	Contains synonyms (values and selection might diffe	er)
•		•
_		
4 01 111	essage at startup	
Show this m		
Show this m	1	
✓ <u>Show this m</u> <u>H</u> elp		Close

Columns that contain
unsupported featuresEach column with a formatting not supported is listed here.
The columns can be used in the Poster. However, no
formatting will be applied. Also, some binned columns

from older versions are not supported.

The table below explains which features and settings can be transferred to a Poster.

Note: Since version 8.0, DecisionSite Client includes a new type of Bar Chart, which replaces Bar Charts and Histograms version 7.x. Bar Charts and Histograms of version 7.x must be converted to 8.x bar charts in DecisionSite Client before being published as a Poster.

Note: All Spotfire DecisionSite users can launch Spotfire DecisionSite Client from within a Poster. This will provide full DecisionSite functionality.

Tip: Move the mouse pointer over the visualization template in the Create Poster dialog to display a ToolTip text which states any unsupported properties of the visualization.

Aspect Supported Comme

Visualizations		
2D Scatter Plot	Yes	Note: All available coloring options are not supported. See 2D Scatter Plot Markers below for more information.
3D Scatter Plot	No	
Bar Chart	Yes	
Bar Chart version 7.x	No	Needs to be converted to Bar Chart 8.x in DecisionSite Client.
Histogram version 7.x	No	Needs to be converted to Bar Chart 8.x in DecisionSite Client.
Line Chart	No	
Profile Chart	Yes	
Pie Chart	Yes	
Heat Map	Yes	Heat maps using a mixture of color ranges and categorical values, which became possible with DecisionSite Client 9.0, are not supported by DecisionSite Posters. Change the coloring to a traditional continuous range prior to publishing the Poster, if needed.
Table	No	
General Visualization Properties		
X and Y-axis labels	Yes	Labels will always appear in the Poster. Horizontal or Vertical labels can be set, but no other label settings will be transferred.
X and Y-axis grid	Yes	
Visualization Annotations	Yes	
Marked Records	Yes	Only if the data set is embedded in the Poster.
Data Range	Yes	
Margins	No	Margins will not be transferred to the Poster, but ToolTips are available on labels that are abbreviated.
HTML Details-on- Demand	No	You can create a custom Web Search when publishing the Poster.

Statistical Measures	No	
Show Deselected	No	
Trellis	Yes	
Zoom	Yes	
Query Devices		
Range Sliders	Yes	
Check Boxes	Yes	
Radio Buttons	Yes	
Item Slider	Yes	
Full Text Search	Yes	Simple Search will be interpreted as Regular Expression.
Column		
Column Annotations	Yes	Shown as a tooltip icon in the Poster query devices.
Column Transformation		
Original Scale	Yes	
Log Scale	Yes	Also note that Categorical Coloring on a transformed column is not supported. In such a case the coloring will be changed to Fixed color.
Other Scale	No	Will be transformed to Original Scale, and the selection is set to All.
2D Scatter Plot Properties		
X and Y-axis Column	Yes	
Background Image	Yes	Must be a BMP, PNG or JPG image.
Background Image Position	Yes	
2D Scatter Plot Markers		
Fixed Color	Yes	
Continuous Color	Yes/No	Note: Only continuous color schemes with two gradients, ranging from "min" to "max" are supported by Posters. Three color gradients or advanced coloring is not supported. See Advanced Color below for more information.
Categorical Color	Yes	Categorical Coloring on a transformed column is

		not supported. In such a case the coloring will be changed to Fixed color.
Advanced Coloring	No	The scatter plot in Posters only supports purely categorical color schemes, or continuous color schemes with one range (from "min" to "max"). If there is a mixture of ranges and categorical values in the scatter plot, or if it uses more than one color range, or if the scatter plot uses one color range with starting/ending points that are not "min" and "max" respectively, then the coloring is not supported. This will give a warning when trying to publish the scatter plot. The scatter plot can still be published as a Poster, but the colors will most likely be wrong.
Shape	Yes	Squares, Circles and Triangles are supported. All other markers will be transformed to filled squares.
Size	Yes	
Size By	Yes	
Drawing Order	No	
Jitter	Yes	
Rotate	No	
Line Connection	Yes	
Bar Chart Properties		
X-Axis Column	Yes	
Background Image	Yes	Must be a BMP, PNG or JPG image.
Bar Chart Bars		
Fixed Color	Yes	
Categorical Color	Yes	Categorical Coloring on a transformed column is not supported. In such a case the coloring will be changed to Fixed color.
Show deselected	No	
Width	Yes	
Outline Bars	Yes	
Labels	No	No text labels above the bars, however, bar chart tool tips displays the information found in DecisionSite Client bar labels.
Stacked bars	Yes	
Side-by-side bars	Yes	
100% stacked bars	No	
100% side-by-side bars	No	
Drop empty bars	Yes	

Binning	Yes	The number of bins in DecisionSite Client will be the same in DecisionSite Posters.
Sort bars	Yes	
Profile Chart Properties		
Numeric Columns	Yes	Supported although not together with Date, DateTime, Time.
Date, DateTime, Time Columns	Yes	Supported although not together with Numeric.
Same Scale for All	Yes	Only supported when all columns are of the same type of scale, that is, either Original scale or Log scale.
String Columns	Yes	
Background Image	Yes	Must be a BMP, PNG or JPG image.
Profile Chart Profiles		
Fixed Color	Yes	
Continuous Color	Yes	
Categorical Color	Yes	Categorical Coloring on a transformed column is not supported. In such a case the coloring will be changed to Fixed color.
Individual Scale	Yes	
Same Scale	Yes	
Labels	No	
Line Width	No	
Line Width By	No	
Break on Empty	Yes	
Pie Chart Properties		
X-Axis Column	Yes	
Y-Axis Column	Yes	
Background Image	Yes	
Pie Chart Pies		
Fixed Color	Yes	
Categorical Color	Yes	
Show deselected	No	
Average Color	Yes	Not on String Columns
Number of Color Bands	No	
Size	Yes	

Fixed Size	Yes	
Size by Records Count	Yes	
Size by Average	Yes	Only for Numeric columns.
Size by Sum	Yes	Only for Numeric columns.
Labels	No	DecisionSite Posters uses ToolTips to display this information instead.
Jitter	No	
Heat Map Properties		
Column colors	Yes	
Color range	Yes	
Advanced colors	No	If the heat map uses a mixture of continuous color ranges and categorical values it cannot be published by the Poster Designer.
Show deselected	Yes	
Row labels	Yes	
Dendrogram	Yes	

Differences between DecisionSite Client and DecisionSite Posters:

Bar Charts:

• In DecisionSite Client labels are used to display information about bars. In DecisionSite Posters this information is displayed using ToolTips when hovering over a bar.

Pie Charts:

- In DecisionSite Client labels are used to display information about sectors. In DecisionSite Posters this information is displayed using ToolTips when hovering over a sector.
- In DecisionSite Client, marking is displayed as a continuous line around the edge of a pie. In DecisionSite Posters, marking is indicated as separate lines beside each sector that has records included in the marking.

Heat Maps:

- Cluster node similarity ToolTip is not supported.
- The dendrogram menu is not supported.
- Cannot zoom in column dendrogram.

Number Formatting:

- Combining scientific notation and parentheses negative format will force negative format to default.
- Combining the parentheses negative format and default number of decimals will force two decimals. To avoid this, set the number of decimals explicitly in DecisionSite Client.
- Combining the thousands separator and default number of decimals will force two decimals. To avoid this, set the number of decimals explicitly in DecisionSite Client.

Shared Ranges:

• Some plots that use Shared Ranges look different in Posters compared to DecisionSite Client. In DecisionSite Client 9.0 and forward, shared ranges are only shared between

columns of compatible types. In Posters, as well as in earlier versions of DecisionSite Client, shared ranges could be applied to a mixture of column types.

- Compatible types are:
 - A) Numeric columns: integer, real
 - B) String columns
 - C) Date columns: date, timestamp
 - D) Time columns

In other words, if two incompatible columns use the same color scheme, their color ranges will be calculated individually in DecisionSite Client 9.0, but DecisionSite Posters will still use shared ranges.

10.4.6.5 Poster Data

You can choose from two kinds of data links. One choice is to embed the data into the Poster. That way, the data is stored within the Poster, and will not be altered if you later change the original data set.

The other alternative is only available if you have imported data into Spotfire DecisionSite by use of Information Links. If created in this way, you can choose to save the Poster with an active data link to the original data so that the Poster will always be based on the latest data, and will be (automatically) updated every time a user opens the Poster. If the range of the data should become larger after the publishing date, the entire data set will still be opened in the Poster regardless of the initial query device settings, etc.

Note: It is not possible to use the linked data option if you have added a column (binned, add columns, calculation, etc.) to a data set imported via Information Links. Also, information about which records are currently marked cannot be stored in a Poster with linked data, this is only possible using embedded data.

10.4.6.6 Poster Background Images

Scatter Plots, Bar Charts, Profile Charts and Pie Charts can display a background image behind the markers, which can be useful when working with geographical maps, etc.



BMP, PNG and JPG images that are used as background images in DecisionSite Client can be published in a Poster; other formats are invalid. Position properties set in DecisionSite Client are carried over to the Poster to align the image properly.

