

BIONUMERICS Tutorial:

Creating charts

1 Introduction

The *Charts and statistics* window in BIONUMERICS provides a uniform charting interface and uses robust and logical concepts to guarantee that most if not all charting and plotting needs can be answered. Not less than 16 major types of charts are available BIONUMERICS. The basis for every chart is the *data source*, which contains different *properties* (see Figure 1). A property can e.g. be a string (information field) or a character value.

In this tutorial you will learn how to create some of the most commonly used chart types in BIONUMERICS and how to alter the appearance of a chart. For detailed information on the different chart types and available fit models we refer to the manual.

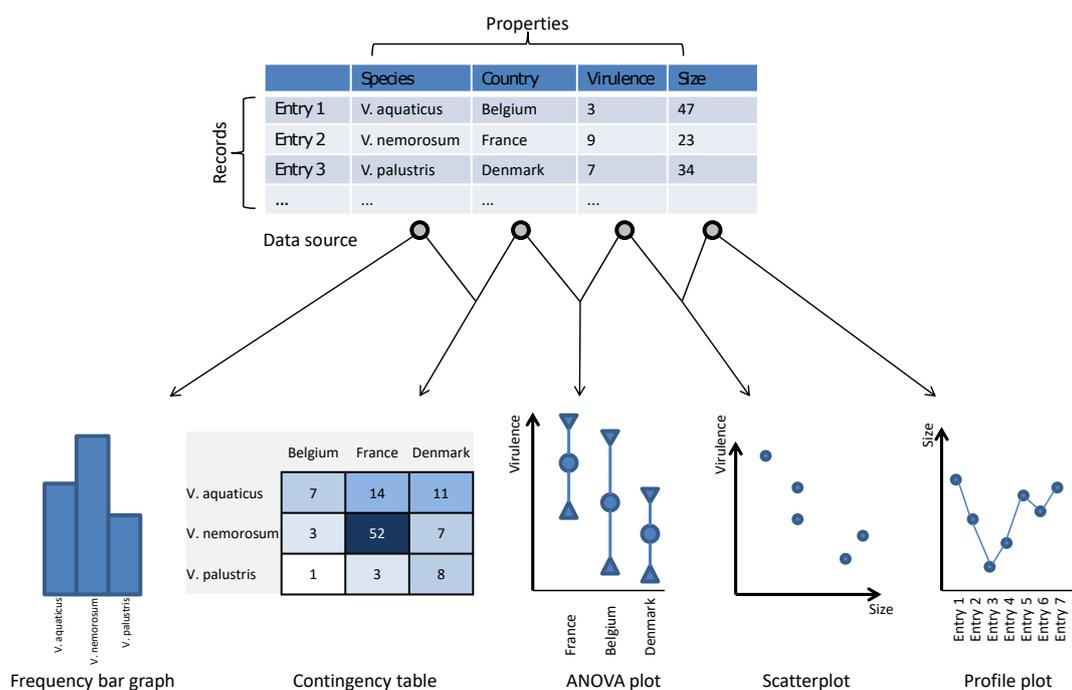


Figure 1: The data source and resulting charts.

2 Preparing the database

The **DemoBase Connected** will be used in this tutorial and can be downloaded directly from the *BIONUMERICIS Startup* window or restored from the back-up file available on our website:

1. To download the database directly from the *BIONUMERICIS Startup* window, click the  button, located in the toolbar in the *BIONUMERICIS Startup* window. Select **DemoBase Connected** from the list and select **Database > Download** (). Confirm the download action.
2. To restore the database from the back-up file, first download the file `DemoBase_Connected.bnbk` from <https://www.applied-maths.com/download/sample-data>, under 'DemoBase Connected'. In the *BIONUMERICIS Startup* window, press the  button, select **Restore database**, browse for the downloaded file and select **Create copy**. Specify a name and click **<OK>**.



In contrast to other browsers, some versions of Internet Explorer rename the `DemoBase_Connected.bnbk` database backup file into `DemoBase_Connected.zip`. If this happens, you should manually remove the `.zip` file extension and replace with `.bnbk`. A warning will appear ("If you change a file name extension, the file might become unusable."), but you can safely confirm this action. Keep in mind that Windows might not display the `.zip` file extension if the option "Hide extensions for known file types" is checked in your Windows folder options.

A text file with additional chart information can be downloaded from the Applied Maths website (<https://www.applied-maths.com/download/sample-data>, click on "Chart data file").

1. Download the file `Chart_data.zip` from the Applied Maths website and extract the content.
2. Open the database **DemoBase Connected**.
3. Select **File > Import...** (, **Ctrl+I**) in the *Main* window to call the *Import* dialog box.
4. Choose the option **Import fields (text file)** under the **Entry information data** item in the tree and click **<Import>**.
5. Browse for the downloaded and unzipped `Chart_data.txt` file and press **<Next>**.
6. In the *Import rules* dialog box highlight the row that corresponds to **Key** and press **<Edit destination>**.
7. In the *Edit data destination* dialog box, highlight **Key** and press **<OK>**.
8. Select the fields **Age**, **Date**, **Country** and **Serotype** using the **Ctrl-key** and press **<Edit destination>** again.
9. In the *Edit data destination* dialog box, highlight **Entry info field** and press **<OK>**.
10. In the *Create new* dialog box that appears, leave the default names unaltered and press **<OK>** and confirm the action.

The *Import rules* dialog box should now look like in Figure 2.

11. Press **<Next>** to move to the next page and press **<Finish>**.
12. Enter **Chart data** as name for the template and press **<OK>**.

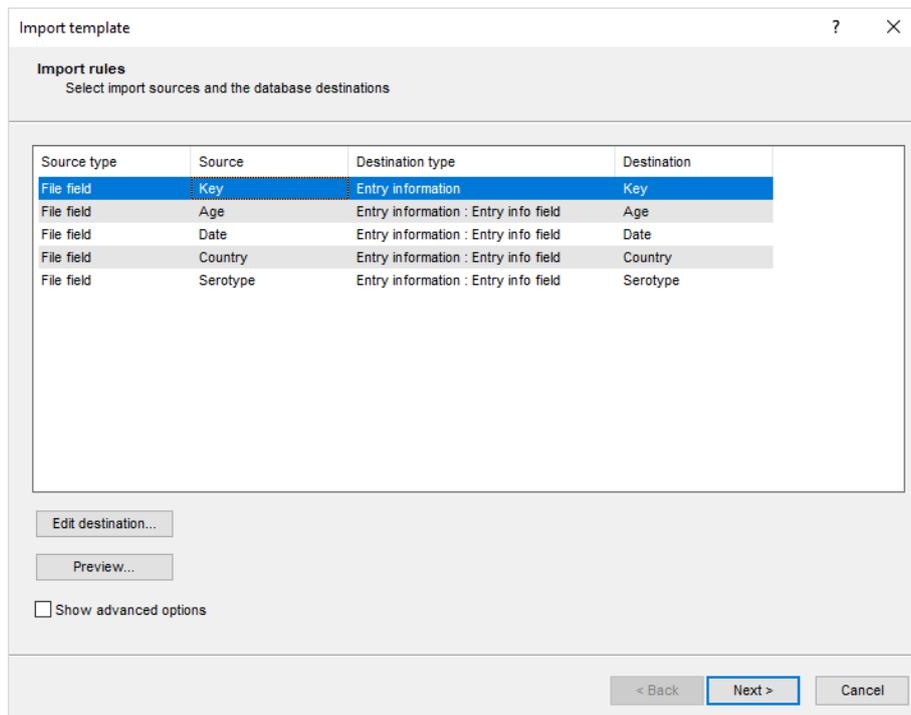


Figure 2: The import template mapping rules.

