

BioNumerics Tutorial:

Importing carbon source oxidation data from Omnilog csv files

1 Aim

Sequential measurements that express an evolution of one parameter in function of another (e.g. enzymatic activity, growth curves, etc.) are called *trend type data* and can be imported and analyzed in our BioNumerics software package.

In this tutorial you will learn how to import trend data in your BioNumerics database, how to fit a curve through the measurement points, and how to deduce parameters from the curve function to compare the samples.

2 Preparing the database

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

1. To download the database directly from the *BioNumerics Startup* window, click the **Download example databases** link, located in the lower right corner of the *BioNumerics 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 <http://www.applied-maths.com/download/sample-data>, under 'DemoBase Connected'.

In the *BioNumerics 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.

3 Example data

The example Omnilog data files from which we will import data in this tutorial can be downloaded from the Applied Maths website: go to <http://www.applied-maths.com/download/sample-data> and click on 'Trend data sample files'.

1. Open one of the files (e.g. `G@Ge107@004.csv`) to examine the data that will be imported.

Each file contains information about the utilization of carbon substrates of a certain strain (see Figure 1):

1	Data File	Setup Time	Position	Plate Type	Strain Type	Sample Number	Strain Name	Strain Number	Other	Hour	A01	A02	A03	A04
2	C:\Users\Documents\	4/27/2012 2:41:14 PM	2-A	PM01			Vercingetorix palustris	G@Gel07@004	0.00	17.00	16.00	11.00	11.00	
3	C:\Users\Documents\	4/27/2012 2:41:14 PM	2-A	PM01			Vercingetorix palustris	G@Gel07@004	0.25	20.00	26.00	11.00	16.00	
4	C:\Users\Documents\	4/27/2012 2:41:14 PM	2-A	PM01			Vercingetorix palustris	G@Gel07@004	0.50	16.00	32.00	11.00	11.00	
5	C:\Users\Documents\	4/27/2012 2:41:14 PM	2-A	PM01			Vercingetorix palustris	G@Gel07@004	0.75	17.00	48.00	14.00	12.00	
6	C:\Users\Documents\	4/27/2012 2:41:14 PM	2-A	PM01			Vercingetorix palustris	G@Gel07@004	1.00	23.00	63.00	21.00	17.00	
7	C:\Users\Documents\	4/27/2012 2:41:14 PM	2-A	PM01			Vercingetorix palustris	G@Gel07@004	1.25	21.00	72.00	28.00	16.00	
8	C:\Users\Documents\	4/27/2012 2:41:14 PM	2-A	PM01			Vercingetorix palustris	G@Gel07@004	1.50	22.00	88.00	29.00	17.00	
9	C:\Users\Documents\	4/27/2012 2:41:14 PM	2-A	PM01			Vercingetorix palustris	G@Gel07@004	1.75	23.00	101.00	37.00	17.00	
10	C:\Users\Documents\	4/27/2012 2:41:14 PM	2-A	PM01			Vercingetorix palustris	G@Gel07@004	2.00	23.00	110.00	40.00	18.00	
11	C:\Users\Documents\	4/27/2012 2:41:14 PM	2-A	PM01			Vercingetorix palustris	G@Gel07@004	2.25	19.00	117.00	42.00	16.00	
12	C:\Users\Documents\	4/27/2012 2:41:14 PM	2-A	PM01			Vercingetorix palustris	G@Gel07@004	2.50	19.00	123.00	53.00	13.00	

Figure 1: Csv file: an example.

- The **Hour** column contains the X-values (= time points). Each panel is screened every 15 minutes.
- The 96 columns labeled with **A01** to **H12** contain the Y-values (= the data signal).
- The first row describes the columns.
- Additional columns are present containing plate and strain information.

4 Create a trend data experiment

1. In the *BioNumerics Startup* window, double-click on the **DemoBase Connected** database to open it.
2. In the *Main* window, click on  in the toolbar of the *Experiment types* panel and select **Trend data type** from the list (see Figure 2).

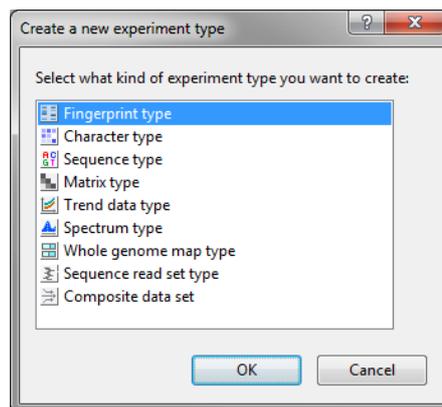


Figure 2: The *Create a new experiment type* dialog box.

3. Press **<OK>**, enter a name, for example **Omnilog** and press **<Finish>** to complete the creation of the new trend data type.