Background Images are particularly useful when running Spotfire Map Interaction Services. This product gives users an easy way of linking data that includes both longitudinal and latitudinal information to geographic images and data. It also provides a means to dynamically interact with geographic data within Spotfire DecisionSite.

10.5 Microsoft PowerPoint Presentation

10.5.1 Exporting Visualizations to PowerPoint

The Microsoft® PowerPoint® Presentation tool exports the selected visualizations to PowerPoint®. Each visualization is added as a new slide along with the annotation, legend and title.

Tip: Also note, other Export options can be found under the File menu.

► To export visualizations to PowerPoint®:

- 1. Create visualizations in Spotfire DecisionSite.
- 2. If necessary, edit the titles and annotations of the visualizations.
- Select File > Export > Microsoft® PowerPoint® Presentation.... Response: The Microsoft® PowerPoint® Presentation dialog is displayed.
- 4. Click to select the visualizations you want to export.

Comment: To select all visualizations click **Select All**. For multiple selection, press **Ctrl** and click on the desired visualizations or click one visualization and drag to select the subsequent ones.

- 5. Select if you want to Create a new presentation or Add to an open presentation.
- 6. If desired, select a different type of **Picture format**.

Comment: The visualization can be exported in a EMF, JPG or PNG format.

- 7. If desired, change the **Font size** of the exported labels.
- 8. Click OK.

Response: If Create a new presentation is chosen, PowerPoint® is started and the selected visualizations are shown in a new presentation. If Add to an open presentation is chosen, the selected visualizations are appended to the end of an open presentation.

Note: Microsoft® PowerPoint® must be installed on the machine for this tool to be used.

10.5.2 Microsoft PowerPoint Presentation Dialog

Microsoft® PowerPoint® Presentation	×
Select visualizations Scatter Plot Bar Chart My Data Table	
Subertrue Create a new presentation Image: Subertrue Create a new presentation Image: Subertrue Add to an open presentation My presentation.ppt Image: Subertrue Picture format: Font size: Portable Networks Graphics (png) Image: Subertrue	
Help OK Cancel	

Option	Description
Select visualizations	The list box shows the titles of all visualizations available for PowerPoint® export. Click a visualization name to include the visualization in the PowerPoint® presentation. For multiple selection, press Ctrl and click the desired visualizations.
Select All	Click this button to select all available visualizations.
Create a new presentation	This exports the Spotfire DecisionSite visualizations to a new PowerPoint® presentation.
Add to an open presentation	This appends pictures of the selected visualizations as new slides at the end of an open presentation. If several presentations are open, select one from the drop-down list box.
Picture format	Select a visualization output format from the drop-down list. Choose from PNG, JPG, or EMF formats.
Font size	Select whether to use a Small, Normal, Large or Extra Large font size when exporting to PowerPoint®. The selection made here affects all labels in the visualization, including the axis labels and the legend.

The image in the dialog shows what the PowerPoint® presentation might look like.

► To reach the Microsoft® PowerPoint® Presentation dialog:

Select File > Export > Microsoft® PowerPoint® Presentation....

10.6 Microsoft Word Presentation

10.6.1 Exporting Visualizations to Word

The Microsoft® Word Presentation tool exports the selected visualizations to Microsoft® Word. Each visualization is added to a new page in a Word document, along with the annotation, legend and title.

Tip: Also note, other Export options can be found under the File menu.

► To export visualizations to Word:

- 9. Create visualizations in Spotfire DecisionSite.
- 10. If necessary, edit the titles and annotations of the visualizations.
- Select File > Export > Microsoft® Word Presentation.....
 Response: The Microsoft® Word Presentation dialog is displayed.
- Click to select the visualizations you want to export.
 Comment: To select all visualizations click Select All. For multiple selection, press
 Ctrl and click on the desired visualizations or click one visualization and drag to select the following.
- 13. If desired, select a different type of **Picture format**. Comment: The visualization can be exported in a EMF, JPG or PNG format.
- 14. If desired, change the Font size of the exported labels.
- 15. Click OK.

Response: Word is started and a new document including the selected visualizations is displayed.

Note: Microsoft® Word must be installed on the machine for this tool to be used.

10.6.2 Microsoft Word Presentation Dialog

Scatter Plot Bar Chart	
My Data Table	
	Select All
PAGETITLE	Picture format:
	Portable Networks Graphics (.png) 💌
Lagard Bart Tatadonal - Lagard Bart Bartan - Lagard Bart Video Tatadon - Lagard Bart Video Tatadon - Lagard Bart Video Tatadon	Font size:

Option	Description
Select visualizations	The list box shows the titles of all visualizations available for Word export. Click a visualization name to include the visualization in the Word report. For multiple selection, press Ctrl and click the desired visualizations.
Select All	Click this button to select all available visualizations.
Picture format	Select a visualization output format from the drop-down list. Choose from PNG, JPG, or EMF formats.
Font size	Select whether to use a Small, Normal, Large or Extra Large font size when exporting to Word. The selection made here affects all labels in the visualization, including the axis labels and the legend.

The image in the dialog shows what the Word report might look like.

► To reach the Microsoft® Word Presentation dialog:

Select File > Export > Microsoft® Word Presentation....

10.7 Export as Web Page

10.7.1 Exporting Visualizations as a Web Page

The Export as Web Page tool exports the current visualizations as an HTML file and a set of images. You can also include the legend, annotations, the SQL query involved and information on the currently marked records.

Tip: Also note, other Export options can be found under the File menu.

► To export visualizations as a web page:

- 1. Create the desired visualizations and set the query devices. If you want to mark any records, do so now.
- 2. If you use multiple visualizations, then organize these so that they are all visible and of the right proportions.

Comment: The visualizations will be included in the report just the way you see them in the visualization area. If the visualizations are tiled, then they will appear tiled in the report. Use **Window > Auto Tile** to automatically organize your visualizations.

3. Select File > Export > Web Page....

Response: The Export as Web Page dialog is displayed.

- 4. Enter a report header. This text will appear at the top of the report.
- 5. Check the options you wish to include in the report.
- 6. Select a graphic file format for the exported images.
- 7. Click Save As...

Response: You will be prompted to select a file name and folder for the report. The report is now saved as an HTML file in the directory you specified. A subdirectory with the same name as the HTML file is created in which all the pictures are stored. To send the report to someone, you need to copy both the HTML file and its corresponding subdirectory. If you selected to **View report after saving option**, your report will be displayed in a browser.

10.7.2 Export as Web Page Dialog

🚰 Export as Web Page 🛛 🔀
Report <u>h</u> eader
My report
Include in web page
I Legend
Annotations
SQL Query
Table of marked record(s)
Pictures Output format: png 💌
✓ View report after saving
Help Save As Cancel

Option

Description

Report header	This text will appear at the top of the report.
Legend	Select this box to include the legend in the report.
Annotations	Select this box to include visualization annotations in the report. Note that column annotations are not included.
SQL Query	Select this box to include the SQL query (corresponding to the current query device settings) in the report.
Table of marked record(s)	Select this box to include a table with the currently marked records.
Output format	Select a graphics file format for the images included in the report.
View report after saving	Select this box if you want to launch the report in your default browser after it has been saved.
Save As	Click here when you have made the desired settings. You will be asked to specify a name and folder for the generated HTML file.

► To reach the Export as Web Page dialog:

Select File > Export > Web Page....

10.8 Export SDFile

10.8.1 SDFile Export Dialog

This dialog is used to export the current data set as an SDFile. In contrast to the SDFile Export tool that can be reached from the Structure Viewer, you cannot select any columns that exist in the structure connection unless they are also available in the data set.

⊙ SDFile Export		<u>×</u>	<
Molfile structure column:		Records to export:	
Structure <molfile></molfile>		 All 	
		C Marked	
Force DB compliant column names		C Selected	
Available data set columns:		Lolumns to include in SDFile:	
Column Name		Column Name	
Enter text here		Enter text here	
		LC/MS	
	Add >		
	< Remove		
	Atom Un		
	Move up		
	Move Down		
Help		OK Carcal	
- Holp		Calcer	1

Description

Option

Molfile structure column	Displays the available structure columns. Select the one you wish to export. If no structure column is available in the actual data set (for example, if you have set up a structure connection to an ISIS database and this has been shown with Structures in Table) you will not be able to export the structures using this tool. Use the Export SDFile functionality from the Structure Viewer instead.
Force DB compliant column names	Select this check box to make sure that the column names of the created SDFile are database compliant.
Records to export	Select whether to export data for All, Marked or Selected records only.
Available data set columns	Displays the available columns in the current data set in Spotfire DecisionSite.
[Enter text here]	Type any text to search for a specific column in the list.
Columns to include in SDFile	Displays the columns that you have selected to export as an SDFile.
[Enter text here]	Type any text to search for a specific column in the list.
Add >	Adds the selected columns to the list of Columns to Include in SDFile.

< Remove	Moves selected columns from the list of Columns to Include in SDFile back to the list of Available data set columns.
Move Up	Moves the selected rows in the Columns to include in SDFile list up one step. The order of the columns in this list determines the order of the columns in the resulting SDFile.
Move Down	Moves the selected rows in the Columns to include in SDFile list down one step.

► To reach the Export SDFile dialog:

Select File > Export > SDFile....

