BIONUMERICS Tutorial:

Importing sugar metabolization data from text 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 Example data

The example text files from which we will import data in this tutorial contain trend data for 6 strains and can be downloaded from the Applied Maths website: go to https://www.applied-maths.com/download/sample-data and click on 'Trend data sample files'.

1. Open one of the files (e.g. `BSU1072.txt`) to examine the data that will be imported.

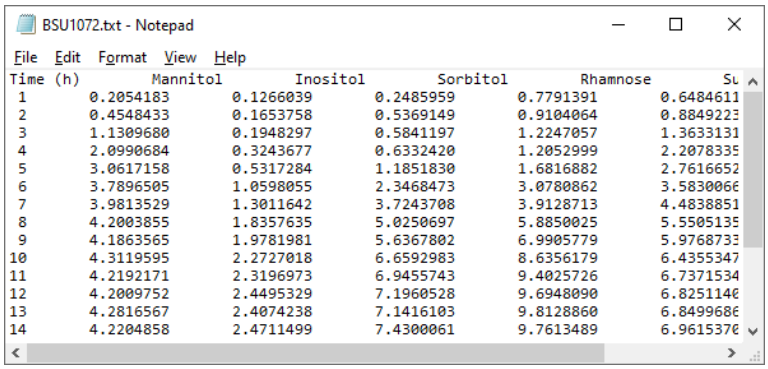


Figure 1: Text file: an example.

The text file contains a header, followed by the actual data in tabular format. In this table, the first column contains the X-values (= time points, expressed in hours) and the other columns contain the Y-values (= sugar concentration, expressed in mM). The first row describes the curve names (= sugar names).

3 Creating a trend data type experiment

1. Create a new database (see tutorial ”Creating a new database”) or open an existing database.

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).

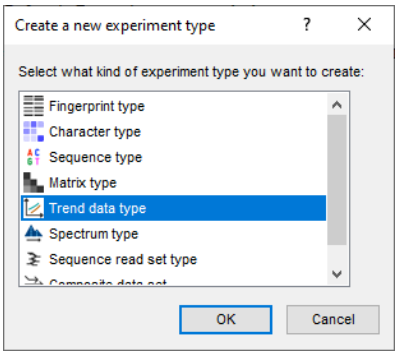


Figure 2: New Trend data type.

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

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

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

The *Trend type* window is initially empty. Trend curves can be added either manually (***Trend-Curves*** > ***Add new trend curve...***) or during import (see 4).

4 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***> (see Figure 3).

3. Press <***Browse***> and browse for the downloaded text files in the `Carbon sources` folder.

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

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 text files are listed in the grid.

5. Select first row in the list and click <***Edit destination***> or simply double-click on the row. Select ”X-axis” as the BIONUMERICS destination field under ***Trend curve value*** in the *Edit data destination* dialog box and press <***OK***> (see Figure 5).

6. Click on ”Mannitol” and whilst holding the **Shift**-key, click on ”Lactose” to make a multiple selection of the 6 trend data curves.

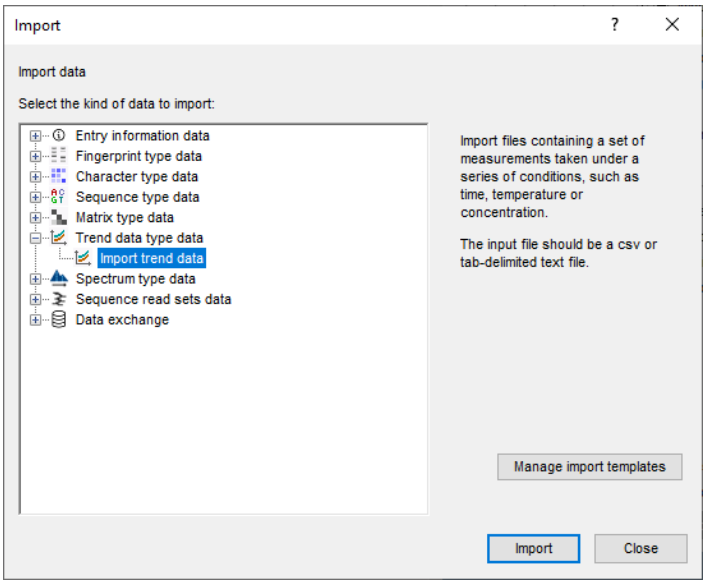


Figure 3: Import tree.