13. Make sure the created template is selected and press **<Next>** to move to the next page.

The last step of the wizard indicates that existing entries will be updated.

14. Press **<Finish>**.

The entry information is imported and displayed in the *Database entries* panel.

3 Bar graph

3.1 Example 1

1. Select a few entries in the *Database entries* panel of the *Main* window (not those labeled as STANDARD in the **Genus** field) using the **Ctrl-key**. Alternatively, use the **space bar** to select a highlighted entry or click the ballot box next to the entry.
2. Highlight the *Comparisons* panel in the *Main* window and select **Edit > Create new object... (+)** to create a new comparison for the selected entries.
3. To clear the selection, press the **F4-key**.
4. In the *Comparison* window, select **Statistics > Chart and statistics... (F7)**.
5. Select **PhenoTest characters** under **Experiment character values** in the dialog box that pops up and press **<OK>**.
6. Choose **Bar Graph** in the next step and press **<Next>**.
7. Choose an entry from the list and press **<Next>**.

- In the final step choose **Name** as **Label** and press <**Finish**>.

A bar graph is created in the *Chart area* panel of the *Charts and statistics* window displaying the character set of the selected entry. The rectangular bar of each character has a length proportional to the character value. We will now add a second bar graph to compare the characters between two entries.

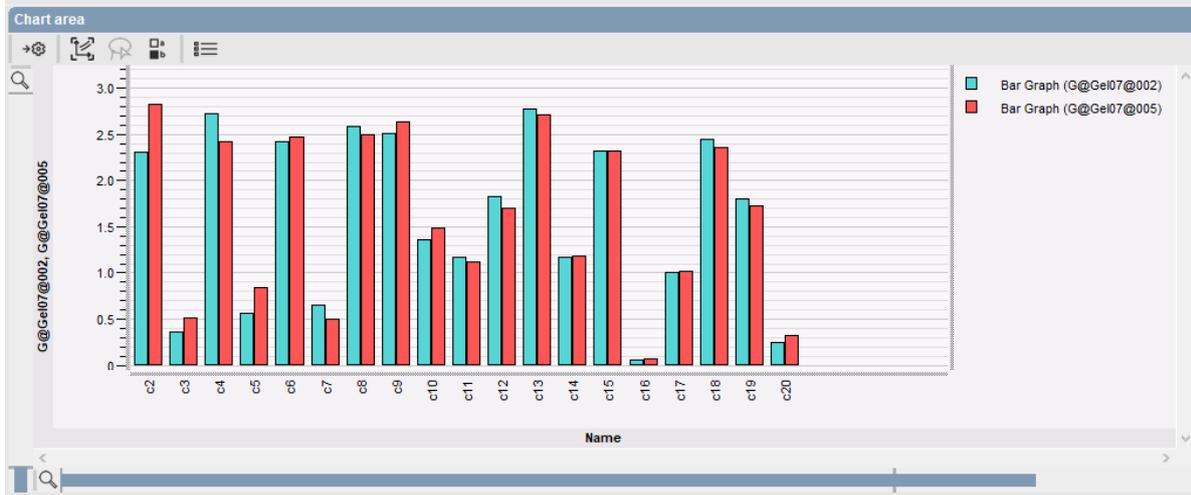


Figure 3: Bar graph displaying the character sets of two entries.

- In the *Data source overview* panel, select another entry under **Entry values**.
- Select **Plot** > **Add new plot from selected properties...** (+).
- Click on **Bar graph** and press <**Next**>.
- Press <**Finish**> again to obtain the bar graph.

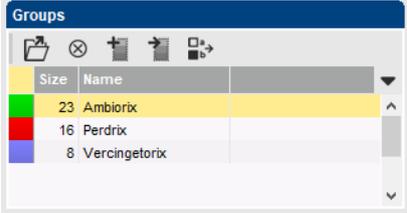
The result looks as in Figure 3. More entries can be added to the chart in the same way.

- Close the *Charts and statistics* window with **File** > **Exit**.
- Close the *Comparison* window with **File** > **Exit** without saving the comparison.

3.2 Example 2

- Select all entries in the *Database entries* panel of the *Main* window with **Ctrl+A**, and unselect those labeled as STANDARD in the **Genus** field.
- Highlight the *Comparisons* panel in the *Main* window and select **Edit** > **Create new object...** (+) to create a new comparison for the selected entries.
- To clear the selection, press the **F4**-key.
- In the *Comparison* window, right-click in the header of the "Genus" field in the *Information fields* panel and select **Create groups from database field** from the menu. Alternatively select **Groups** > **Create groups from database field**.
- Press <**OK**> to create groups based on the "Genus" names.

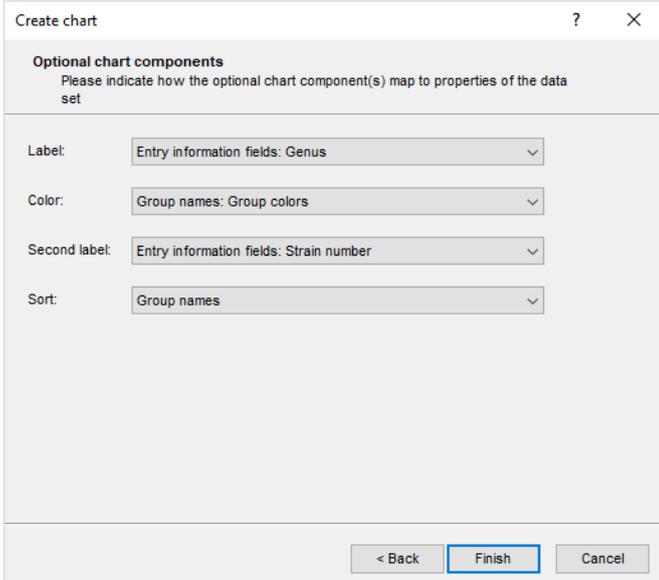
The three groups appear in the *Groups* panel along with their color, size and name (see Figure 4).



Size	Name
23	Ambiorix
16	Perdrix
8	Vercingetorix

Figure 4: The *Groups* panel.

20. In the *Comparison* window, select **Statistics > Chart and statistics...** (F7).
21. Select **Comparison entries** in the dialog box that pops up and press <OK>.
22. Choose **Bar Graph** in the next step and press <Next>.
23. Choose a character value from the list (e.g. **FAME: Values: 18:0**) and press <Next>.
24. In the final step choose **Entry information fields: Genus** as **Label**, **Group names: Group colors** as **Color**, **Entry information fields: Strain number** as **Second label**, **Group names** as **Sort** method and press <Finish> (see Figure 5).



Create chart

Optional chart components
Please indicate how the optional chart component(s) map to properties of the data set

Label: Entry information fields: Genus

Color: Group names: Group colors

Second label: Entry information fields: Strain number

Sort: Group names

< Back Finish Cancel

Figure 5: Chart components.

A bar graph is created in the *Chart area* panel of the *Charts and statistics* window. The rectangular bar of each database entry has a length proportional to the value of the selected FAME character.

Ideally, we would like to see the genus and species information as chart labels, rather than only the genus name. Since only one chart label can be displayed at a time, we will create a *derived property*, containing the first character of the genus name and the full species name.

25. In the *Data source overview* panel, select **Genus (Label)** under **Current view**.
26. Select **Dataset > New derived property...** (⊞+).
27. Select **Abbreviate** and press <Next> and <Finish>.

A derived property **Abbreviate (Genus)** now branches off from the **Genus (Label)** property.