The *Experiment types* panel now lists the trend data type **Omnilog**.

4. Open the *Trend type* window by double-clicking on **Omnilog** in the *Experiment types* panel.

The *Trend type* window is initially empty. Trend curves can be added either manually (*TrendCurves > Add new trend curve...*) or during import (see 5).

5 Importing trend data

1. Select **File > Import...** (📁, **Ctrl+I**) to open the *Import* dialog box.
2. Choose the option **Import trend data** under the **Trend data type data** item in the tree and press **<Import>**.

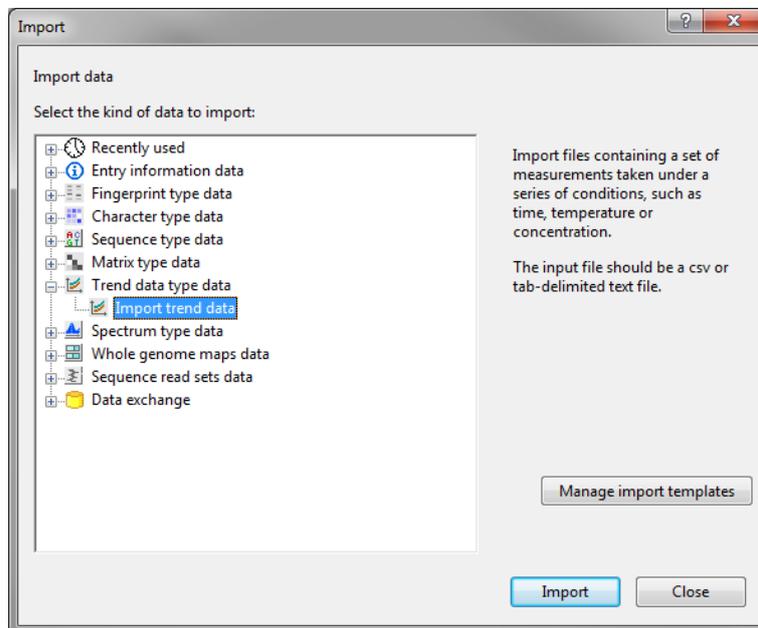


Figure 3: Import tree.

3. Press **<Browse>** and browse for the downloaded csv files in the Omnilog folder.

The *Input* wizard page is updated (see Figure 4).

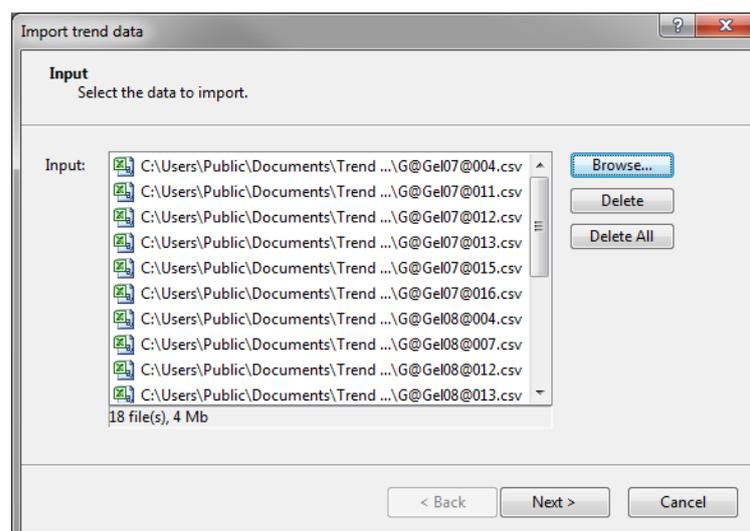


Figure 4: The *Input* wizard page.

4. Press **<Next>**.

As this is the first time we import trend data into the database, we need to create a new import template by specifying **Import rules**.

All columns detected in the selected csv files are listed in the grid.

5. Select the *Strain Number* row in the list and click **<Edit destination>** or simply double-click on the row. Select "Key" as the destination field and press **<OK>**.
6. Select the *Hour* row in the list and click **<Edit destination>**. Select "X-axis" as the BioNumerics destination field under *Trend curve value > Omnilog* in the *Edit data destination* dialog box and press **<OK>** (see Figure 5).

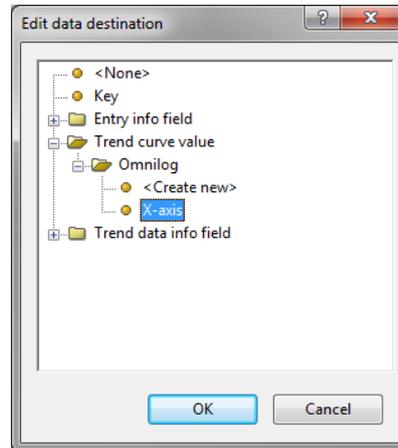


Figure 5: The *Edit data destination* dialog box.