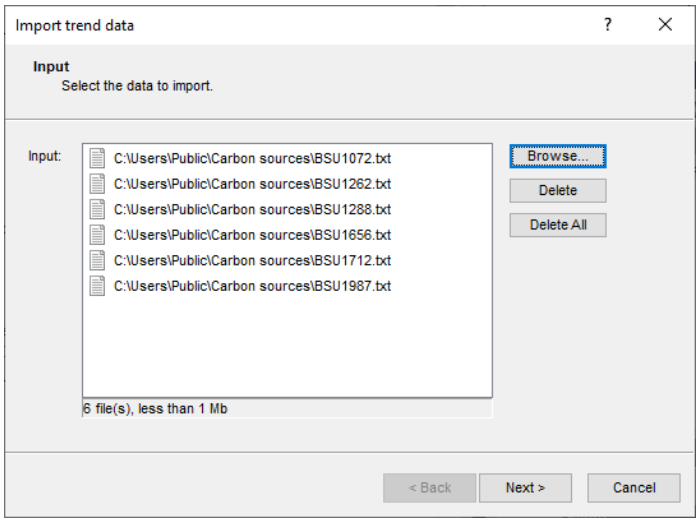


Figure 4: The *Input* wizard page.

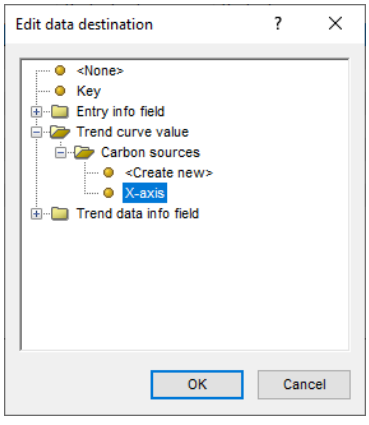


Figure 5: Edit data destination.

7. Press <***Edit destination***>, select ”Carbon Sources” under ***Trend curve value*** as destination and click <***OK***> (see Figure 6).

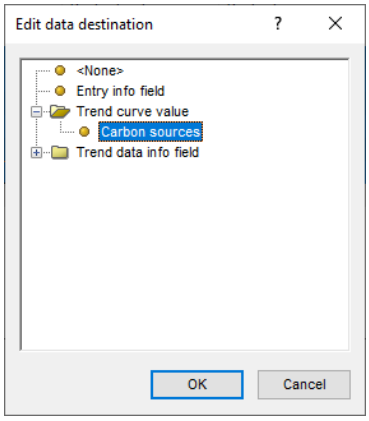


Figure 6: Edit data destination.

BIONUMERICS 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.

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

9. Select the last row in the grid, i.e. the row containing the ***File name***, click <***Edit destination***> and link the field to the ”Key” field. Press <***OK***>.

The grid is updated and should now look like in Figure 7.