28. In the *Data source overview* panel, select the derived property **Abbreviate (Genus)** and while holding down the **Ctrl-key** select **Species**. Select **Dataset > New derived property...** (🔍+) again.
29. Choose the option **Merge two strings** and press **<Next>**.
30. Select **Abbreviate (Genus)** as **String 1**, **Species** as **String 2** and replace the comma with a space in the **Template** text box so that the template looks as "**^1 ^2**" (see Figure 6).

Figure 6: Merge two strings.

31. Press **<Finish>** to add the derived property to the *Data source overview* panel.
32. Right-click on the new derived property in the *Data source overview* panel (**Merge two strings**) and choose **Use as Chart Label**.
33. Choose **Plot > Edit active plot properties...** (📊), specify **Taxon** as **X axis label** and press **<OK>**.

The result looks as in Figure 7.

34. Close the *Charts and statistics* window with **File > Exit**.
35. Save the comparison by selecting **File > Save** (💾, **Ctrl+S**).
36. Specify the name **All** and press **<OK>**.
37. Close the comparison with **File > Exit**.

The comparison **All** is now listed in the *Comparisons* panel of the *Main* window.

4 Profile chart

4.1 Example 1

1. In the *Database entries* panel of the *Main* window, double-click on an entry to open its *Entry* window.
2. Select **File > Charts and statistics...** (📊, **F7**).

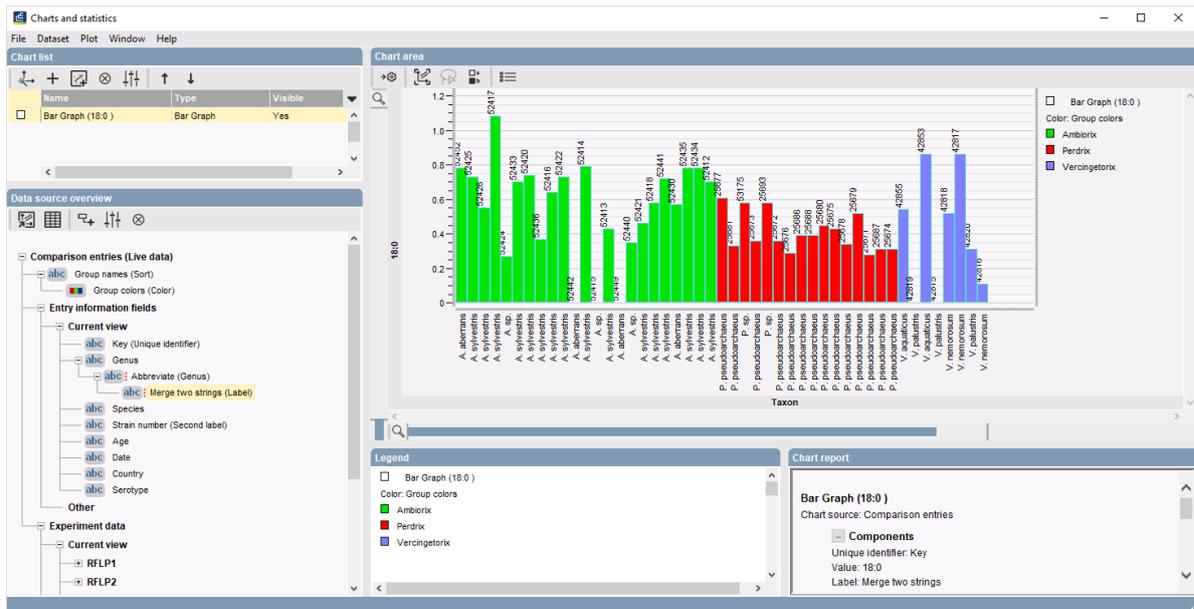


Figure 7: Bar graph.

3. In the *Create chart* dialog box, select **RFLP1 Curve** under **Fingerprint experiments** and press **<OK>**.
4. Select **Profile chart** in the next step and press **<Next>**.
5. Highlight **Value** in the next step and press **<Next>** and **<Finish>**.

A profile chart of densitometric values from the **RFLP1** profile for the selected entry appears in the *Chart area* panel (Figure 8).

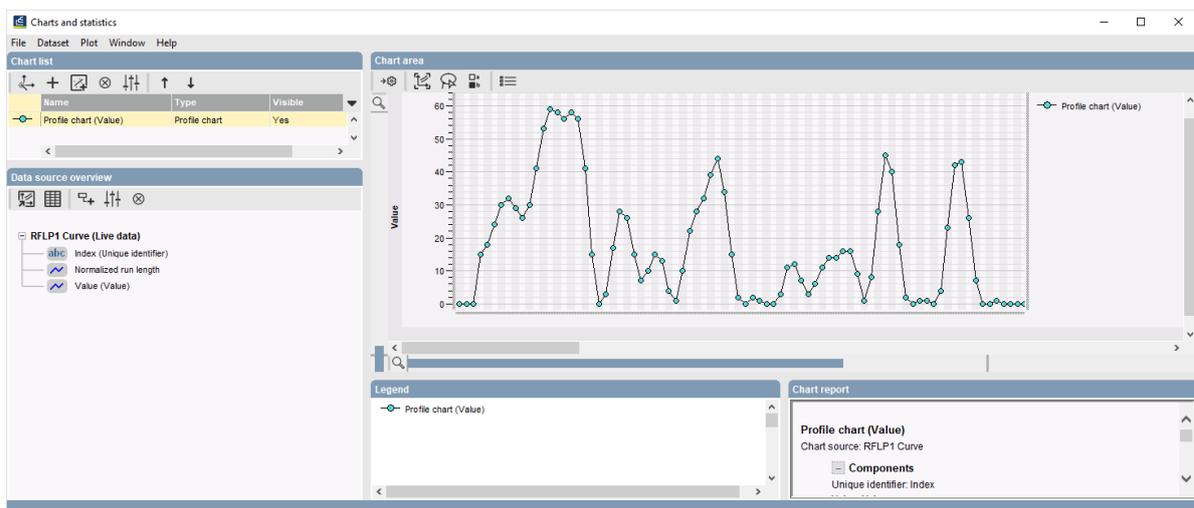


Figure 8: Profile chart from curve data.

We will now use the copy and paste functions to display another curve in the same *Charts and statistics* window.

6. Bring the *Main* window back into focus without closing the *Charts and statistics* window.
7. Double-click on another entry in the *Main* window to open its *Entry* window.

8. Select **File > Charts and statistics...** (📊, F7).
9. In the *Create chart* dialog box, select **RFLP1 Curve** under **Fingerprint experiments** and press **<OK>**.
10. Select **Profile chart** in the next step and press **<Next>**.
11. Highlight **Value** in the next step and press **<Next>** and **<Finish>**.

A profile chart of densitometric values from the **RFLP1** profile for the selected entry appears in the *Chart area* panel.

12. Select **Plot > Copy active plot**. Bring the first *Charts and statistics* window into focus and select **Plot > Paste plot**.

The *Charts and statistics* window now contains two charts: the original one (cyan dots) and the pasted one (red dots) (see Figure 9). Note that the original chart has a live data source whereas the pasted chart does not, because it is just a copy which is not linked anymore to its parent *Entry* window.