7. Click on "A01", scroll down the list and whilst holding the **Shift**-key, click on "H12" to make a multiple selection of the 96 trend data curves.
8. Press **<Edit destination>**, select "Omnilog" under *Trend curve value* as destination and click **<OK>** (see Figure 6).

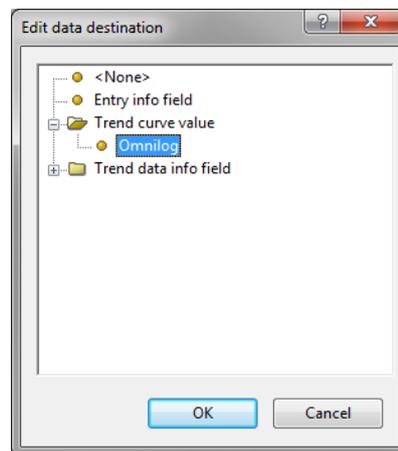


Figure 6: The *Edit data destination* dialog box.

The software tries to map the column names to existing trend data curves. When there is no trend data curve present with the same name, you will be prompted to create the new trend data curves (see Figure 7).

9. Press **<OK>** and then **<Yes>** to confirm the creation of the curves.

The grid is updated and should now look like in Figure 8.

10. Press the **<Preview>** button to verify that all information will correctly be imported in the database (see Figure 9).

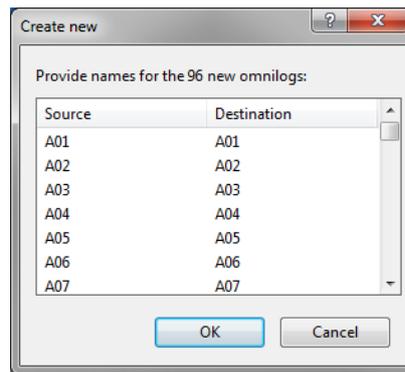


Figure 7: Create new trend data curves.

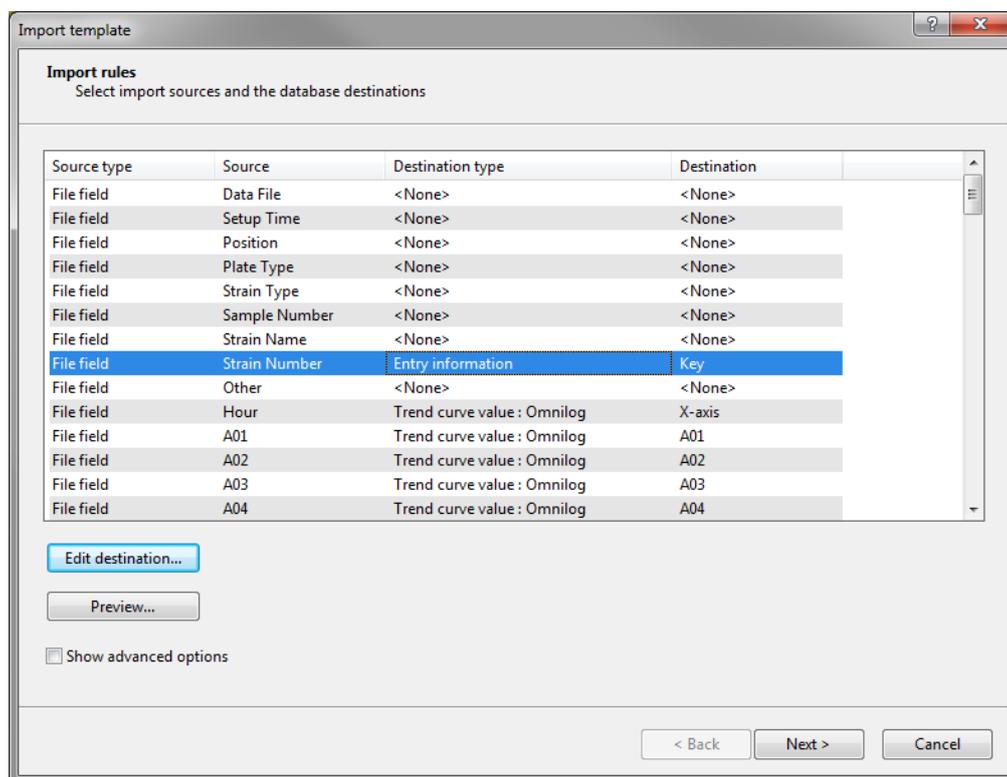


Figure 8: Import rules.