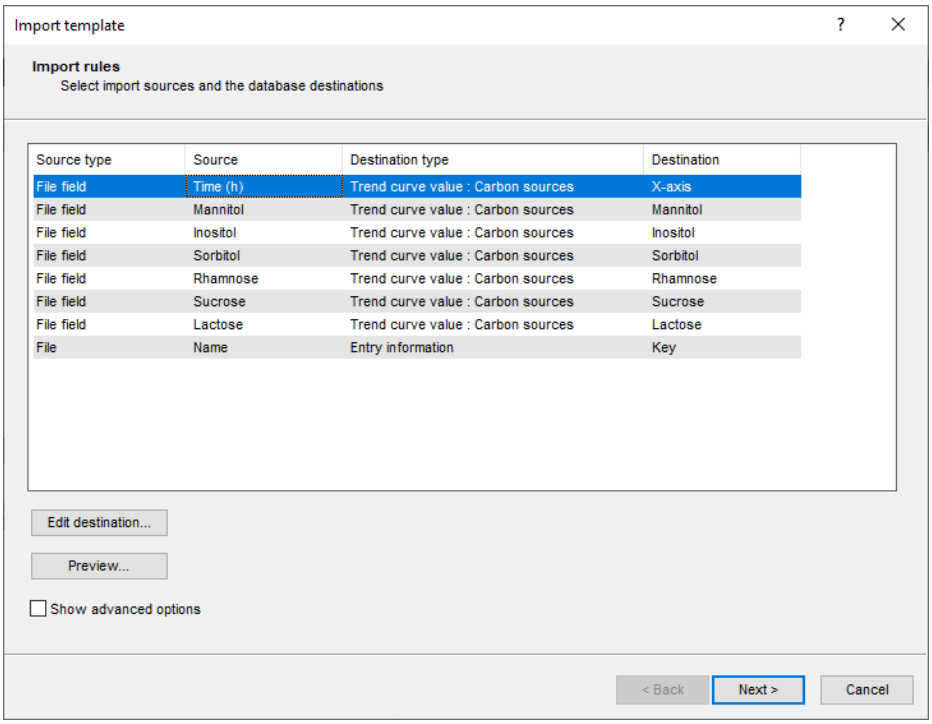
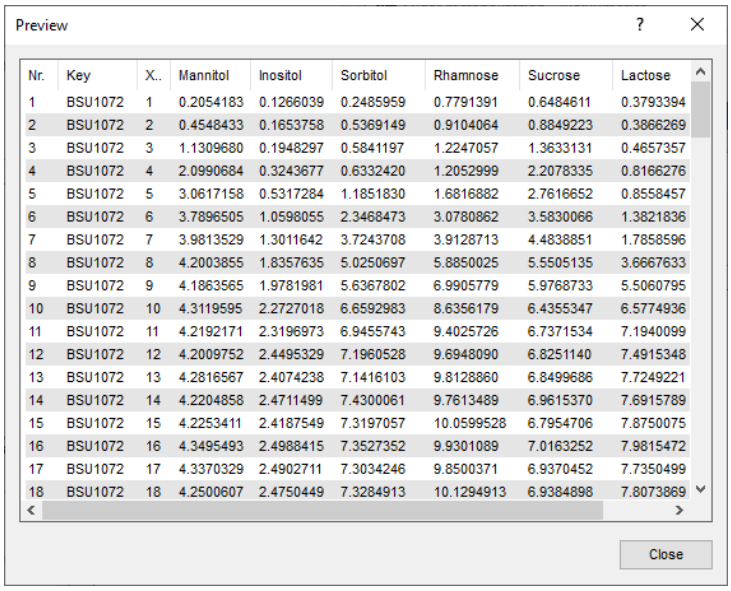


Figure 7: Import rules.

10. Press the <***Preview***> button to verify that all information will correctly be imported in the database (see Figure 8).