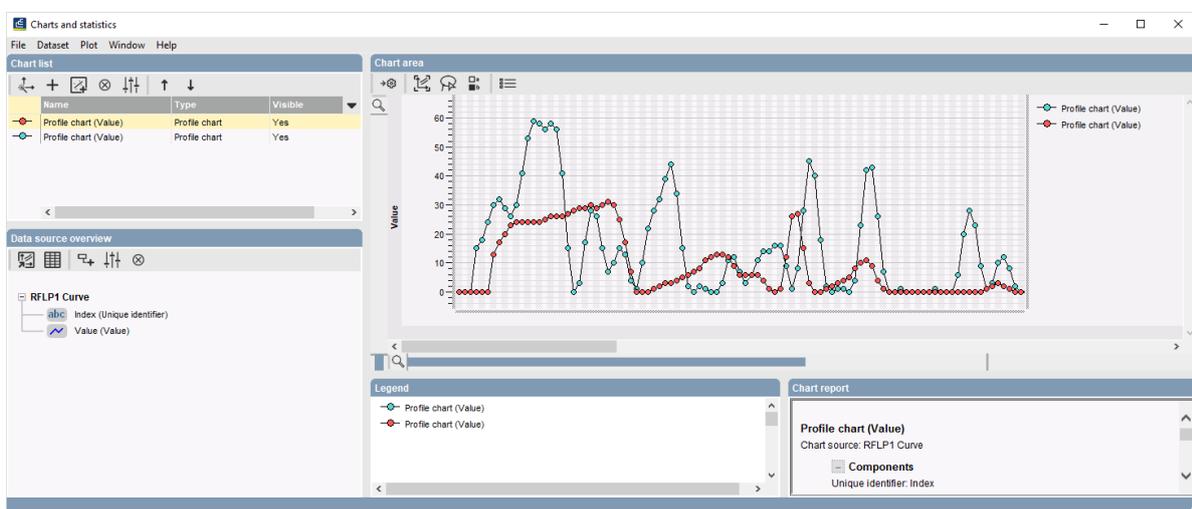


Figure 9: Two profile charts.

13. Close the *Charts and statistics* window with **File > Exit** and close the *Entry* window.

4.2 Example 2

14. Double-click on the comparison **All** in the *Comparisons* panel of the *Main* window to open the saved comparison.



If the comparison **All** is not present in the **DemoBase Connected**, select all entries in the *Main* window with **Ctrl+A** and unselect those labeled as **STANDARD** in the **Genus** field. Highlight the *Comparisons* panel in the *Main* window and select **Edit > Create new object...** (+). In the *Comparison* window, right-click in the header of the "Genus" field in the *Information fields* panel and select **Create groups from database field** from the menu and confirm the creation of the groups.

15. In the *Comparison* window, select **Statistics > Chart and statistics...** (F7).
16. Select **Comparison entries** in the dialog box that pops up and press **<OK>**.

17. Select **Profile chart** in the next step and press <Next>.
18. In the next step choose **PhenoTest: Values: c17** and press <Next>.
19. In the last step choose **Entry information fields: Genus** as **Label** and press <Finish>.

The value for character c17 is now displayed for all entries in the *Chart area* panel of the *Charts and statistics* window. The label **Genus** identifies the entries on the chart.

A chart can be sorted according to a selected string or value property. As an example, we will sort the chart according to the character it is based upon.

20. Right-click on **c17 (Value)** in the *Data source overview* panel under **PhenoTest** and select **Use as Chart Sort** from the floating menu.

Now it becomes clear that there is a correlation between the intensity of the character c17 and the genus. Alternatively, the genus name can also be used as a sort property:

21. Right-click on **Genus (Label)** in the *Data source overview* panel and select **Use as Chart Sort** from the floating menu.

Ideally, we would like to see the genus and species information as chart labels, rather than only the genus name. Since only one chart label can be displayed at a time, we will create a *derived property*, containing the first character of the genus name and the full species name.

22. Highlight **Genus** in the *Data source overview* panel (probably indicated as **Genus (Label) (Sort)**) and select **Dataset > New derived property...** (☰+).
23. In the *Create derived property* wizard, select **Abbreviate** and press <Next>.
24. Leave the options on the second page to their defaults and press <Finish>.

A derived property **Abbreviate (Genus)** now branches off from the **Genus** property.

25. Select the derived property **Abbreviate (Genus)** and while holding down the **Ctrl-key**, select **Species**.
26. Select **Dataset > New derived property...** (☰+) to create a new derived property.
27. Select **Merge two strings** to concatenate the abbreviated genus name and the species name into a new string and press <Next>.
28. In the next page, choose **Abbreviate (Genus)** as **String 1** and **Species** as **String 2**. As **Template**, replace the comma between ^1 and ^2 by a space so that the template looks as " ^1 ^2 " (see Figure 10).
29. Press <Finish> to create the new derived property.
30. Right-click on the new derived property **Merge two strings** and select **Use as Chart label** from the floating menu.

This derived property can also be used to sort the chart:

31. Right-click on the derived property **Merge two strings** and select **Use as Chart Sort** from the floating menu.

The profile chart can further be supplied with additional information fields. For example, a *chart point label* can be added as follows:

32. Right-click on **Strain number** in the *Data source overview* panel and select **Use as Chart Point label** from the floating menu.

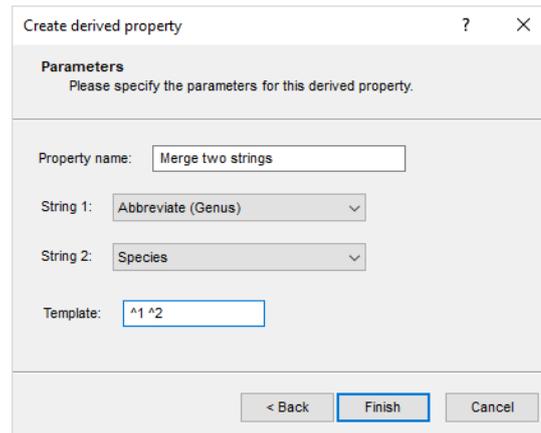


Figure 10: Merge two strings.

The strain numbers are now displayed as additional information on top of the chart points. The current profile chart displays just one character for the selected set of entries. The legend shows the symbol and color used for this chart (see Figure 11).

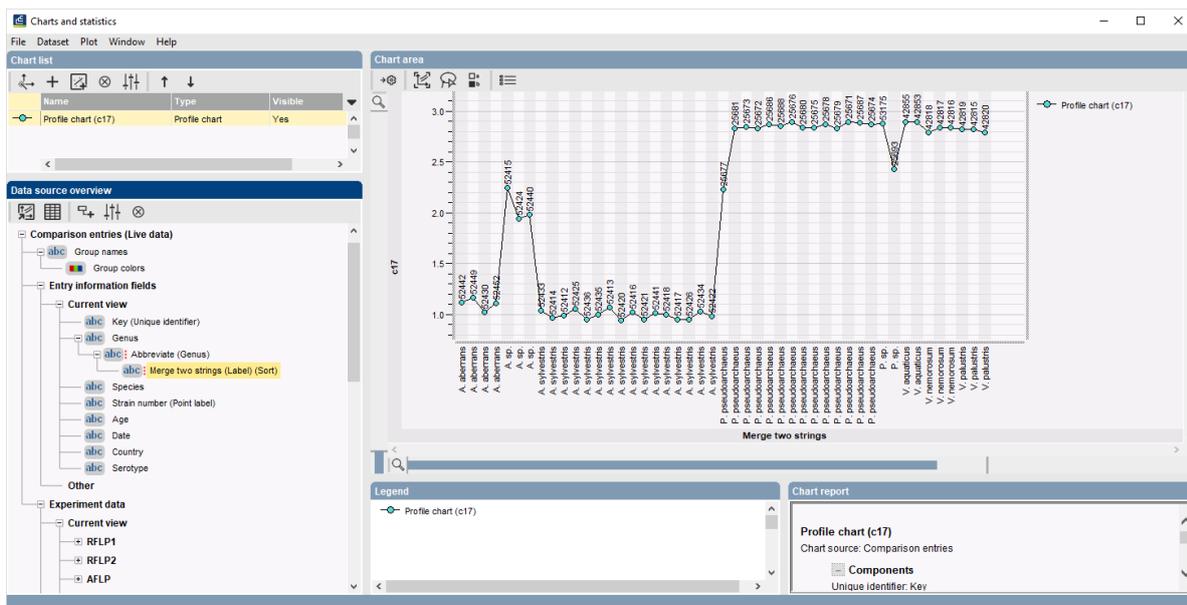


Figure 11: One profile chart.