11. Press **<Next>** to proceed to the *Import links* dialog box.
12. Make sure "Key" is checked and press **<Finish>**.

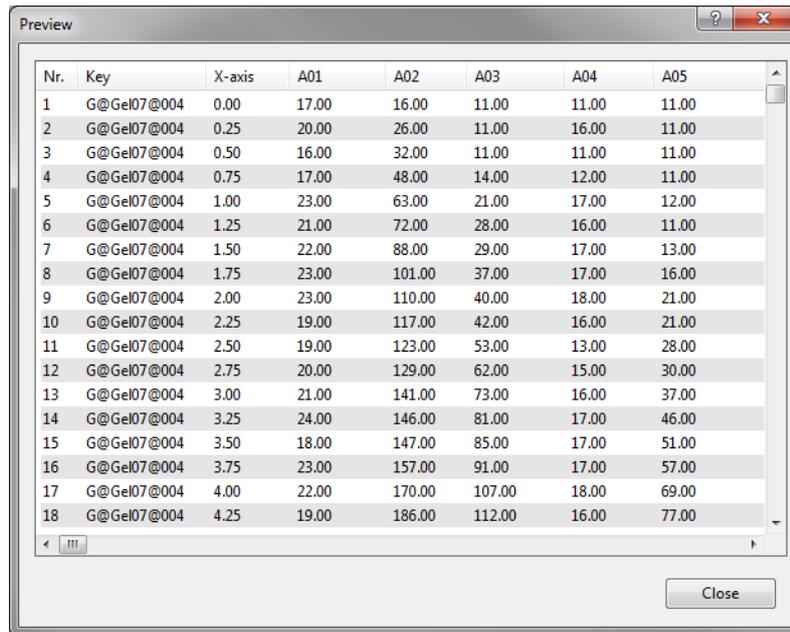
The import template needs to be saved to be able to use it again later on.

13. Enter a **Name** for the import template (e.g. "Omnilog template") and optionally a **Description**. Press **<OK>**.
14. Highlight the newly created template and click **<Next>**.

This next dialog will indicate that 18 entries will be updated during import (see Figure 10).

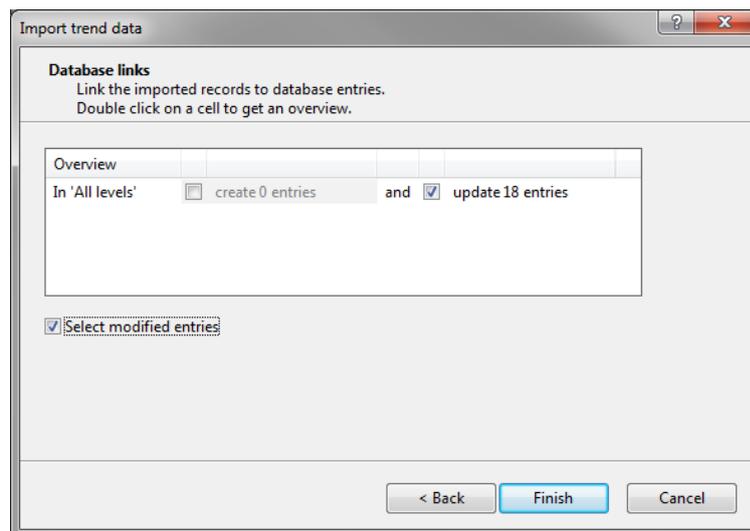
15. Press **<Finish>** to start the actual import. The progress of the import is shown while database information is added to the BioNumerics database.

All entries for which data is imported are automatically selected in the *Database entries* panel.



Nr.	Key	X-axis	A01	A02	A03	A04	A05
1	G@Gel07@004	0.00	17.00	16.00	11.00	11.00	11.00
2	G@Gel07@004	0.25	20.00	26.00	11.00	16.00	11.00
3	G@Gel07@004	0.50	16.00	32.00	11.00	11.00	11.00
4	G@Gel07@004	0.75	17.00	48.00	14.00	12.00	11.00
5	G@Gel07@004	1.00	23.00	63.00	21.00	17.00	12.00
6	G@Gel07@004	1.25	21.00	72.00	28.00	16.00	11.00
7	G@Gel07@004	1.50	22.00	88.00	29.00	17.00	13.00
8	G@Gel07@004	1.75	23.00	101.00	37.00	17.00	16.00
9	G@Gel07@004	2.00	23.00	110.00	40.00	18.00	21.00
10	G@Gel07@004	2.25	19.00	117.00	42.00	16.00	21.00
11	G@Gel07@004	2.50	19.00	123.00	53.00	13.00	28.00
12	G@Gel07@004	2.75	20.00	129.00	62.00	15.00	30.00
13	G@Gel07@004	3.00	21.00	141.00	73.00	16.00	37.00
14	G@Gel07@004	3.25	24.00	146.00	81.00	17.00	46.00
15	G@Gel07@004	3.50	18.00	147.00	85.00	17.00	51.00
16	G@Gel07@004	3.75	23.00	157.00	91.00	17.00	57.00
17	G@Gel07@004	4.00	22.00	170.00	107.00	18.00	69.00
18	G@Gel07@004	4.25	19.00	186.00	112.00	16.00	77.00

Figure 9: Preview of the parsed data.