Nr.	Key	X..	Mannitol	Inositol	Sorbitol	Rhamnose	Sucrose	Lactose
1	BSU1072	1	0.2054183	0.1266039	0.2485959	0.7791391	0.6484611	0.3793394
2	BSU1072	2	0.4548433	0.1653758	0.5369149	0.9104064	0.8849223	0.3866269
3	BSU1072	3	1.1309680	0.1948297	0.5841197	1.2247057	1.3633131	0.4657357
4	BSU1072	4	2.0990684	0.3243677	0.6332420	1.2052999	2.2078335	0.8166276
5	BSU1072	5	3.0617158	0.5317284	1.1851830	1.6816882	2.7616652	0.8558457
6	BSU1072	6	3.7896505	1.0598055	2.3468473	3.0780862	3.5830066	1.3821836
7	BSU1072	7	3.9813529	1.3011642	3.7243708	3.9128713	4.4838851	1.7858596
8	BSU1072	8	4.2003855	1.8357635	5.0250697	5.8850025	5.5505135	3.6667633
9	BSU1072	9	4.1863565	1.9781981	5.6367802	6.9905779	5.9768733	5.5060795
10	BSU1072	10	4.3119595	2.2727018	6.6592983	8.6356179	6.4355347	6.5774936
11	BSU1072	11	4.2192171	2.3196973	6.9455743	9.4025726	6.7371534	7.1940099
12	BSU1072	12	4.2009752	2.4495329	7.1960528	9.6948090	6.8251140	7.4915348
13	BSU1072	13	4.2816567	2.4074238	7.1416103	9.8128860	6.8499686	7.7249221
14	BSU1072	14	4.2204858	2.4711499	7.4300061	9.7613489	6.9615370	7.6915789
15	BSU1072	15	4.2253411	2.4187549	7.3197057	10.0599528	6.7954706	7.8750075
16	BSU1072	16	4.3495493	2.4988415	7.3527352	9.9301089	7.0163252	7.9815472
17	BSU1072	17	4.3370329	2.4902711	7.3034246	9.8500371	6.9370452	7.7350499
18	BSU1072	18	4.2500607	2.4750449	7.3284913	10.1294913	6.9384898	7.8073869

Figure 8: Preview of the parsed data.

11. Press <***Next***> to proceed to the *Import links* dialog box.

12. Check ***Key*** under ***Import links*** 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. “Carbon sources template”) and optionally a ***Description***. Press <***OK***>.

14. Highlight the newly created template and click <***Next***>.

This next dialog will indicate that 6 new entries will be created during import (see Figure 9).

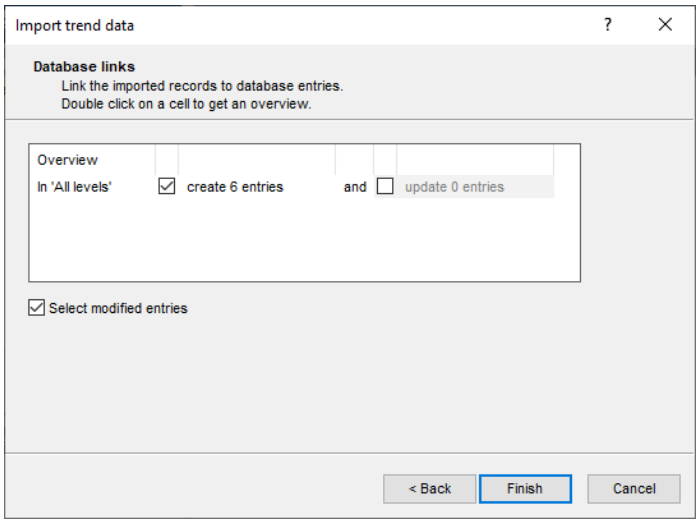


Figure 9: Create 6 new entries.

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

The entries are displayed in the *Database entries* panel and all entries are automatically selected (see Figure 10).