By selecting additional numerical properties as chart values, a profile chart can display multiple characters in the same graph:

33. Right-click on **c19** in the *Data source overview* panel under **PhenoTest** and select **Use as Chart Value**.

The chart now displays a profile for the two characters. The legend still lists one profile chart, but containing multiple components. Alternatively, you can also display the second character profile in a separate chart, which has the advantage that you can assign different colors or symbols to the profiles.

34. First, remove character c19 from the current profile by right-clicking on **c19 (Value)** in the *Data source overview* panel under **PhenoTest** and selecting **Use as Chart Value** from the floating menu.

35. Click on **c19**, hold down the **Ctrl-key** and click on the derived property **Merge two strings**.
36. Create a new chart with **Plot > Add new plot from selected properties...** (+).
37. Select **Profile chart** and press <**Next**>.
38. Press <**Finish**> to create the profile chart.

The chart area is updated and the two characters are listed with a different color in the legend panel.

39. Close the *Charts and statistics* window with **File > Exit**.

5 Contingency table

5.1 Example 1

1. In the *Database entries* panel of the *Main* window, make sure all entries are selected except the "STANDARD" entries. With this selection, create a *Charts and statistics* window with **Analysis > Chart and statistics...** (📊, F7).
2. Select **Currently selected entries** and press <**OK**>.
3. Select **Contingency table** in the next step and press <**Next**>.
4. Choose **Entry information fields: Country** as **Column** and **Entry information fields: Serotype** as **Row** and press <**Finish**> (see Figure 12).

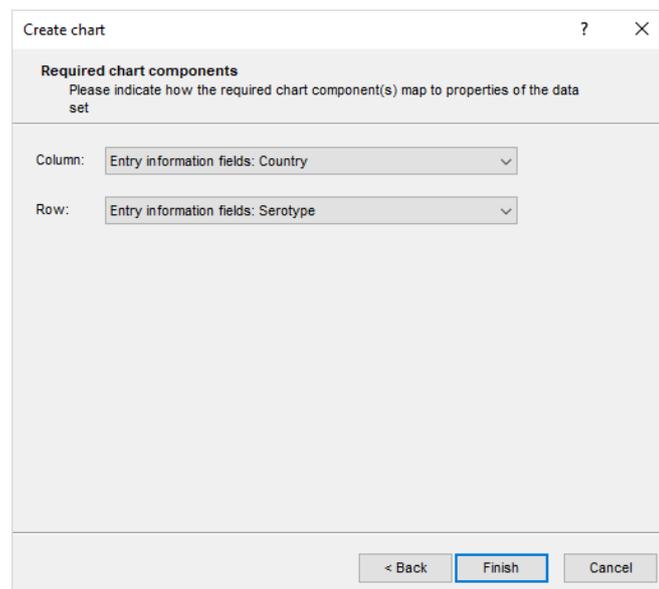


Figure 12: Chart components.

By default, the contingency table displays the member counts per cell and the cells are colored according to the member counts using a color scale blue-green-yellow-orange-red. In addition, the order of the cells is determined by the appearance in the database (see Figure 13).

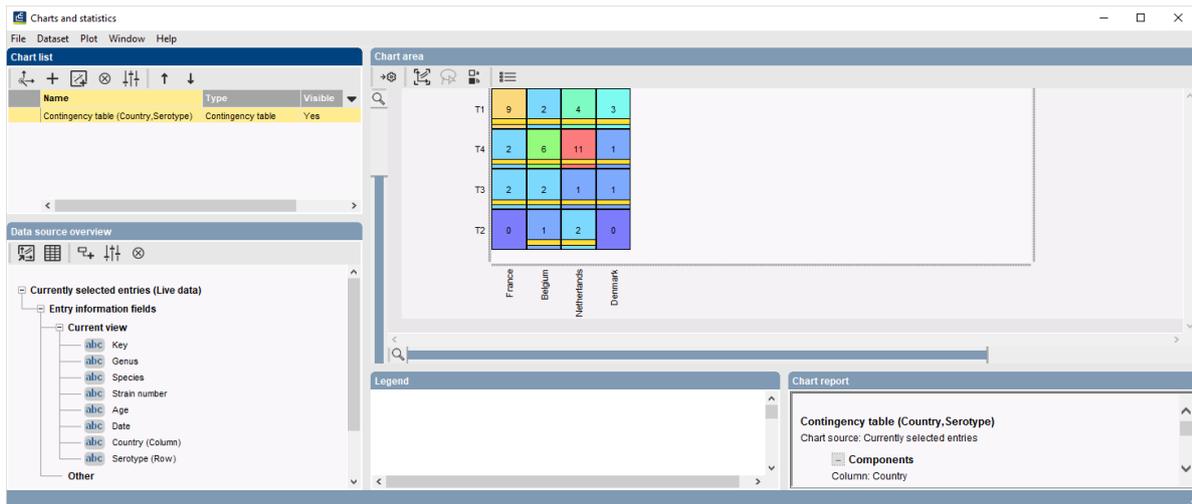


Figure 13: Contingency table.

The currently selected entries are shown in the contingency table as yellow bars in the cells. The width of the bar in a cell is proportional to the relative number of entries selected within the cell.

5. To clear the selection, press the **F4**-key.
6. Select the entries of a particular cell by clicking in the cell while holding down the **Ctrl**-key. To select multiple cells at once, hold down the **Shift**-key while dragging the mouse over the cells to select.
7. To change the appearance settings, select **Plot > Edit active plot properties...** (⌘+P).
8. Select **Alphabetical** as **Column sort** and **Row sort**.
9. Choose **Row percentages** as **Quantification** and **Gray scale** as **Cell background**. Press **<OK>** to apply the changes.
10. Close the *Charts and statistics* window with **File > Exit**.

5.2 Example 2

11. Repeat the steps in 5.1, but now choose **3D contingency chart** as plot type and choose **Entry information fields: Country** as **First category** and **Entry information fields: Genus** as **Second category**.

The 3D contingency chart displays the frequency distribution in a 3D bar graph (see Figure 14).

12. Drag the mouse of the image to rotate the 3-D view in all directions.
13. Close the *Charts and statistics* window with **File > Exit**.