10.9 Exporting Details-on-Demand

Spotfire DecisionSite provides the possibility to export the information about the active or the marked markers. If the **Details-on-Demand (HTML)** option is selected under the **View** menu, the **File > Export > Details-on-Demand** option is available. Selecting it will launch an external browser, Netscape or Internet Explorer, in which the details of the records will be presented. **Tip:** Also note, other Export options can be found under the File menu.

10.10 Export Current Visualization

- ▶ To save an image of the current visualization to a file:
 - 1. Select File > Export > Current Visualization.

Export Visualization Options
Title Include title
Scatter Plot
Visualization Preserve aspect ratio
Width: 722 Height: 541
OK Cancel

- 2. Enter the title to be included at the top of the image.
- 3. Enter the size of the exported image. If you check **Preserve aspect ratio**, the heightwidth ratio of the exported image will be the same as that of the visualization on screen.
- 4. Click OK.
- 5. Select a location, name and format for the file. The formats available are Windows BMP, JPEG and PNG.

Tip: The current visualization can be copied to the Windows Clipboard as a vector graphic (Windows Metafile) to be pasted into another application. This is accomplished through the **Copy Special > Visualization** option under the **Edit** menu. In the Metafile format each block of text, marker, line, etc. is an independent object that can be manipulated.

10.11 Export Database Queries

The current query device settings can be exported as a SQL database query. This is done by selecting the **Export** > **SQL Query...** option from the **File** menu. When you do this, a dialog containing the query appears. The query can be edited at this stage by clicking in the edit box and entering or erasing text. By clicking **Save As...** the query can be saved to the file system.

Tip: Also note, other Export options can be found under the File menu.



10.12 Export Legend Image

This option will place an image of the legend describing the columns that are used for size, color, rotation, etc. on the Windows Clipboard.

To make this option available you must first display the Legend in Spotfire DecisionSite. There are three ways to do this:

- Select Legend command from the View menu
- Use the keyboard shortcut [Ctrl + L]
- Click the button on the toolbar



The legend in Spotfire DecisionSite (above) and the bitmap exported (below)



When you select the **File > Export > Legend** option, a **Save As...** dialog opens and you can browse to where you want to save the legend image; you are able to choose BMP or JPG format.

10.13 Export Data

All the data loaded into memory and used by Spotfire DecisionSite can be exported using this option. Records that have been removed by deleting marked markers will of course not be among the exported data. All other records—even those not currently portrayed in visualizations or those deselected by query devices—will be exported. The format of the data is as comma separated values (.csv).

When you select the **File** > **Export** > **Data** option, a **Save As...** dialog opens and you can browse to the location where you want to save the file, and save it under any viable name you wish. Available formats are TXT (tab separated columns), CSV (default list separator), SKV (semicolon), Spotfire Text Data Format and two versions of Microsoft ADO Persisted Record set (XML and ADTG binary format).

To export as Persisted Record set you need MDAC 2.5 or later installed on your computer. You can also open Persisted Record sets in DecisionSite Client via **File > Open...** and selecting **All Files** (*.*).

Note: Data are per default exported exactly the way they are currently displayed. This means that the export of a formatted Date, Time or DateTime column may result in data loss. For example, if a Date column is formatted to be displayed as "Day of week, Monday first (day name)", the exported data will not contain the information about year and month which was originally in the data, but only the string showing day of week. Optionally, you can turn off this setting and always export the original data from the Advanced tab of the Tools > Options dialog.

Tip: You can export data directly from the Table visualization by right-clicking and selecting **Export Data...**.

Also note, other Export options can be found under the File menu.

10.14 Printing

► To print the document with the current Print Layout settings:

- 6. Select File > Print...
- 7. Select a printer from the drop-down list.
- 8. Optionally, click **Properties** and adjust your printer settings.
- 9. Click OK.

Use the **Print Preview** option on the **File** menu to see how your printout will appear with the current Print Layout settings.

Print Layout

Spotfire DecisionSite printouts may contain any of the information available in the visualizations.

To control which information to include select Print Layout Options... from the File menu.

Option	Explanation
Header	The printed document will have a header stating Date, File name, Time.
Include title	Select this check box to include a title, and enter a title in the text field.
Include visualization	Deselect this check box if you do not want to print the visualization.
Keep aspect ratio	Select this option if you want to keep the aspect ratio of the visualization when printed on paper.
Auto fit to page	Select this option if you want the printed visualization to automatically resize to cover as much of the page as possible.
Footer	The printed document will have a footer stating the text you enter in this field.
Include query	Selecting this option provides information on the filtering you have done using the query devices.
Include Details-on-Demand	Selecting this option includes the Details-on-demand information in the printed document.
Include legend	Selecting this option includes the legend in the printed document.
Force single page layout	Selecting this option causes as much information as possible to fit onto one page, and only prints that.
Frame around areas	Selecting this option displays frames around the various includes sections.
Annotation	This tab provides an option to include the visualization annotation.

11 Quick Reference

11.1 Menus

11.1.1 File Menu

Option	Hotkey	Description
Open	Ctrl+O	Opens an existing document. A browse dialog opens where you can search for files in various formats to open in Spotfire DecisionSite. You can also enter a URL in the File name field, and access data from a web server.
Apply Template		Applies settings from an SFT or SFS file. HTML templates for presenting Details-on-Demand will be imported from the external SFS file.
Save	Ctrl+S	Saves the active document. If the document has never been saved before, this will open the same dialog as Save As
Save As	F12	Saves the document with another name, in another format, or in another location.
Close		Closes the active document. You will be prompted for saving changes.
Open from Library		Opens an item from the DecisionSite Library. A Library dialog opens where you can browse the Library for an Analysis, Guide, or Poster you want to open. See Open From Library for more information.
Publish Analysis to Library		Publishes the current Analysis to the Library. A dialog opens in which you specify details on how to publish. See Publishing Analyses to Library for more information.
Publish Poster to Library		Publishes a DecisionSite Poster to the Library. A dialog opens that allows you to design your Poster. See Publishing Posters to Library for more information.
Import >		
> Import Data	Ctrl+D	This allows you to import data in any supported format (ODBC, text files, clipboard, etc), and to apply data conditioning. See Importing Data for more information.
> Open Information Link		Launches the Information Library where you can open information links and retrieve the data. To access the online help for this application, you must first start the application by selecting it from the menu.
Export >		

> Details-on-Demand HTML		Exports information about marked or active objects as text.
> Current Visualization		Exports the current visualization. An image of the currently active visualization is exported as a JPG or BMP image file. A Save As dialog is opened and you can navigate to where you want to save your image.
> SQL Query		Exports the settings of the query devices as an SQL query.
> Legend		Exports the legend. An image of the legend, the description of which columns are used for size, color, etc. is exported as a JPG or BMP image file. A Save As dialog is opened and you can navigate to where you want to save your image.
> Data		Exports data as Tab Separated Values. A Save As dialog opens and you can save all the records in the data set as tab separated text.
> Microsoft® PowerPoint® Presentation		Exports the selected visualizations to PowerPoint®. See Exporting Visualizations to PowerPoint.
> Microsoft® Word Presentation		Exports the selected visualizations to Microsoft® Word. See Exporting Visualizations to Word.
> Web Page		Exports the visualization as a Web Page.
Print Layout Options		Changes the report layout.
Print Preview		Displays full pages. Shows a preview of the visualization as it will be printed with the settings that will apply.
Print	Ctrl+P	Prints the active visualization. A Print dialog is opened where you can choose printer and printer settings.
Switch DecisionSite >		Switch to another DecisionSite.
Login to DecisionSite >		
> Log Out		Log out of the current DecisionSite Analytics Server.
> Log into Server		Log into a DecisionSite Analytics Server.
> Change Password		Change your current password to a new one.
> Unlock New License		Opens the Add Software tool, where Spotfire Administrators can enter a product key to unlock more features to Spotfire DecisionSite.
# Most recent files		The four most recently opened documents can be opened from the list.
Exit		Quit the application. You are prompted to save open documents.

11.1.2 Edit Menu

Option	Hotkey	Description
Сору	Ctrl+C	Copies the records corresponding to the markers, bars and pies marked with the lasso or rectangle marking tool to the Windows clipboard in text format. It also copies an image of the visualization to the clipboard, which can be pasted into other applications by using a Paste Special option.
Copy Special >		
> Marked Records		Copies the set of marked records to the Clipboard. Data in all the records that have been marked is copied to the Clipboard in text format.
> Selected Records		Copies the selected records to the Clipboard. Data in the records that fulfill all query device constraints is copied to the Clipboard in text format.
> All Records		Copies all records to the Clipboard.
> Visualization		Copies the current visualization to the Clipboard. An image in vector graphics format of the active visualization is copied to the Clipboard. This image can be pasted into another application as a Windows Metafile.
Paste	Ctrl+V	Inserts Clipboard contents. The contents of the clipboard are pasted into a new Spotfire DecisionSite visualization. The Clipboard should contain data as text in one of the formats recognized by Spotfire DecisionSite.
Reset to All	Ctrl+R	Resets all query devices and zoom bars to show all records. Color, size, marking and other properties are unaffected.
Mark Selected	Ctrl+A	Marks all visible (selected) records. Records not selected by the current query device settings are not marked.
Marked Record(s)		
> Unmark	Ctrl+E	Resets the set of marked records. Unmarks all marked records.
> Invert	Ctrl+I	Inverts the set of marked records. Marks all unmarked records and unmarks the set of marked records.
> Select	Ctrl+M	Sets the selection to the marked records. Creates a temporary filter so that only the marked records are visible.
> Undo Select	Ctrl+Shift+M	Undoes all record selections without resetting the query devices.
> Delete	Del	Deletes the set of marked records. The marked records are removed from the data set in

		Spotfire DecisionSite's memory. This operation cannot be undone but does not affect the original data unless that file is intentionally overwritten with the diminished data.
Properties	Ctrl+Enter OR Alt+Enter	Set document properties. The Properties dialog opens in which parameters governing the appearance of the visualization can be set, annotations made, etc.