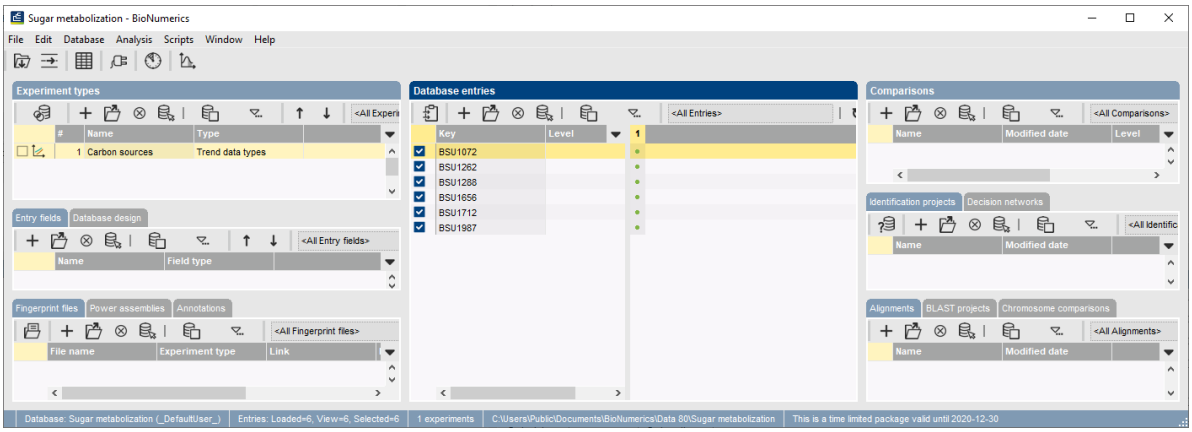


Figure 10: The *Main* window after import of the data.

The imported trend data is stored in the trend data type **Carbon sources**.

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

The 6 trend data curves are displayed in the *Curves* panel of the *Trend type* window (see Figure 11).

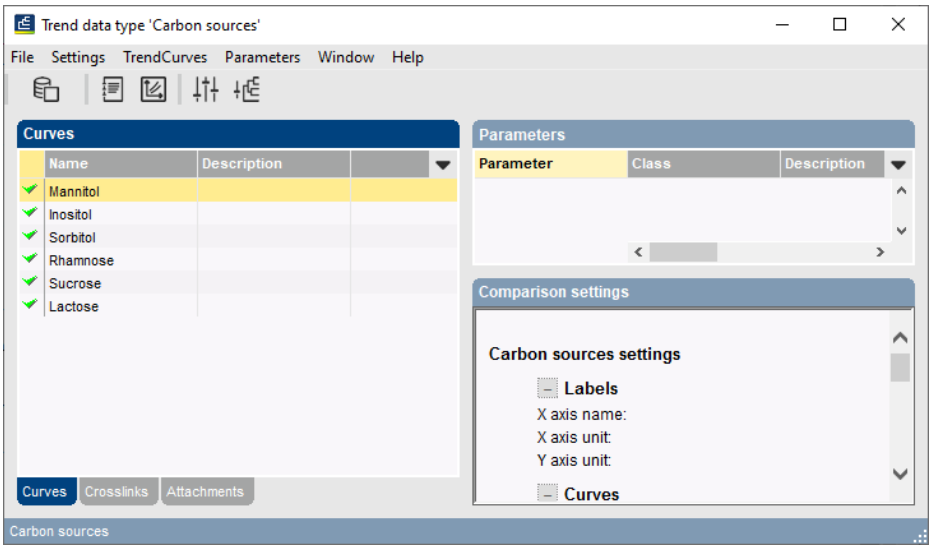


Figure 11: The *Trend type* window.

5 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).

Bacterial growth and activity is usually analyzed using a *Logistic growth* fit.

2. Choose ***Logistic growth*** and check both ***Use offset*** and ***Use generalized formula***.

3. Press <***OK***> to set the curve model.

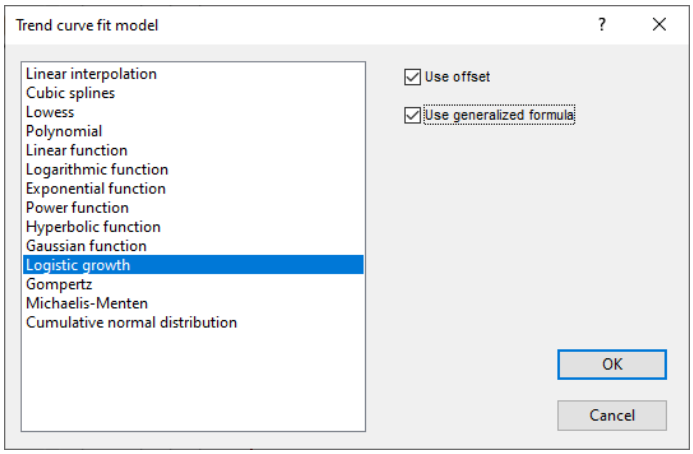


Figure 12: Set trend curve model.