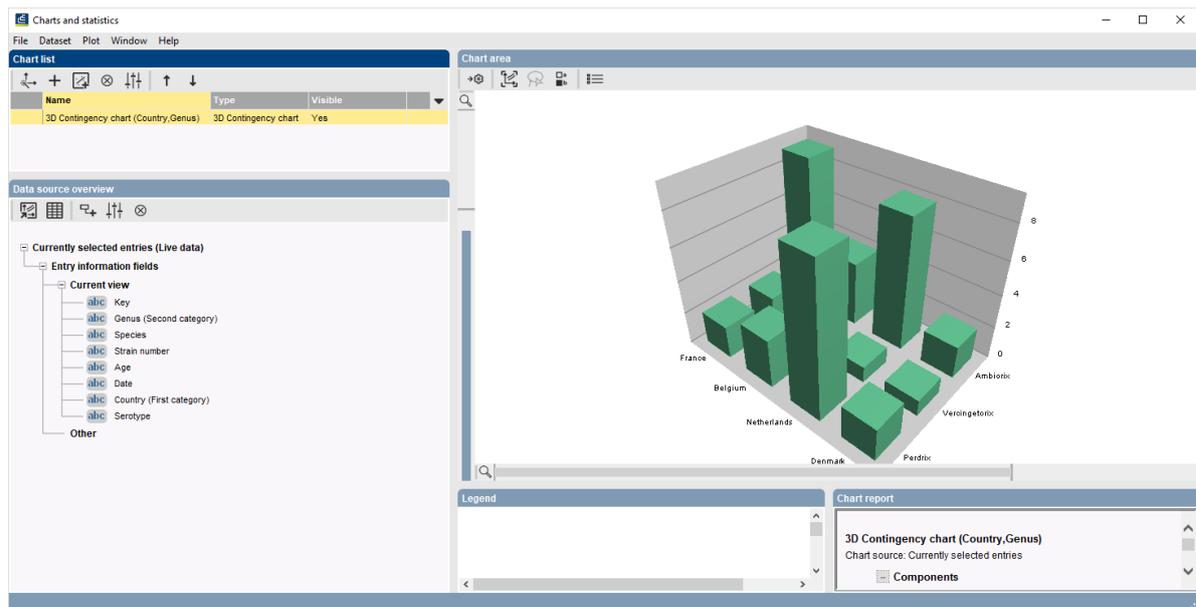


Figure 14: 3D contingency chart.

6 Scatter chart

6.1 Example 1

1. Double-click on the comparison **All** in the *Comparisons* panel of the *Main* window to open the comparison.



If the comparison **All** is not present in the **DemoBase Connected**, select all entries in the *Main* window with **Ctrl+A** and unselect those labeled as **STANDARD** in the **Genus** field. Highlight the *Comparisons* panel in the *Main* window and select **Edit > Create new object...** (+). In the *Comparison* window, right-click in the header of the "Genus" field in the *Information fields* panel and select **Create groups from database field** from the menu.

2. In the *Comparison* window, select **Statistics > Chart and statistics...** (F7).
3. Select **Comparison entries** in the dialog box that pops up and press <OK>.
4. Select **Scatter chart** in the next step and press <Next>.
5. In the next step choose **PhenoTest: Values: c17** as **X axis** and **PhenoTest: Values: c19** as **Y axis** and press <Next>.
6. In the last step, select **Entry information fields: Strain number** as **First Label** and press <Finish>.

The two characters are now displayed in an X-Y coordinate system with c17 as X axis and c19 as Y axis. Each dot in the scatter chart represents an entry plotted according to its respective values for c17 and c19. It can be seen from this chart that the scatter for these two characters is not random.

The *Entry* window can be revealed from the chart area by double-clicking on a dot. Additionally, it is also possible to select entries in the chart area using **Ctrl+click** or by holding down the **Shift**-key while dragging the mouse arrow over the dots to select.

In dense areas with on the scatter chart, the **Strain number** information may become illegible, and therefore using symbols or colors may be more informative.

7. First, remove the entry labels from the scatter chart by right-clicking on **Strain number** in the *Data source overview* panel and selecting **Use as Chart First Label**.
8. Right-click on **Group colors** under **Group names** in the *Data source overview* panel and select **Use as Chart Color** from the floating menu.

The chart area now looks as in Figure 15.

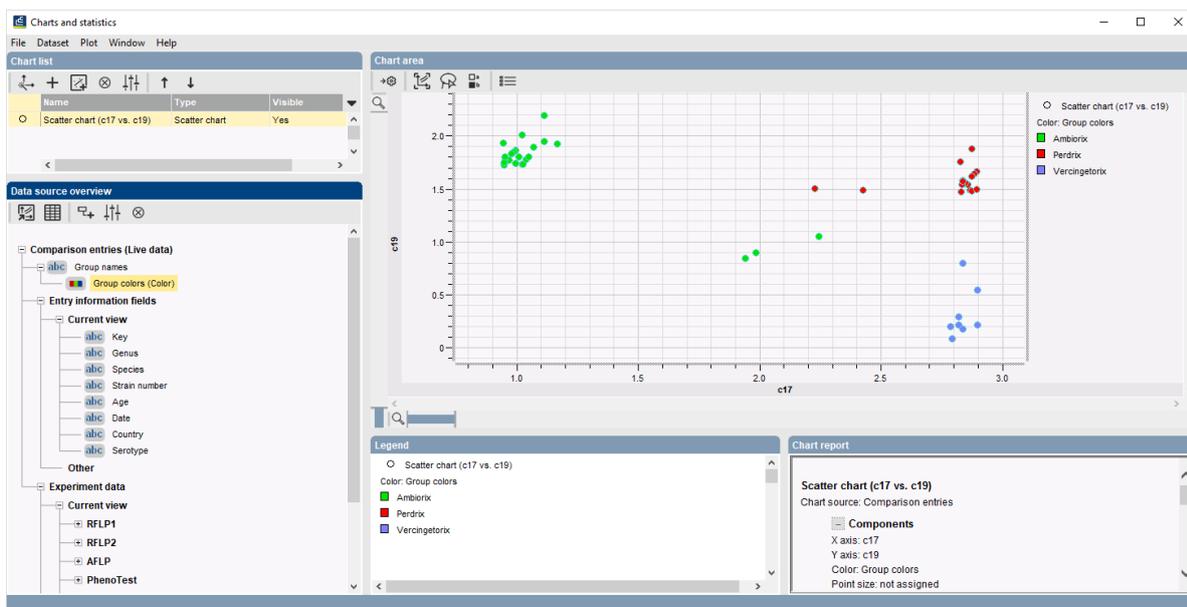


Figure 15: Scatter plot of two characters.

9. Close the *Charts and statistics* window with **File > Exit**.

6.2 Example 2

10. Repeat the steps in 6.1, but now choose **3D Scatter chart** as plot type and choose **PhenoTest: Values: c17**, **PhenoTest: Values: c18** and **PhenoTest: Values: c19** as X, Y and Z axis respectively.
11. In the last step of the wizard choose **Group names: Group colors** as **Color** label and press **<Finish>**.

The 3D Scatter chart displays the data as a collection of points in a 3-D space, with the values of three selected characters determining the position on the X, Y and Z axis (see Figure 16).

12. Drag the mouse of the image to rotate the 3-D view in all directions.
13. Close the *Charts and statistics* window with **File > Exit**.

7 Frequency bar graph

1. Double-click on the comparison **All** in the *Comparisons* panel of the *Main* window to open the comparison.

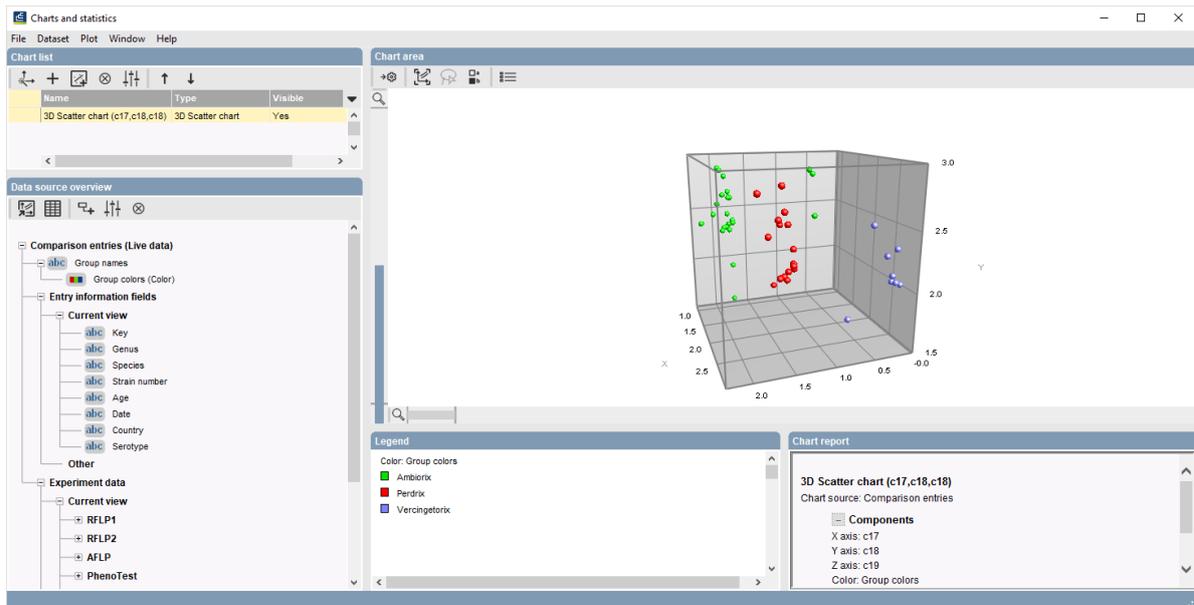


Figure 16: 3D Scatter chart.