11.1.3 View Menu

Checkmarks in front of the options indicate that they are active; selection toggles this status.

Option	Hotkey	Description
Toolbars		Show or hide the toolbar.
Status Bar		Show or hide the status bar.
Workbook		Show visualizations with tabs.
Full Screen	F11	Full screen mode, on/off.
Details-on-Demand (Text)		Show or hide text Details-on-Demand.
Details-on-Demand (HTML)		Show or hide HTML Details-on-Demand.
Details-on-Demand (External Browser)		Launches an external browser displaying the Details-on-Demand.
Query Devices		Show or hide the query devices.
Legend	Ctrl+L	Show or hide the Legend.
Guides Toolbar		Show or hide the Guides toolbar.
Guides		Show or hide the Guides pane.
Getting Started		Show or hide the Getting Started welcome screen.

11.1.4 Visualization Menu

Option	Hotkey	Description
New Scatter Plot	Ctrl+1	Creates a new scatter plot visualization. A two- dimensional visualization is created. See Scatter Plots.
New 3D Scatter Plot	Ctrl+2	Creates a new scatter plot visualization. A three- dimensional visualization is created. See Scatter Plots.
New Bar Chart	Ctrl+4	Creates a new bar chart visualization. See Bar Charts.
New Pie Chart	Ctrl+5	Creates a new pie chart visualization. See Pie Charts.
New Line Chart	Ctrl+6	Creates a new bar chart visualization. See Line Charts.
New Profile Chart	Ctrl+7	Creates a new bar chart visualization. Profile

		Charts.
New Heat Map	Ctrl+8	Creates a new heat map visualization. See Heat Maps.
New Table	Ctrl+9	Creates a new table visualization. See Tables.
View Tip		Invokes the View Tip Dialog. Thumbnail views of visualizations are presented and can be quickly analyzed.
Duplicate Visualization	Ctrl+U	Creates a duplicate of the selected visualization.

11.1.5 Data Menu

Option	Description
Add Columns	Allows you to incorporate new columns into your current data set. See Add Columns Overview.
New Column >	
> By Binning	Allows you to sort your data into different groups or bins using different methods. See the Different Binning Methods.
> From Marked Records	Creates a new column from the currently marked records. See New Column from Marked Records.
> From Expression	Allows you to add a new column calculated from other columns in your data set. See Workflow of the New Column from Expression Tool.
Normalization	Allows you to normalize your data in various ways and to do fold change calculations. See Normalization Overview.
Column Normalization	Allows you to standardize the values in selected columns using a number of different normalization methods. See Column Normalization Overview.
Row Summarization	Allows you to combine values from multiple samples into a single column. See Performing a Row Summarization.
Pivot Data	Allows you to rotate and aggregate your data in order to use it in a better way. See Pivoting the Data Set.
Depivot Data	Allows you to transform your data to a tall and skinny format. See Depivoting the Data Set.
Transpose Data	Rotates your data set so that columns become records and vice versa. See Transpose Data Overview.
Clustering >	
> Hierarchical Clustering	Arranges records in a dendrogram (a tree graph) based on the similarity between them. See Hierarchical Clustering Method Overview.
> Hierarchical Clustering on Keys	Groups compounds with similar sets of substructures. See Hierarchical Clustering on Keys.
> Self-Organizing Maps	Groups records using an algorithm based on neural networks. See Self-Organizing Maps Overview.
> K-means Clustering	A non-hierarchical clustering, which groups records into a

	defined number of clusters based on their similarity. See K-means Clustering Overview.
> Principal Component Analysis	Reduces the dimensionality of a data set without significant loss of information. See Understanding PCA.
Pattern Detection >	
> Treatment Comparison	Provides methods for distinguishing between different treatments for an individual record. See Treatment Comparison Overview.
> Profile Search	Calculates the similarity to a selected profile for all records in the data set and adds the result as a new column. See Profile Search Overview.
> Coincidence Testing	Compares two columns and investigates whether or not the seeming similarity between the two distributions is a coincidence. See Coincidence Testing Overview.

11.1.6 Tools Menu

Option	Description
Structure Analytics >	
> Structure Viewer	Launches the Structure Viewer tool which allows you to examine chemical structures from an ISIS database and manage lists of compound identifiers generated by this tool. See Structure Viewer Overview.
> Structures in Table	Launches the Structures in Table tool which allows you to incorporate structure images from an ISIS database into a table visualization. See Displaying Structures in a Table Visualization.
> Structure Search	Launches the Structure Search tool which provides several search algorithms which retrieve molecules with similarities to the master structure. See Searching for Compounds Using Structure Search.
> R-group Search	Launches the R-group Search tool which helps you to perform searches for molecules with specified or unspecified R-groups. Note: You need to have ISIS/Draw installed on your computer to reach this tool. See Performing an R-group Search.
> List Search	Launches the List Search tool which allows you to search for structures using a list or compound identifiers. See Using List Search.
> Add Structure Keys	Launches the Add ISIS Keys tool which allows you to import keys from an ISIS database; this information is added to the data set as a new column. See Adding Structure Keys.
> Structure Connection	Launches the ISIS Connection tool where you can connect to a local or remote Integrated Scientific Information System (ISIS) database. See ISIS Connection Overview.
> Advanced Preferences	Launches a dialog where you can view and edit rules regarding which structure editor and renderer you prefer to use in your structure analytics tools. See Advanced

	Preferences.
Portfolio	Launches the Portfolio tool where you can arrange records into lists. See Portfolio Overview.
List Logic	Launches the List Logic tool where you can compare lists using Boolean operators. See Comparing Lists Using List Logic.
Web Links	Enables you to send a query to an external web site to search for information about marked records. See Web Links Overview.
Compound Details >	
> IDdb3 Drug Search	Allows you to search the Investigational Drugs database (IDdb3) using the active record in Spotfire DecisionSite or an entered drug name as search criterion. See Searching the IDdb3 Database.
Computation Services	Allows you to connect to a calculation server and add any type of statistical or mathematical calculations to your analysis. This can be a server running R, SAS, S-PLUS or custom servers.
Distance Calculator	Calculates the distance between two markers in a scatter plot.
Decision Tree	Explaining the behavior of one column as a function of other columns in a data set. See Decision Tree Overview.
Statistics >	
> Box Plot	Helps to visualize key statistical measures, such as median, mean and quartiles. See Box Plot Overview.
> Summary Table	Displays statistical information numerically. See Summary Table Overview.
> Normal Probability Plot	Helps you to investigate to what extent a data set exhibits normal distribution. See Normal Probability Plot Overview.
> Profile Anova	Provides a method for locating records where there is a significant difference between one group of columns and another group. See Profile Anova Overview.
> Column Relationships	Helps you to investigate the relationships between different column pairs. See Column Relationships Overview.
Create Information Link	Launches the Information Builder tool where you can create and open <i>information links</i> . This tool has its own help file. To see Information Builder help, start the tool and select Help .
Information Designer	Launches the Information Designer tool where you can set up database connections. This tool has its own help file. To see Information Designer help, start the tool and select Help .
Administration >	
> DecisionSite Administrator	Only available for users with Administrator privileges. Launches the DecisionSite Administrator tool where you can manage DecisionSite users and groups. You can organize users into groups, define profiles for the individual user and

	group, and assign licenses to groups and users. To see DecisionSite Administrator help, start the tool and select Help .
> DecisionSite Library	Only available for users with Administrator privileges. Starts DecisionSite Library which provides easy-to-access publishing of Analyses, Guides, and Posters. See What is DecisionSite Library.
> DecisionSite Library Administrator	Only available for users with Administrator privileges. Edit who is allowed to create new Library Sections, configure DecisionSite Library and Poster settings.
> Server Usage	Only available for users with Administrator privileges. Opens the log file dssaccess.sfs in DecisionSite, for an easy analysis and overview. This file contains information about all logins and logouts from all DecisionSite Clients to the DecisionSite Analytics Server. It shows which user logged in/out and when. The log is always enabled, and it is unaffected by Log Configuration File settings.
Customize	Customize menu and toolbars. A dialog box opens with four tabs on which you can choose appearances and customize toolbars, commands and menus.
Options	The Options dialog lets you specify visualization settings such as fonts, axis labels, default file location and much more. Here you can also choose to save personal settings.
Select Language	The Select Language dialog lets you change the language of the main menus and the online help, if you have access to any language pack. Note: The dialog texts and any submenus will still be displayed in English.