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*** > ***Model parameters...*** to call the *Trend curve parameters* dialog box.

5. Select ***Logistic growth*** and check ***Use model***.

For taxonomy or typing purposes one might be interested in combining data from multiple parameters into one clustering or identification.

6. Enable the parameters ***Final value (Max)*** (i.e. the maximum value derived from the curve) and ***Maximum slope (Smax)*** (i.e. the maximum growth rate) (see Figure 13) and press <***Exit***>.

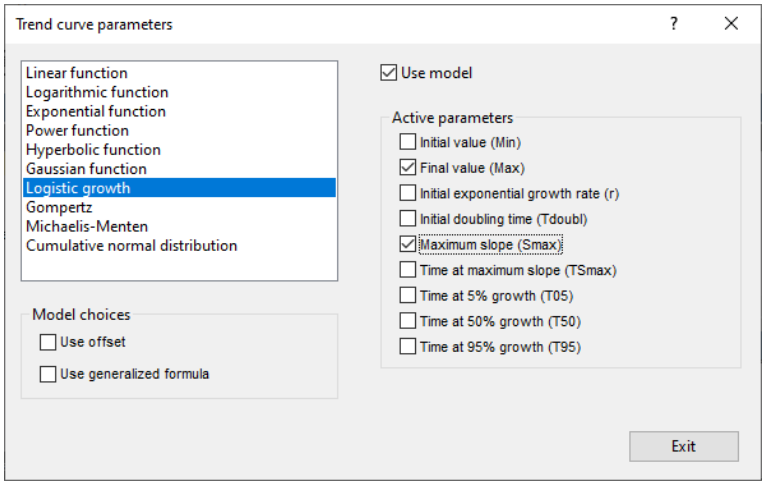


Figure 13: Trend curve parameters.

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

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

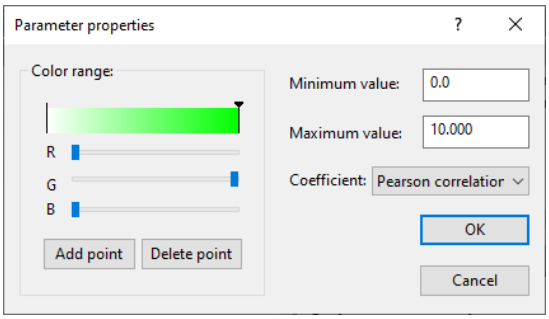


Figure 14: Parameter properties.

8. Change the color scale of the selected parameter using the red, green and blue sliders and close the *Parameter properties* dialog box.

9. Change the color scale for the other parameter and close the dialog.

The color scales specified will be used when displaying the parameter values in the *Comparison* window (see 6).

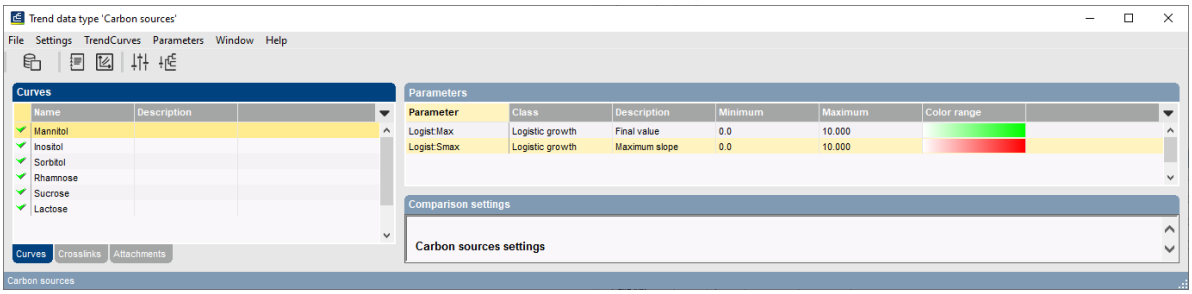


Figure 15: The *Trend type* window with two parameters defined.