Database links
Link the imported records to database entries.
Double click on a cell to get an overview.

Overview				
In 'All levels'	<input type="checkbox"/> create 0 entries	and	<input checked="" type="checkbox"/> update 18 entries	

Select modified entries

< Back Finish Cancel

Figure 10: Update entries in the database.

The imported trend data is stored in the trend data type **Omnilog**.

16. Double-click on the experiment **Omnilog** in the *Experiment types* panel.

The 96 trend data curves are displayed in the *Curves* panel of the *Trend type* window. Optionally a **Description** can be given to each curve:

17. Click twice on a cell in **Description** column. The information will appear highlighted and can be edited (see Figure 11).

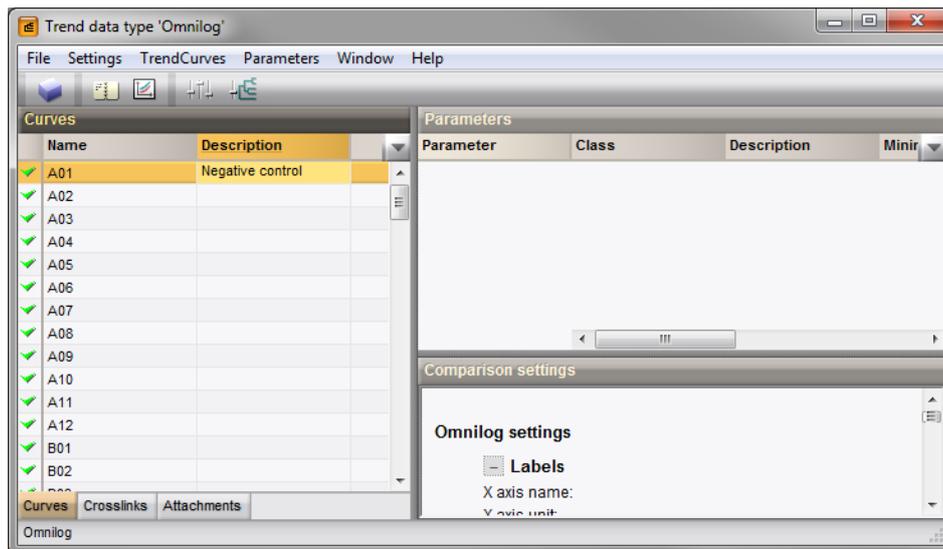


Figure 11: The *Trend* type window.

6 Defining parameters

For visualization and comparison purposes, a default *curve fit model* needs to be specified.

1. In the *Trend* type window select **Settings > Default trend curve model...** to call the *Trend curve fit model* dialog box (see Figure 12).

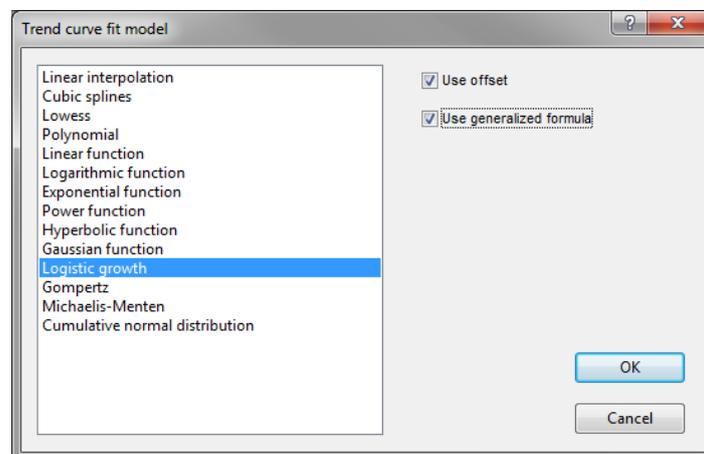


Figure 12: Set trend curve model.

2. Choose a fit, e.g. **Logistic growth** and check both **Use offset** and **Use generalized formula**.
3. Press **<OK>** to set the curve model.

Before any analysis can be done, parameters have to be defined. Parameters can be deduced from the model function (**Parameters > Model parameters...**) or from the original data points (**Parameters > Statistics parameters...**).

4. In the *Trend* type window select **Parameters > Statistics parameters...** to call the *Statistics parameters* dialog box.
5. Check **Mean** for the **Y value** and press **<OK>** (see Figure 13).

Since all curves have been measured using the same time scale (= same X values), the mean intensity is a relative measure for the Area Under the Curve (= AUC).