11.1.7 Guides Menu

Option	Description
Data Analysis >	
> Pivot results	Starts the Guide Pivot results in the Guides pane.
> Review HTS data	Starts the Guide Review HTS data in the Guides pane.
> Key-based clustering	Starts the Guide Key-based clustering in the Guides pane.
> Rule of 5	Starts the Guide Rule of 5 in the Guides pane.
> Create SAR Table using Information Link	Starts the Guide Create SAR Table using Information Link in the Guides pane.
> Structure similarity scores	Starts the Guide Structure similarity scores in the Guides pane.

> Explore categories	Starts the Guide Explore categories in the Guides pane.
> Venn logic	Starts the Guide Venn logic in the Guides pane.
> Group data using hierarchical clustering	Starts the Guide Group data using hierarchical clustering in the Guides pane.
Tutorials >	
> Explore a film database	Starts the Tutorial Explore a film database in the Guides pane.
> Find interesting stocks	Starts the Tutorial Find interesting stocks in the Guides pane.
Run from File	Launches an Open dialog where you can Browse to the Guide file that you want to run. See Running Guides Locally.
Run from Library	Opens an item from the DecisionSite Library. A Library browser opens where you can browse the Library for an Analysis, Guide, or Poster you want to open. See Open From Library.
Create and Edit Guide	Opens the Analysis Builder tool where you can create and edit Guides. See Analysis Builder overview.
Publish to Library	Publishes the current Analysis to the Library. A dialog opens in which you specify detail on how to publish. See Publish Analysis to Library.

11.1.8 Window Menu

Option	Hotkey	Description
Close	Ctrl+F4	Closes the active visualization.
Close All		Closes all visualizations.
Auto Hide Axis Selectors		Hides axis selectors. When hidden this gives greater room for the visualizations.
Hide Window Frame		Hides window frame. With multiple visualizations displayed, greater room is available for the visualizations when frame and title bar are hidden.
Auto Tile		Auto tiles the visualizations. Arranges all the open visualizations to fill the visualization window.
Cascade		Arranges windows so they overlap. Each window is staggered so that all title bars are accessible.
Tile Horizontal		Arranges visualizations as non overlapping horizontal tiles.
Tile Vertical		Arranges visualizations as non overlapping vertical tiles.

(#) Visualizations

Pressing the key representing the number in front of the visualization title, activates that visualization.

11.1.9 Help Menu

Help menu		
Option	Hotkey	Description
Help Topics	F1	Launches the online Help, where you can search for specific topics or subjects.
PDF Manuals		Opens a web page where you can download printable manuals in PDF format.
What's New		Lists all the new features and latest information for Spotfire DecisionSite.
Ask Spotfire Support		Opens the Support web page with information on how to contact Spotfire support.
Support Diagnostics		Use this tool to verify that everything that is needed to run DecisionSite has been installed, and has the correct version. For example, Internet Explorer version, Operating System version, correct DLLs, etc.
Structure Analytics Diagnostics		Launches the Structure Analytics Diagnostics tool. If you should run in to any problems with the configuration and set up of your Structure Analytics tools, you can retrieve information about what went wrong here.
About Spotfire DecisionSi	te	Displays program information, version number and copyright. License information is also found here.

11.2 Query Device Pop-Up Menu

Right-clicking in the query device window brings up a pop-up menu to let you modify query devices, generate new columns, change the kind of query device used, alter scale transformations, etc.

Option	Description
Check Boxes	If the column contains less than 500 unique values you can choose to have check boxes as query device. Values deselected by other query device constraints have red labels.
Radio Buttons	If the column contains less than 500 unique values you can choose to have radio buttons as query device. Only one of the values may be selected at a time.
Range Slider	Range sliders can be used to select numeric data.
Item Slider	Item sliders can be used to select alphanumeric data.
full-text search	Full-Text Search can search a string for any combination of characters using Boolean logic.

None	Select none of the records with values in this column.	
All	Select all records with values in this column.	
Data Range	Select all records with values in this column.	
From Selected	Changes the data range to span only the selected records. Three small dots are displayed at the end of the slider to indicate that the current data range is not the full range.	
Reset	Resets the data range to its original full width.	
Show Empty Values	Display records even though values are empty (null).	
Show Full Name	The query device is given another row with the entire name of the column.	
Sort	Sorts the order of the Query Devices.	
Original	Resets the original order.	
by Annotation	Sorts alphabetically by Annotation.	
by Name	Sorts alphabetically by Name.	
by Type	Sorts by type of Query Device.	
Move	Moves the query device.	
To the Top	Moves the query device to the top of the window.	
Up	Moves the query device up one position in the window.	
Down	Moves the query device down one position in the window.	
To the Bottom	Moves the query device to the bottom of the window.	
Hide	Makes the query device invisible. Selecting the Show Query Devic option on the Columns tab of the Properties dialog box makes the device visible again.	
New Column		
By Binning	Create a new column by binning, a dialog box allows you to choose column to be binned and then a wizard Guides you through the binning process.	
From Expression	Create a new column from mathematically operations on data, a wizard guides through the construction of the expression.	
From Marked Records	Create a new column. Each record is given a value indicating whether it is marked or not.	
Set Property		
Color	The colors of the markers, pies or bars are governed by the values of the records in the column. If there are less than 20 items in the column the coloring will be set to categorical, otherwise it will be continuous.	
Size	The sizes of the markers, pies or bars are governed by the values of the records in the column.	
Axis		
X	Set the X-axis to the column represented by the current Query Device.	
Y	Set the y-axis to the column represented by the current Query	

	Device.		
Z	Set the Z-axis to the column represented by the current Query Device.		
Original Scale	All changes to the scale of the column are removed.		
Ln(1+x) Scale	Logarithm base e scale $[ln(x+1)]$.		
Log Scale	Logarithm base 10 scale $[log_{10}(x)]$.		
Exp Scale	Exponential scale base e [e ^x].		
Exp10 Scale	Exponential scale base 10 [10 ^x].		
Inverse Scale	Inverse scale [1/x].		
Reverse Sorting	Reverse scale		
Edit Annotation	Go to the dialog that lets you edit the annotation for this column.		

11.3 Visualization Pop-up Menu

If you right-click in a visualization you will bring up a pop-up menu with shortcuts to some of the most used commands. The pop-up menu is slightly different in some of the visualizations. Right-clicking on an item label (marker label, bar label, etc.) will also display the Copy Special option which allows you to copy either the value of the label, or, if you are using structure marker labels, the chemical structure.

Option	Hotkey	Description
Zoom >		
> Zoom to Selection		Zooms to the selected records.
> Reset Zooming		Resets the zoom bars to the original state (no zooming).
Trellis		Opens the Properties dialog to the Trellis tab, where you can split the visualization to display different subsets of your data.
Marked Record(s) >		
> Delete	Del	Deletes the set of marked records. The marked records are removed from the data set in Spotfire DecisionSite's memory. This operation cannot be undone but does not affect the original data unless that file is intentionally overwritten with the diminished data.
> Unmark	Ctrl+E	Resets the set of marked records. No records will be marked after you have executed this operation.
> Invert	Ctrl+I	Inverts the set of marked records. Marks all unmarked records and unmarks the set of marked records.
> Select	Ctrl+M	Sets the selection to the marked records. Creates a temporary filter so that only the marked records are visible.
> New Column		Opens the New Column from Marked Records

Scatter plots

		dialog, where you can add a new column showing whether records are included in the marked group or not.
> Create New Portfolio List		Creates a new list with the marked records to the Portfolio. The list is placed as the last item on root level.
> Add to Portfolio List		Adds the marked records from the visualization into your currently active Portfolio list.
Annotate		Opens the Properties dialog to the Annotations tab, where you can provide the visualization with a description of your choice.
Сору	Ctrl+C	Copies the records corresponding to the markers, bars and pies marked with the lasso or rectangle marking tool to the Windows clipboard in text format. It also copies an image of the visualization to the clipboard, which can be pasted into other applications by using a Paste Special option.
Duplicate Visualization		Creates a duplicate of the selected visualization.
Structure Marker Labels >		Allows you to specify a structure column to use in the labels. Once structure marker labels are used, you also have the option to right-click on a structure label and select Structure Search, R- group Search or Export to File directly from the pop-up menu. You can also use Copy Special > Copy Structure to copy that specific structure as an image or as a structure element (depending on the application where you paste your structure.
> Connection		Allows you to change the connection used to display the structures into a different structure database.
> Renderer		Allows you to specify which renderer to use for drawing the structures in the labels. Here, you also have the option to change the settings for the selected renderer, or to turn off smooth drawing of structures.
> Remove		Reverts to use the column specified on the Scatter Plot Properties Markers tab in the labels instead of the structures.
Reset Navigation		Available for 3d scatter plots only. Resets the visualization to the original view.
Properties	Alt+Enter	Opens the Properties dialog n which parameters governing the appearance of the visualization can be set, annotations made, etc.
Bar charts		

Option	Hotkey	Description
Zoom >		
> Zoom to Selection		Zooms to the selected records.