10. Select ***Settings*** > ***General settings...*** ( ) to call the *Curve settings* dialog box (see Figure 16).

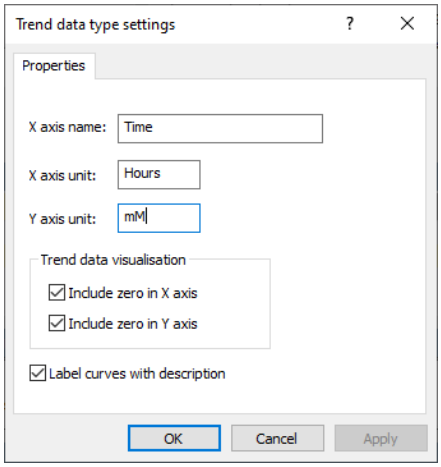


Figure 16: General settings.

11. Enter “Time” as ***X axis name***, “Hours” as ***X axis unit***, and “mM” as ***Y axis unit*** (see Figure 16). Press <***OK***>.

12. Close the *Trend type* window with ***File*** > ***Exit***.

6 Displaying trend data

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

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.

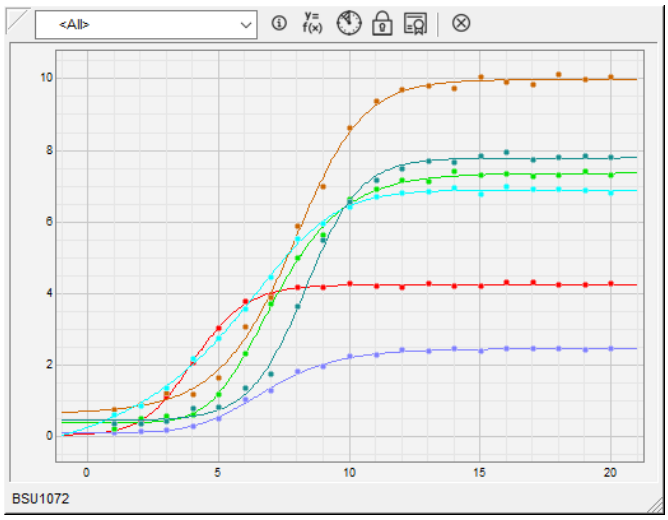


Figure 17: Experiment presence card.

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. To select all entries at once select **Ctrl+A**.

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

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

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

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

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

7. Make sure a few entries are selected in the *Main* window.

8. Highlight the *Comparisons* panel in the *Main* window and select ***Edit*** > ***Create new object...*** (+) to create a new comparison for the selected entries.

9. Click on the next to the experiment name **Carbon sources** in the *Experiments* panel to display the selected curve model parameters in the *Experiment data* panel (see Figure 19).

10. Select ***TrendData*** > ***Show parameter values colors*** to display the values of the parameters together with the color as defined in the *Trend type* window (see 5).