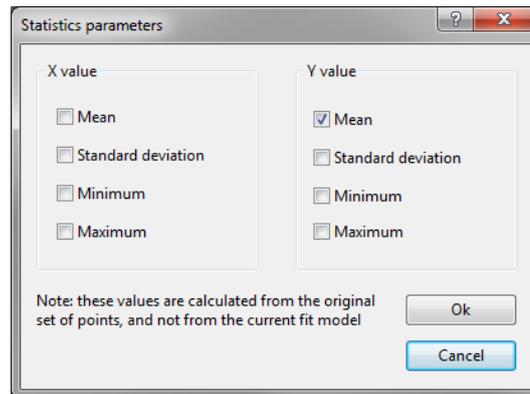


Figure 13: The *Statistics parameters* dialog box.

The *Parameters* panel now contains the selected parameter to be used for comparison (see Figure 15). Our imported samples can now be compared based on the selected parameter rather than based on all original data points.

6. Select *Parameters* > *Parameter properties...* to call the *Parameter properties* dialog box (see Figure 14).

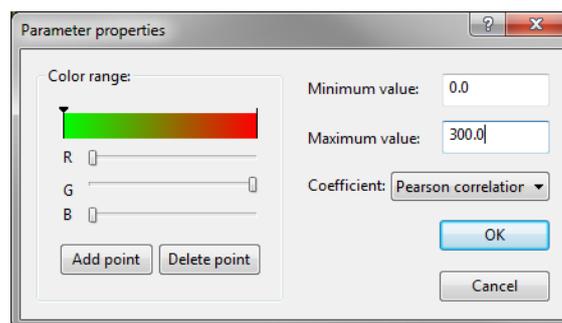


Figure 14: Parameter properties.

7. Change the color scale of the selected parameter using the red, green and blue sliders.
8. Change the *Maximum value* to “300”, make sure *Pearson correlation* is selected as similarity *Coefficient* and close the *Parameter properties* dialog box.

The color scale specified will be used when displaying the parameter values in the *Comparison* window (see 7).

9. Select *Settings* > *General settings...* (⌘+T) to call the *Curve settings* dialog box (see Figure 16).
10. Enter “Time” as *X axis name* and “Hours” as *X axis unit*. Press <OK>.
11. Close the *Trend type* window with *File* > *Exit*.

7 Displaying trend data

1. Click on a colored dot in the *Experiment presence* panel of the *Main* window representing an *Omnilog* trend data type for a particular entry.

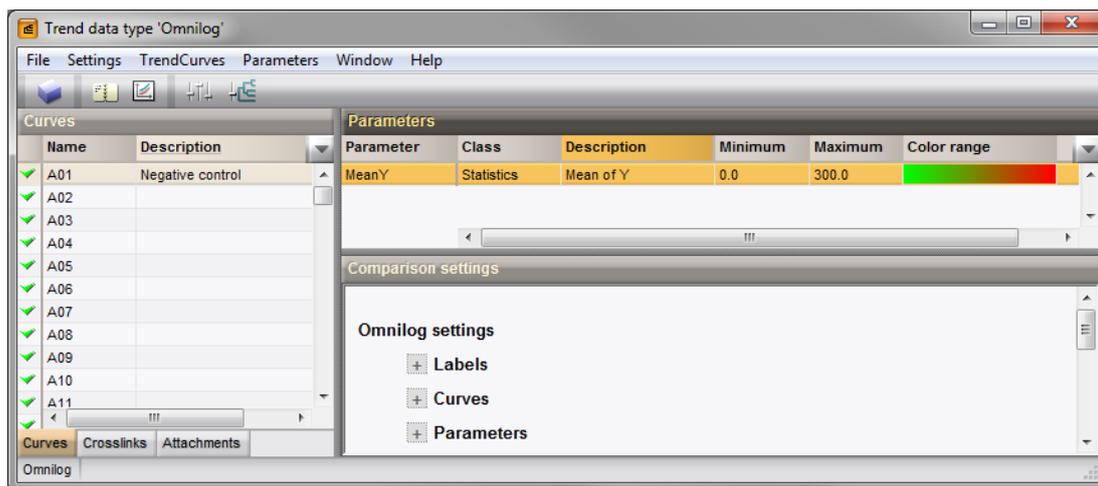


Figure 15: The *Trend type* window with one parameter defined.

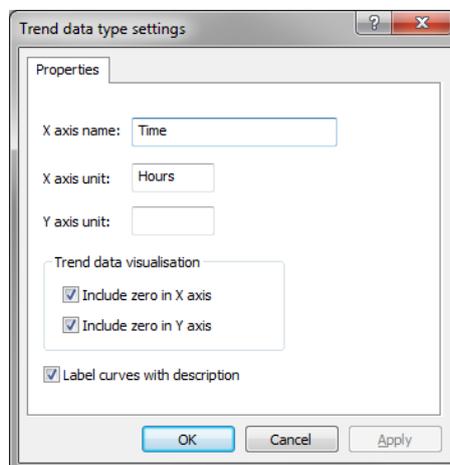


Figure 16: General settings.