> Reset Zooming		Resets the zoom bars to the original state (no zooming).
Trellis		Opens the Properties dialog to the Trellis tab, where you can split the visualization to display different subsets of your data.
Marked Record(s) >		
> Delete	Del	Deletes the set of marked records. The marked records are removed from the data set in Spotfire DecisionSite's memory. This operation cannot be undone but does not affect the original data unless that file is intentionally overwritten with the diminished data.
> Unmark	Ctrl+E	Resets the set of marked records. No records will be marked after you have executed this operation.
> Invert	Ctrl+I	Inverts the set of marked records. Marks all unmarked records and unmarks the set of marked records.
> Select	Ctrl+M	Sets the selection to the marked records. Creates a temporary filter so that only the marked records are visible.
> New Column		Opens the New Column from Marked Records dialog, where you can add a new column showing whether records are included in the marked group or not.
> Create New Portfolio List		Creates a new list with the marked records to the Portfolio. The list is placed as the last item on root level.
> Add to Portfolio List		Adds the marked records from the visualization into your currently active Portfolio list.
Sort		
> Descending		Sorts the bars from the highest to the lowest bar.
> Ascending		Sorts the bars from the lowest to the highest bar.
> Reverse		Reverses the current sort order.
> Reset		Resets the sorting to the original order.
Annotate		Opens the Properties dialog to the Annotations tab, where you can provide the visualization with a description of your choice.
Сору	Ctrl+C	Copies the records corresponding to the markers, bars and pies marked with the lasso or rectangle marking tool to the Windows clipboard in text format. It also copies an image of the visualization to the clipboard, which can be pasted into other applications by using a Paste Special option.
Duplicate Visualization		Creates a duplicate of the selected visualization.
Properties	Alt+Enter	Opens the Properties dialog n which parameters governing the appearance of the visualization can be set, annotations made, etc.

Option	Hotkey	Description
Zoom >		
> Reset Zooming		Resets the zoom bars to the original state (no zooming).
Trellis		Opens the Properties dialog to the Trellis tab, where you can split the visualization to display different subsets of your data.
Marked Record(s) >		
> Delete	Del	Deletes the set of marked records. The marked records are removed from the data set in Spotfire DecisionSite's memory. This operation cannot be undone but does not affect the original data unless that file is intentionally overwritten with the diminished data.
> Unmark	Ctrl+E	Resets the set of marked records. No records will be marked after you have executed this operation.
> Invert	Ctrl+I	Inverts the set of marked records. Marks all unmarked records and unmarks the set of marked records.
> Select	Ctrl+M	Sets the selection to the marked records. Creates a temporary filter so that only the marked records are visible.
> New Column		Opens the New Column from Marked Records dialog, where you can add a new column showing whether records are included in the marked group or not.
> Create New Portfolio List		Creates a new list with the marked records to the Portfolio. The list is placed as the last item on root level.
> Add to Portfolio List		Adds the marked records from the visualization into your currently active Portfolio list.
Annotate		Opens the Properties dialog to the Annotations tab, where you can provide the visualization with a description of your choice.
Сору	Ctrl+C	Copies the records corresponding to the markers, bars and pies marked with the lasso or rectangle marking tool to the Windows clipboard in text format. It also copies an image of the visualization to the clipboard, which can be pasted into other applications by using a Paste Special option.
Duplicate Visualization		Creates a duplicate of the selected visualization.
Properties	Alt+Enter	Opens the Properties dialog n which parameters governing the appearance of the visualization can be set, annotations made, etc.

Pie charts

Option Zoom >	Hotkey	Description
> Reset Zooming		Resets the zoom bars to the original state (no zooming).
Trellis		Opens the Properties dialog to the Trellis tab, where you can split the visualization to display different subsets of your data.
Marked Record(s) >		
> Delete	Del	Deletes the set of marked records. The marked records are removed from the data set in Spotfire DecisionSite's memory. This operation cannot be undone but does not affect the original data unless that file is intentionally overwritten with the diminished data.
> Unmark	Ctrl+E	Resets the set of marked records. No records will be marked after you have executed this operation.
> Invert	Ctrl+I	Inverts the set of marked records. Marks all unmarked records and unmarks the set of marked records.
> Select	Ctrl+M	Sets the selection to the marked records. Creates a temporary filter so that only the marked records are visible.
> New Column		Opens the New Column from Marked Records dialog, where you can add a new column showing whether records are included in the marked group or not.
> Create New Portfolio List		Creates a new list with the marked records to the Portfolio. The list is placed as the last item on root level.
> Add to Portfolio List		Adds the marked records from the visualization into your currently active Portfolio list.
Same Scale for All		Sets all line charts to use the same scale. (Same as the 'One for all' scale mode option in the Properties dialog.)
Cascade All		Sets the Scale and Position of all columns so that each of them will occupy a separate slot of the window height.
Maximize All		Set the Scale and Position on every column so they utilize the whole height of the window.
Show Markers		Displays (or hides) markers in the line chart.
Annotate		Opens the Properties dialog to the Annotations tab, where you can provide the visualization with a description of your choice.
Сору	Ctrl+C	Copies the records corresponding to the markers, bars and pies marked with the lasso or rectangle marking tool to the Windows clipboard in text

Line charts
		format. It also copies an image of the visualization to the clipboard, which can be pasted into other applications by using a Paste Special option.
Duplicate Visualization		Creates a duplicate of the selected visualization.
Properties	Alt+Enter	Opens the Properties dialog n which parameters governing the appearance of the visualization can be set, annotations made, etc.

Profile charts

Option	Hotkey	Description
Zoom >		
> Zoom to Selection		Zooms to the selected records.
> Reset Zooming		Resets the zoom bars to the original state (no zooming).
Trellis		Opens the Properties dialog to the Trellis tab, where you can split the visualization to display different subsets of your data.
Marked Record(s) >		
> Delete	Del	Deletes the set of marked records. The marked records are removed from the data set in Spotfire DecisionSite's memory. This operation cannot be undone but does not affect the original data unless that file is intentionally overwritten with the diminished data.
> Unmark	Ctrl+E	Resets the set of marked records. No records will be marked after you have executed this operation.
> Invert	Ctrl+I	Inverts the set of marked records. Marks all unmarked records and unmarks the set of marked records.
> Select	Ctrl+M	Sets the selection to the marked records. Creates a temporary filter so that only the marked records are visible.
> New Column		Opens the New Column from Marked Records dialog, where you can add a new column showing whether records are included in the marked group or not.
> Create New Portfolio List		Creates a new list with the marked records to the Portfolio. The list is placed as the last item on root level.
> Add to Portfolio List		Adds the marked records from the visualization into your currently active Portfolio list.
Same Scale for All		Sets all profile charts to use the same scale. (Same as the 'All columns use same scale' scale mode option in the Properties dialog.)
Annotate		Opens the Properties dialog to the Annotations tab, where you can provide the visualization with a description of your choice.

Сору	Ctrl+C	Copies the records corresponding to the markers, bars and pies marked with the lasso or rectangle marking tool to the Windows clipboard in text format. It also copies an image of the visualization to the clipboard, which can be pasted into other applications by using a Paste Special option.
Duplicate Visualization		Creates a duplicate of the selected visualization.
Structure Marker Labels >		Allows you to specify a structure column to use in the labels. Once structure marker labels are used, you also have the option to right-click on a structure label and select Structure Search, R- group Search or Export to File directly from the pop-up menu. You can also use Copy Special > Copy Structure to copy that specific structure as an image or as a structure element (depending on the application where you paste your structure.
> Connection		Allows you to change the connection used to display the structures into a different structure database.
> Renderer		Allows you to specify which renderer to use for drawing the structures in the labels. Here, you also have the option to change the settings for the selected renderer, or to turn off smooth drawing of structures.
> Remove		Reverts to use the column specified on the Scatter Plot Properties Markers tab in the labels instead of the structures.
Properties	Alt+Enter	Opens the Properties dialog n which parameters governing the appearance of the visualization can be set, annotations made, etc.

Heat maps

Option	Hotkey	Description
Zoom >		
> Reset Zooming		Resets the zoom bars to the original state (no zooming).
Trellis		Opens the Properties dialog to the Trellis tab, where you can split the visualization to display different subsets of your data.
Marked Record(s) >		
> Delete	Del	Deletes the set of marked records. The marked records are removed from the data set in Spotfire DecisionSite's memory. This operation cannot be undone but does not affect the original data unless that file is intentionally overwritten with the diminished data.
> Unmark	Ctrl+E	Resets the set of marked records. No records will be marked after you have executed this operation.

> Invert	Ctrl+I	Inverts the set of marked records. Marks all unmarked records and unmarks the set of marked records.
> Select	Ctrl+M	Sets the selection to the marked records. Creates a temporary filter so that only the marked records are visible.
> New Column		Opens the New Column from Marked Records dialog, where you can add a new column showing whether records are included in the marked group or not.
> Create New Portfolio List		Creates a new list with the marked records to the Portfolio. The list is placed as the last item on root level.
> Add to Portfolio List		Adds the marked records from the visualization into your currently active Portfolio list.
Show Deselected		Shows (or hides) deselected records in the heat map.
Annotate		Opens the Properties dialog to the Annotations tab, where you can provide the visualization with a description of your choice.
Сору	Ctrl+C	Copies the records corresponding to the markers, bars and pies marked with the lasso or rectangle marking tool to the Windows clipboard in text format. It also copies an image of the visualization to the clipboard, which can be pasted into other applications by using a Paste Special option.
Duplicate Visualization		Creates a duplicate of the selected visualization.
Reset Navigation		Available for 3d scatter plots only. Resets the visualization to the original view.
Properties	Alt+Enter	Opens the Properties dialog n which parameters governing the appearance of the visualization can be set, annotations made, etc.