If the comparison **All** is not present in the **DemoBase Connected**, select all entries in the **Main** window with **Ctrl+A** and unselect those labeled as **STANDARD** in the **Genus** field. Highlight the **Comparisons** panel in the **Main** window and select **Edit > Create new object...** (+). In the **Comparison** window, right-click in the header of the "Genus" field in the **Information fields** panel and select **Create groups from database field** from the menu.

2. In the **Comparison** window, select **Statistics > Chart and statistics...** (F7).
3. Select **Comparison entries** in the dialog box that pops up and press <OK>.
4. Choose **Frequency bar graph (colored)** as chart type and press <Next>.
5. Choose **Entry information fields: Country** as **Category** and the **Group names: Group colors** as **Color** label in the next step (see Figure 17) and press <Finish>.

A frequency bar graph is created in the **Chart area** panel of the **Charts and statistics** window (see Figure 18).

6. Close the **Charts and statistics** window with **File > Exit**.

8 Pie chart histogram

1. In the **Main** window, make sure all entries are selected except the "STANDARD" entries. With this selection, create a **Charts and statistics** window with **Analysis > Chart and statistics...** (📊, F7).
2. Select **Currently selected entries** and press <OK>.
3. Select **Pie chart histogram table** in the next step and press <Next>.
4. Choose **Entry information fields: Genus** as **Column category** and **Entry information fields: Country** as **Row category** and press <Finish>.

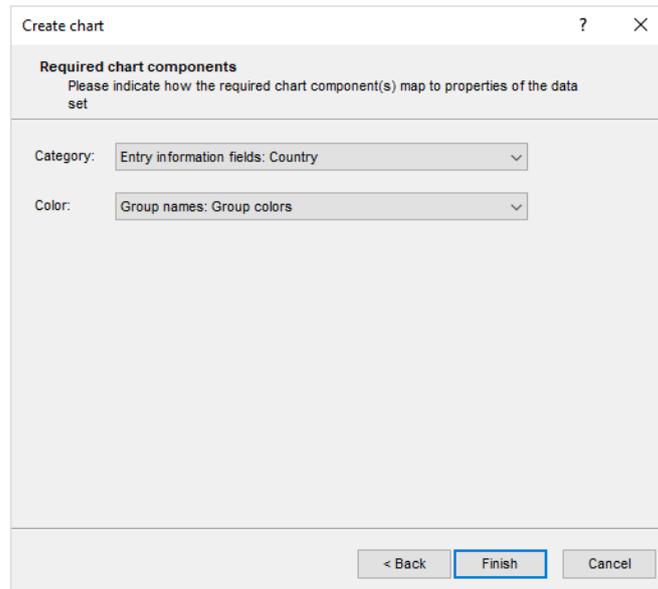


Figure 17: Chart components.

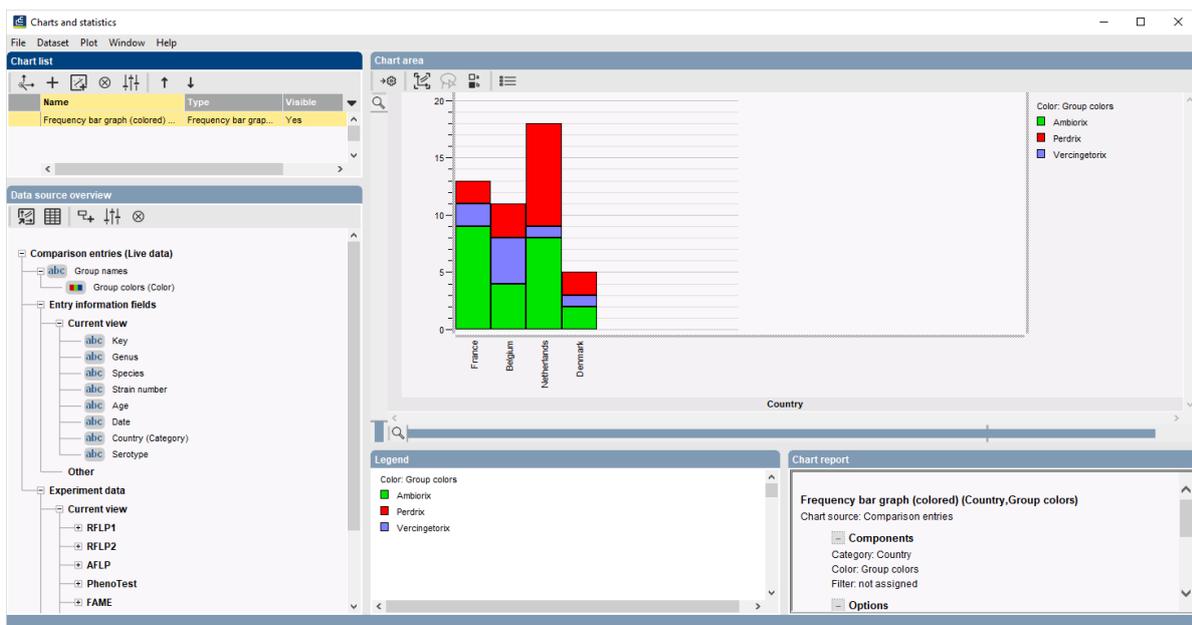


Figure 18: Frequency bar graph.

A pie chart histogram table displays the frequency distribution of the two selected categorical properties, with one category represented as rows, the other as columns (cf. contingency table). The frequency over the row and column category is indicated by the size of the pie charts.

5. Press the **F4**-key to clear the selection.

We will now add a third category (a color property):

6. In the *Data source overview* panel, select **Serotype** and select **Dataset > New derived property...** ($\square+$) to create a new derived property.

7. Choose **Convert to color** and press **<Next>** and **<Finish>**.

- Right-click on the new derived property **Convert to color (Serotype)** and select **Use as Chart Pie chart category** from the floating menu.

The chart area now looks as in Figure 19.