The curves for the selected entry are displayed in the experiment card (see Figure 17). Using the pull-down list in the upper left corner of the card you can choose which curves to display.

2. Close the experiment card by clicking on the triangular button in the upper left corner.

Trend curves can also be displayed for multiple entries at a time in the same window. This is achieved as follows:

3. Select a number of entries in the database for which trend curves are present using the **Ctrl-** and **Shift-** keys.

Selected entries are marked by a checked ballot box (☑).

4. Double-click on the experiment **Omnilog** in the *Experiment types* panel to call the *Trend type* window.

5. Select **File > Create trend data window** (📄) to open the *Trend data* window.

6. Select a trend curve from the drop down list in the toolbar.

The *Curves panel* displays the selected curve for all selected entries in a single plot (see Figure 18).

7. Close the *Trend data* window with **File > Exit**.

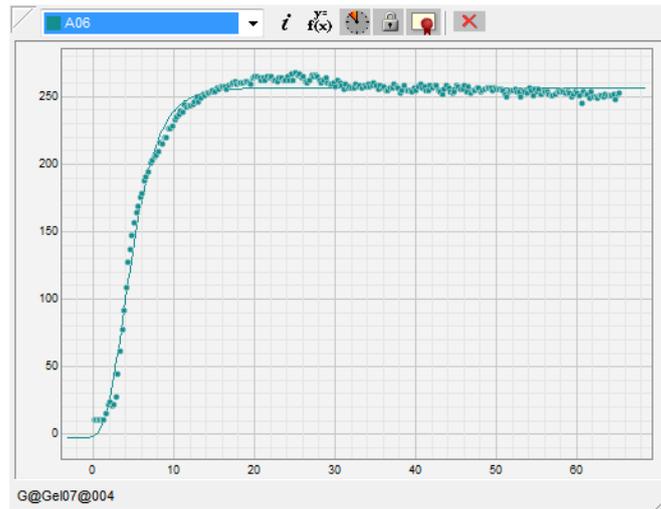


Figure 17: Experiment presence card.