Table visualizations

Option	Hotkey	Description
Marked Records >		
> Delete	Del	Deletes the set of marked records. The marked records are removed from the data set in Spotfire DecisionSite's memory. This operation cannot be undone but it does not affect the original data unless that file is intentionally overwritten with the diminished data.
> Unmark	Ctrl+E	Resets the set of marked records. No records will be marked after you have executed this operation.
> Invert	Ctrl+I	Inverts the set of marked records. Marks all previously unmarked records and unmarks the set of marked records.

> Select	Ctrl+M	Sets the selection to the marked records. Creates a temporary filter so that only the marked records are visible.
> New Column		Opens the New Column from Marked Records dialog, where you can add a new column showing whether records are included in the marked group or not.
> Create New Portfolio List		Creates a new list with the marked records to the Portfolio. The list is placed as the last item on root level.
> Add to Portfolio List		Adds the marked records from the visualization into your currently active Portfolio list.
Сору	Ctrl+C	Copies the set of marked records to the Clipboard. Data in all the records that have been marked is copied to the Clipboard in text format.
Copy Special >		
> Copy Value		Copies the cell value that you right-clicked upon.
> Copy Visualization		Copy the current visualization to the Clipboard. An image in vector graphics format of the active visualization is copied to the Clipboard. This image can be pasted into another application as a Windows Metafile.
Duplicate Visualization		Creates a duplicate of the selected visualization.
Export Data		Opens a dialog where you can select a folder to save the exported data to, specify a file name and determine the type and encoding to use for the new file.
Add Structure Column		Allows you to add a structure column to the table, so that it behaves like a Structures in Table visualization.
Properties	Alt+Enter	Opens the Properties dialog n which parameters governing the appearance of the visualization can be set, annotations made, etc.

If you are running DecisionSite for Lead Discovery you will have access to more options on the pop-up menu. See Structures in Table pop-up menu for more information.

11.4 Toolbar Buttons

The following tables describe the toolbar and shortcuts that you can use to create, open, close, save, and manipulate your visualizations. Look up the action you want to take, and perform one of the alternatives shown.

Most actions can be performed with hot-keys from the keyboard (Keyboard Shortcut), from the menu (Menu Command, or Mouse), or by clicking a toolbar button (Toolbar). The menus can be reached by pressing the Alt key in combination with the underlined letter key. Subsequent underlined letter keys activate the menu items.

	Hotkey	Menu Command, or Mouse	Toolbar Button
Open an existing file or import a database.	Ctrl+O	\underline{F} ile > \underline{O} pen	
Import data from file, clipboard or database, and perform data conditioning.	Ctrl+D	<u>F</u> ile > Import <u>D</u> ata	5
Save the present visualization in the same format as when opened .	Ctrl+S	\underline{F} ile > \underline{S} ave	
Print the active visualization.	Ctrl+P	\underline{F} ile > \underline{P} rint	3
Copy the marked records to the clipboard as text.	Ctrl+C	\underline{E} dit > \underline{C} opy	B
Paste the clipboard contents into Spotfire DecisionSite.	Ctrl+V	\underline{E} dit > \underline{P} aste	(
Reset all query devices and zoom bars.	Ctrl+R	\underline{E} dit > \underline{R} eset to All	C ¹
Create a new 2D scatter plot.	Ctrl+1	<u>W</u> indow > New <u>S</u> catter Plot	
Create a new 3D scatter plot.	Ctrl+2	<u>W</u> indow > New <u>3</u> D Scatter Plot	۲
Create a new bar chart.	Ctrl+4	<u>W</u> indow > New <u>B</u> ar Chart	
Create a new pie chart.	Ctrl+5	<u>W</u> indow > New <u>P</u> ie Chart	
Create a new line chart.	Ctrl+6	<u>W</u> indow > New <u>L</u> ine Chart	\geq
Create a new profile chart.	Ctrl+7	<u>W</u> indow > New P <u>r</u> ofile Chart	MA.
Create a new heat map.	Ctrl+8	Window > New Heat Map	
Create a new table.	Ctrl+9	Window > New Table	
Auto-tile visualizations.		\underline{W} indow > \underline{A} uto Tile	
Place all visualizations so they partially overlap each other.		<u>W</u> indow > Cascade	1
Place all visualizations next to each other.		<u>W</u> indow > Tile Vertical	
Place all visualizations under each other.		<u>W</u> indow > Tile Horizontal	
Open the Properties dialog.	Ctrl+Enter OR Alt+Enter	\underline{E} dit > \underline{P} roperties	
Display legend in separate window.	Ctrl+L	$\underline{V}iew > \underline{L}egend$	

Export the active visualization as an image (BMP or JPG) to disk.	<u>H</u> C	<u>File > Export ></u> Current Visualization	₩
Open browser and display values for the currently marked records.	<u>I</u>	<u>File > E</u> xport > <u>D</u> etails	.
Show the Guides pane. Ct	trl+W V	View > Spotfire DecisionSite	2
Go to Start page.			

11.5 Mouse Shortcuts

11.5.1 Mouse Shortcuts – Scatter Plots and Line Charts

Mouse over marker

A thin ring highlights the marker and all markers containing the record in other visualizations.

Left-click on marker

Activates a record. A persistent ring surrounds the object. Information about the record corresponding to the marker that was clicked displays in the Details-on-Demand window.

Left-drag

Marks the records that are inside the 'rubber band box' delineated by the pointer's diagonal movement. These markers will be given another color. A table of details will be displayed in the Details-on-Demand window. If no markers are surrounded all previously marked objects will be unmarked.

Shift + left-drag

Marks records using the lasso tool. Draw an arbitrary shape around the markers you want to mark. If none are surrounded all objects will be unmarked.

Ctrl + left-drag

Adds markers to the set of marked records using the rectangle 'rubber band box' tool.

Ctrl + Shift + left-drag

Adds markers to the set of marked records using a lasso function.

Ctrl + Shift + left-drag

Adds markers to the set of marked objects using a lasso function to the set of marked records.

Mouse wheel

Zooms in and out in the visualization.

Ctrl + right-click

Zooms in from the visualization.

Ctrl + Shift + right-click

Zooms out from the visualization.

Right-click in visualization

Brings up the visualization context pop-up menu.

11.5.2 Mouse Shortcuts – 3D Scatter Plots

Mouse over marker

Identical to 2D scatter plots

Left-click on marker

Identical to 2D scatter plots.

Ctrl + drag using the right mouse button (or drag using the middle mouse button)

Rotation around the visualization center.

Shift + drag using the right mouse button (or Shift + drag using the middle mouse button)

Zooms in the direction of the view.

Ctrl + Shift + drag using the right mouse button (or Ctrl + Shift + drag using the middle mouse button)

Rotation in the plane of the screen; downwards and right cursor motion rotates clockwise.

Mouse wheel

(or Ctrl + drag using the middle mouse button)

Zooms in and out in the visualization.

Right-click in visualization

Brings up the visualization context pop-up menu.

11.5.3 Mouse Shortcuts – Bar Charts and Pie Charts

Mouse over object

An outline highlights the object and corresponding objects in similar visualizations.

Left-click on object

Activates an object. A persistent outline surrounds the object. Information about the bar or pie that was clicked displays in the Details-on-Demand window.

Left-drag

Marks the pies or bars that are inside the rectangle delineated by the diagonal movement of the pointer. If no bars are surrounded all objects will be unmarked.

Shift + left-drag

Enables marking of bars or pies with the lasso tool. Draw an arbitrary shape around the objects you want to mark. If none are surrounded all objects will be unmarked.

Ctrl + left-drag

Adds bars or pies to the set of marked objects using the rectangle 'rubber band box' tool.

Ctrl + Shift + left-drag

Adds bars or pies to the set of marked objects using a lasso function to the set of marked records.

Mouse wheel

Zooms in and out in the visualization.

Ctrl + right-click

Zooms in from the visualization (only works for pie charts when an axis different than None has been selected).

Ctrl + Shift + right-click

Zooms out from the visualization (only works for pie charts when an axis different than None has been selected).

Right-click in visualization

Brings up the visualization context pop-up menu.

11.5.4 Mouse Shortcuts – Profile Charts

Mouse over profile

A thin contour highlights the profile (record), as well as all markers associated with the record in other visualizations.

Left-click on profile

Activates A persistent contour surrounds the profile. Information about the profile appears in the Details-on-Demand window.

Left-drag

Marks the profiles that are fully or partially inside the 'rubber band box' delineated by the pointer's diagonal movement. These profiles will become thicker. A table of details will be displayed in the Details-on-Demand window. If no profiles are surrounded all previously marked objects will be unmarked.

Shift + left-drag

Enables marking of profiles with the lasso tool. Draw an arbitrary shape around the profile you want to mark. If none are surrounded all profiles will be unmarked.

Ctrl + left-drag

Adds profiles to the set of marked profiles using the rectangle 'rubber band box' tool.

Ctrl + Shift + left-drag

Adds profiles, by using a lasso function, to the set of marked records.