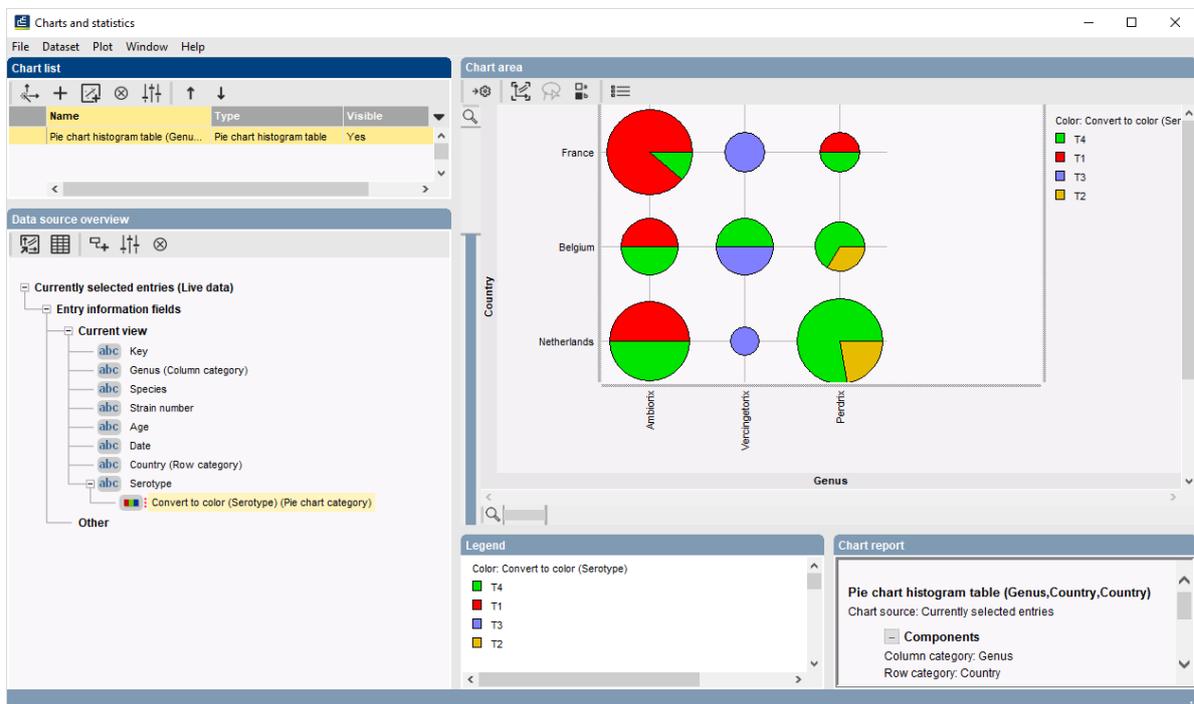


Figure 19: Pie chart histogram.

- Close the *Charts and statistics* window with **File > Exit**.

9 ANOVA chart

Before an ANOVA chart based on the **Age** information can be created, the property of this field needs to be changed from **String** to **Number**:

- In the *Database entries* panel of the *Main* window, right-click on the entry field header **Age**, and select **Field properties ...** from the pop-up menu that appears.

This action opens the *Database field properties* dialog box.

- Change the **Content type** to "Number" and press <OK> to close the dialog.
- In the *Database entries* panel of the *Main* window, make sure all entries are selected except the "STANDARD" entries. With this selection, create a *Charts and statistics* window with **Analysis > Chart and statistics...** (📊, F7).
- Select **Currently selected entries** and press <OK>.
- Select **ANOVA chart** in the next step and press <Next>.
- Choose **Entry information fields: Age** as **Value** and **Entry information fields: Country** as **Category** (see Figure 20).
- Press <Next> and <Finish>.

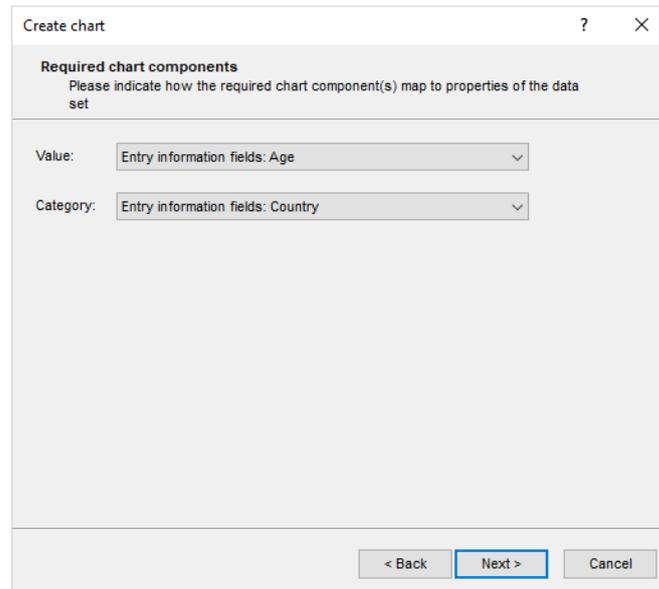


Figure 20: Chart components.

The ANOVA chart is displayed in the *Chart area* panel of the *Charts and statistics* window and summarizes the value property **Age** over the **Country** categories.

Optionally a color property can be added to the chart:

8. Highlight **Genus** in the *Data source overview* panel and select **Dataset > New derived property...** (📄+) to create a new derived property.
9. In the *Create derived property* wizard, select **Convert to color** and press <Next> and <Finish>.
10. Right-click on the new derived property **Convert to color (Genus)** and select **Use as Chart color** from the floating menu.

The chart area now looks as in Figure 21.

11. Close the *Charts and statistics* window with **File > Exit**.

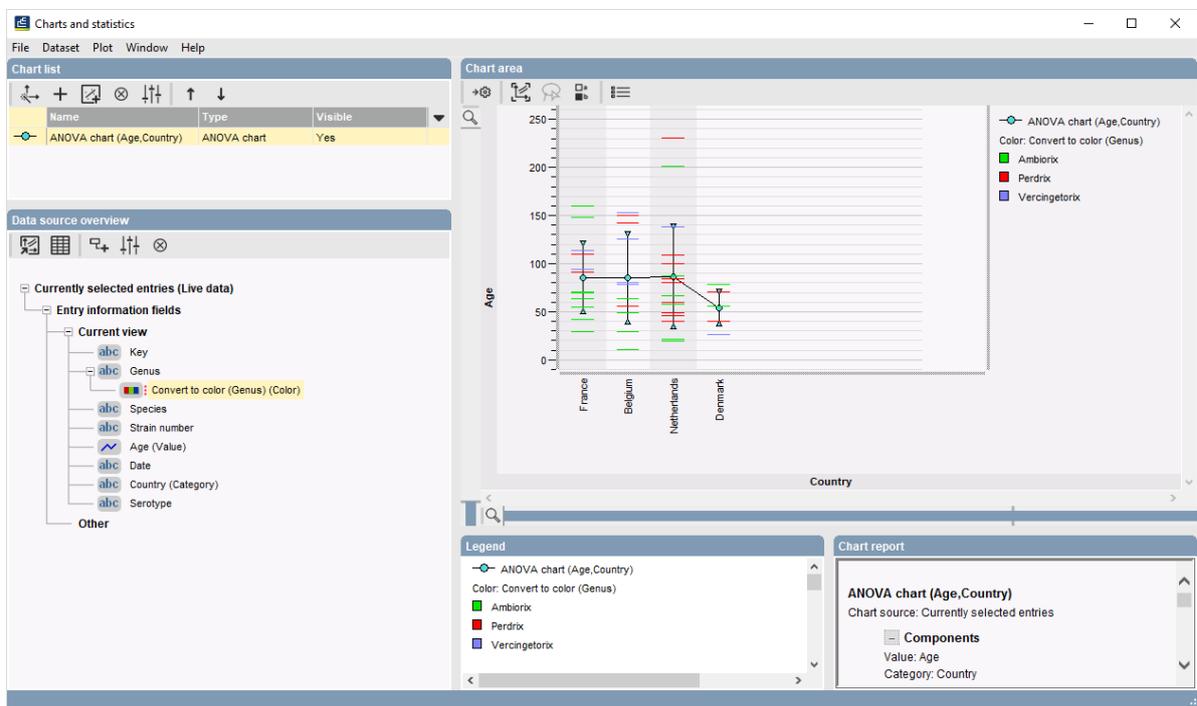


Figure 21: ANOVA chart.