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

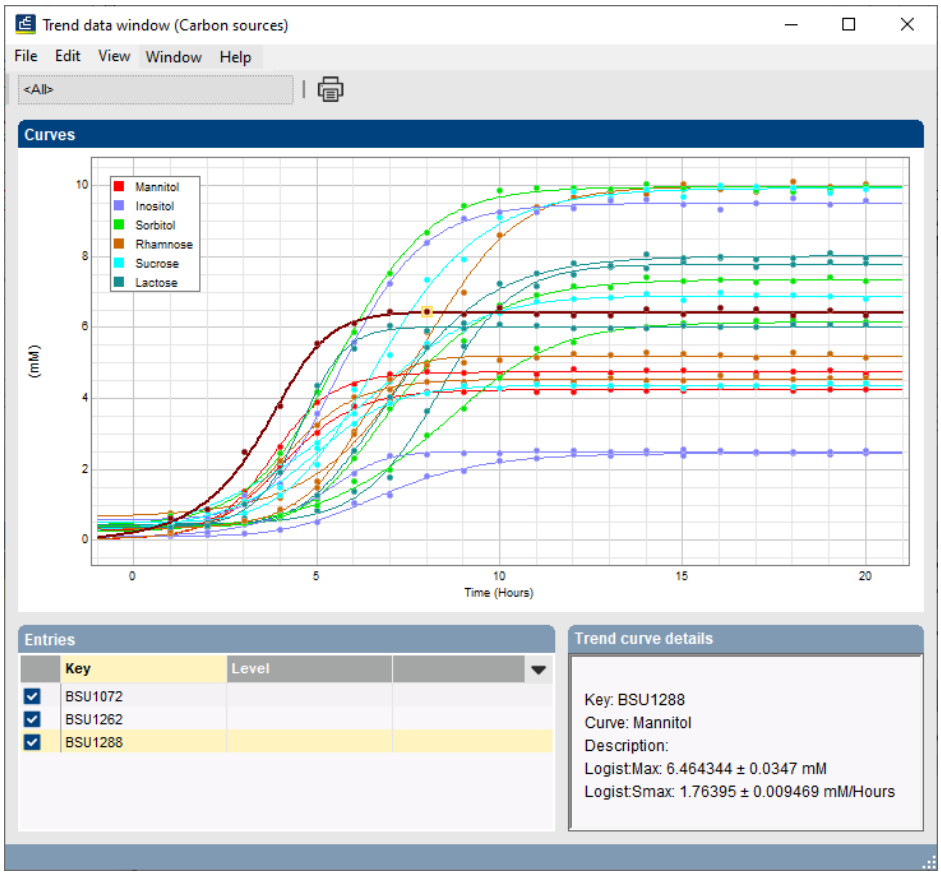


Figure 18: Trend curves displayed for multiple entries at a time.

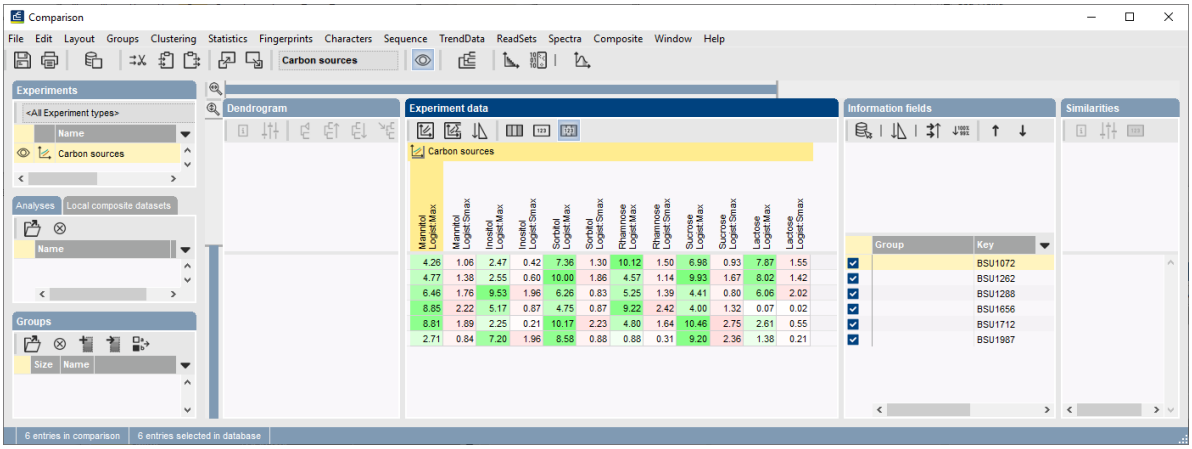


Figure 19: The *Comparison* window.

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

12. A tab-delimited text file of the entries and trend data values contained in the comparison can be exported with ***TrendData*** > ***Export character table***.

13. Selecting ***TrendData*** > ***Create trend data window*** () calls the *Trend data* window again (see Figure 18).

14. A cluster analysis (***Clustering*** > ***Calculate*** > ***Cluster analysis (similarity matrix)...***) can be performed either by comparing the original data points of the curves, or by comparing the parameter values.

15. To calculate correlation and regression on trend data, open the *Trend analysis* window with ***TrendData*** $>$ ***Perform trend analysis*** ( ).