Mouse wheel

Zooms in and out in the visualization.

Ctrl + right-click

Zooms in from the visualization.

Ctrl + Shift + right-click

Zooms out from the visualization.

Right-click in visualization

Brings up the visualization context pop-up menu.

12 Glossary

The glossary only contains brief definitions of the terminology used in Spotfire DecisionSite. Links to more information are available when applicable.

API

The term API stands for Application Programmer's Interface, and is a set of functions available to programmers. These functions cover a wide range of tasks, such as graphics, multimedia, fonts, disk access, memory management, etc.

This functionality allows strong integration with legacy systems and novel applications.

Bar Charts

A visualization displaying the data as bars. The value from each record is added to the bar's total value/ Y-axis height.

Binning

The process of grouping *values* with similar properties together in a way that each Bin contains values that, in some important respect, are similar. Not to be confused with clustering, which means grouping similar *records*.

Bitmap

A file format for graphics. The format is used in Spotfire DecisionSite when copying the graphical presentation of a decision tree to the clipboard.

Browser

A program able to display pages encoded in HTML.

Categorical Coloring

Markers, bars or pie charts are assigned distinct colors depending on their values.

Centroids

The centroids are the center points of clusters. How initial centroids are chosen is determined in the K-means Clustering dialog.

Check Boxes

A Query Device enabling toggling of each data value, to control which will be shown in the visualization and which will not.

Clustering

A technique for grouping objects on the basis of their similarity for a specified set of characteristics. The main objective of a cluster analysis is that objects within a cluster should be more similar to each other than they are to objects in other clusters. Spotfire DecisionSite Statistics offers three different kinds of clustering: Hierarchical Clustering, K-means Clustering and Self-Organizing Maps.

Column

Corresponding fields in a set of records constitute a column. (Records go by the name 'rows', in spreadsheet programs).

Continuous Coloring

Coloring whereby the values in the column determine the shade displayed. The (dissimilar) Begin and End colors selected in the Customize dialog represent the minimum and maximum values in a column. The markers representing records having intermediate values are colored with a blend of the two; depending on their value.

Control

A control is a graphical object (for example an icon, a button or a window) in the user interface that represents the properties or operations of other objects.

CSV

Comma-Separated Values. This is a standardized way to save data sets. Each data record is stored as text, using the default list separator as column separator, and a line feed and return character to mark the end of each record. The default list separator is a property of the Regional Settings of your Windows system.

Data Column

A property in a data set. Each column in your data set is represented by a query device in Spotfire DecisionSite.

Data Conditioning

Any kind of processing performed prior to visualizing or analyzing the data, such as normalization, pivoting, de-pivoting, etc. These features can be accessed upon data import through the Import Data option. It is also possible to use either of the data conditioning tools from the Data menu after retrieving your data.

Data Source

A database, a file, or the clipboard.

DecisionSite Navigator

The precursor to the Guides pane. A browser window integrated into the Spotfire DecisionSite environment, able to communicate with the Spotfire DecisionSite visualization engine.

Delimiter

This is a separator between data values, for example between columns in a data table or between IDs in a search string.

Dendrogram

A dendrogram is a branching diagram which represents a hierarchy of categories based on the degree of similarity or number of shared characteristics.

Deselected Records

The records that do not fulfill the constraints of the query devices.

Details-on-Demand

A window that shows the data in a marked record. The information can be displayed as plain text, HTML styled text in a window or as styled text in an external HTML browser.

Docked Window

By default, the Query Device window, the Details-on-Demand window, and the Legend window are docked; they stick to one of the outer borders of the Spotfire DecisionSite main window but can be moved.

De-pivoted Data

Another word for Tall/Skinny data.

Distance Measures

A type of similarity measures.

Empty Values

Empty values are values that are missing in your data set (has a null value). If you intend to use any type of clustering tool, all empty values need to be replaced or else the clustering will not work. There are several replacement methods but all empty values in a column must be replaced using the same method.

Full-text Search Query Device

A query device with which any string of characters can be located in the column under investigation. Boolean logic can be used to refine the search.

Glyph

One of the shapes representing a data record in a 3D scatter plot.

Graphical User Interface - GUI

This is the graphical presentation of the application that you see on the screen.

HTML

Hyper Text Markup Language. At its simplest, a language for formatting text. One of the primary reasons for the success of HTML and the World Wide Web is the ability to use links within or between documents.

Identifier Column

The identifier column is the column that contains IDs for the records that are used in a certain calculation. The IDs should be unique for all records in the data set (see also Short/Wide).

ISIS

Integrated Scientific Information System from MDL.

ISIS/Draw

A desktop application from MDL, used for creating and editing models of chemical structures.

Item Slider

A query device with which to select a specific value in a range.

Jitter

An option that displaces the visualization objects randomly in the display window, to make overlapping records visible.

Lasso Function

Enclosing a set of markers with the mouse pointer while pressing **Shift** on the keyboard. This marks the records. The resulting encircling can have any shape.

List

A node in a portfolio where you can add records, annotations and other lists.

Marker

One of the shapes representing a data record in a scatter plot. The 3D shapes are also called glyphs.

Marked Record

A marker in a scatter plot becomes marked when captured using the lasso or rectangle method (left mouse button pressed while moving pointer). Marked records are given a definable color to distinguish them from the rest of the data.

Menu Bar

The row of commands visible at the upper border of a Windows program. Clicking any of the menu titles will display sub menus with additional choices.

Menu Item

One of the options available in the menu presented by one of the commands in the menu bar.

MOL File

This is a file format used for chemical structures. Each file contains only one structure.

Navigate Menu

The Navigate menu used to be located in the top left corner of the DecisionSite Navigator. From here you could reach various tools and resources, or log into and log out of the network. In DecisionSite 8.1 the corresponding functions can be reached via the main menus in DecisionSite.

Node

A node is a circle in a decision tree that represents either a record or a cluster of records.

Null Value

Empty value. Cell with no value.

ODBC

Open DataBase Connectivity, a common method of accessing databases.

Pie Chart

A visualization showing data in aggregated "pie segments", which can be split, drilled down into and taken apart.

Pivoted Data

Another word for Short/Wide data.

Pop-up Menu

Menus that are available of you right-click directly in the graphical user interface. The content of the menu depends on where you click.

Portfolio

A portfolio is a data file in XML-format that can be viewed in the Portfolio tool and which makes it possible to work with genes or experimental results in a structured way.

Profile

Synonymous to a record (data point) in Spotfire DecisionSite.

Profile Chart

A visualization type where column names are plotted along the X-axis, and the value in each column on the Y-axis. This means that each record is presented as a line.

Properties

The dialog box enabling changes to query devices, visualization objects—markers, pies, bars, backgrounds and HTML code. Located in the Edit menu. Accessible with [Alt+Enter] Edit > **Properties** and a toolbar button.

Query Device

A tool that selects data having certain values for visualization. There are five kinds of query devices: range sliders, item sliders, full-text searches, check boxes and radio buttons.

Query Device Window

The window where the query devices are located. By default, this window is placed in the upper right corner.

Range Slider

A Query Device used to select a range of data. The default device for numerical data. A range slider enables narrowing, broadening and moving the interval of the selected data of the designated column.

Record

One entry or line in a database or data set. Sometimes called a row.

Sampling

In previous versions of DecisionSite, subsets of data could be extracted using a sampling tool. This is no longer supported.

SAR Table

Structure-Activity Relationship table. The SAR table combines structural and other data about compounds into a single spreadsheet.

Scatter Plot

A visualization type showing the records as markers in a two-dimensional or three-dimensional diagram.

SDFile

This is a file format used for exporting ISIS data. Structure-data files contain structures and data for any number of molecules. SDFiles can be imported into ISIS for Excel.

Selected Records

The records explicitly chosen for display by manipulating the query devices and zoom bars. Do not confuse with the *Marked Records*. The option "Work on: Selected records" in the calculation dialogs means that only the records selected via the query devices are included in the calculations.

Selecting Data

Using the query devices to control which data is visualized.

SFS

The file extension that Spotfire DecisionSite applies when saving data set in its proprietary format.

Short/Wide

A data table format with relatively few rows and many columns, suitable for analysis. The identifier column in a short & wide data table has a unique value for each row, in other words, all data associated with a specific ID is available on one row in the table.

Similarity Measure

Methods for calculating the similarity between data.

SQL

Structured Query Language, a common language used for formulating queries when investigating databases.

Tall/Skinny

A data table format with many rows and relatively few columns, commonly used for automatically generated data, but often not suitable for analysis. The identifier column in a tall & skinny data table contains multiple values, which means that the same ID and information associated with it appear on many rows.

Toolbar

The bar at the top of the application or tool window that contains buttons that are shortcuts to frequent commands on the menus.

Tools

The tools provide the special functions of your DecisionSite, such as clustering or structure analytics. You reach the tools via the **Data** and **Tools** menus.

Trellis plot

A way of splitting a visualization into panes and organizing these in a grid layout.

Visualization

A graphical presentation of data in Spotfire DecisionSite, e.g., scatter plot, pie chart, etc. The query devices control which data is displayed.

Web link

A link to an external web site that lets you send a query about marked records.

Zoom Bar

The bars along the edges of the visualization window. By manipulating them it is possible to zoom in on details of the visualization.

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