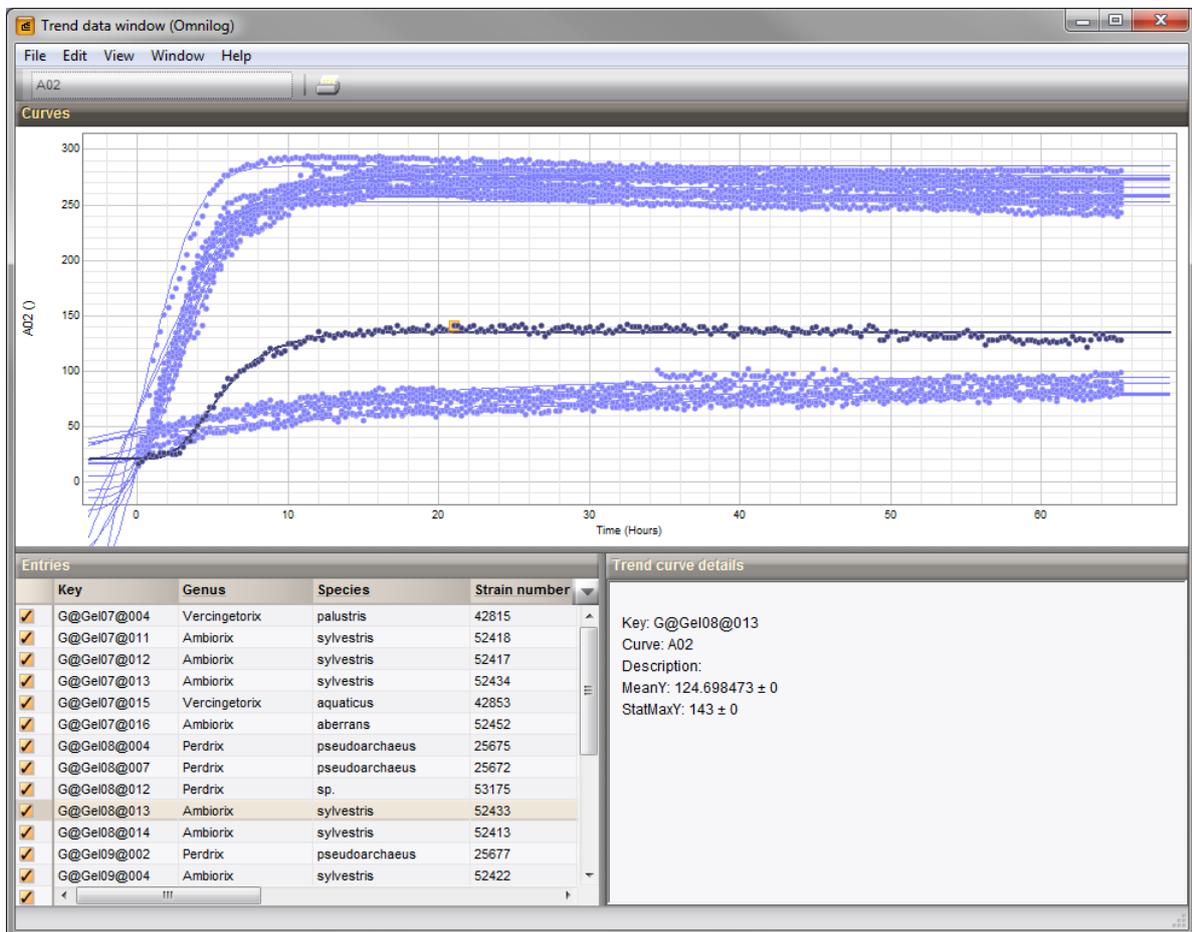


Figure 18: Trend curve displayed for multiple entries.

8. Make sure a few entries in the database are selected for which trend curves are present using the **Ctrl-** and **Shift-** keys.
9. Highlight the *Comparisons* panel in the *Main* window and select **Edit > Create new object...** () to create a new comparison for the selected entries.

10. Click on the  next to the experiment name **Omnilog** in the *Experiments* panel to display the defined parameter(s) in the *Experiment data* panel (see Figure 19).
11. Select *TrendData* > *Show parameter values colors* to display the values of the parameter together with the color as defined in the *Trend type* window (see 6).

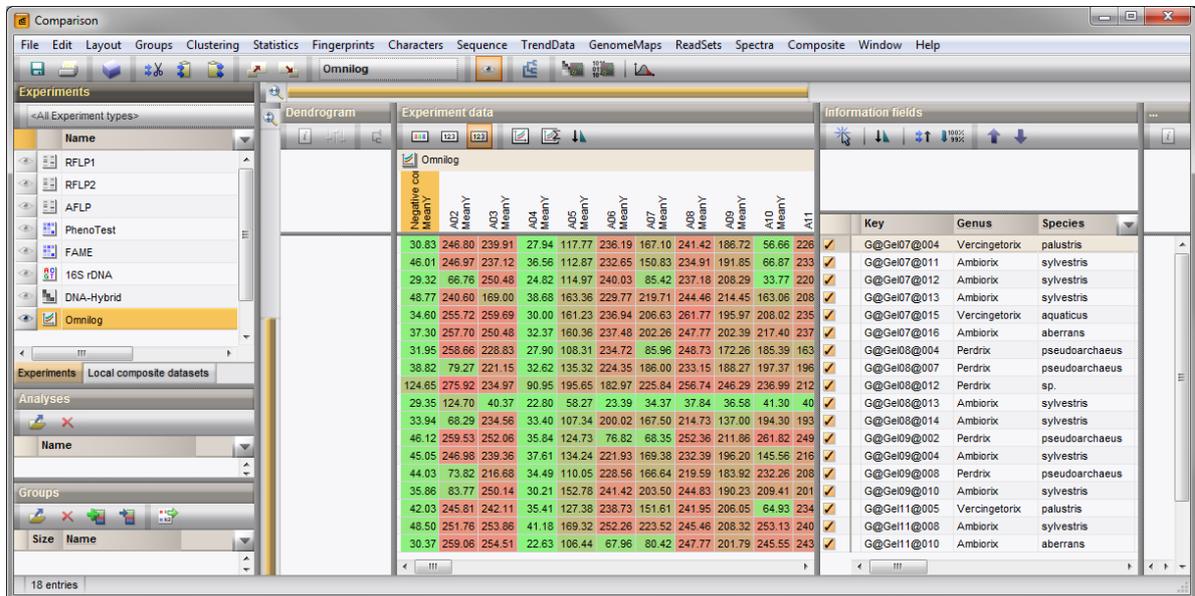


Figure 19: The *Comparison* window.

12. Select a parameter in the *Experiment data* panel, and select *TrendData* > *Sort entries by parameter value* ().

The entries are sorted according to increasing value of the selected parameter.

13. A tab-delimited text file of the entries and trend data values contained in the comparison can be exported with *TrendData* > *Export character table*.
14. Selecting *TrendData* > *Create trend data window* () calls the *Trend data* window again.
15. A cluster analysis (*Clustering* > *Calculate* > *Cluster analysis (similarity matrix)*...) on trend data can be performed either by comparing the original data points of the curves, or by comparing the parameter values.
16. To calculate correlation and regression on trend data, open the *Trend analysis* window with *TrendData* > *Perform trend analysis* (.