BIONUMERICS Tutorial:

Importing spectrum data: peak lists

1 Aim

Comprehensive tools for the import of spectrum data, both raw spectrum data as processed spectrum data are incorporated into BIONUMERICS. In this tutorial the import of peak lists (= processed spectrum data) is illustrated with a sample data set.

2 Sample data

As an exercise, we will import a set of MALDI-TOF peak lists from different isolates and species. The set can be downloaded from the Applied Maths website: go to https://www.applied-maths.com/download/sample-data and click on "Demo spectra peak lists". When the download is complete, unzip the file.

3 Preparing a sample database

3.1 Creating a new database

1. Double-click on the BIONUMERICS icon () on the desktop.
2. In the *BIONUMERICS Startup* window, press the  button to enter the *New database* wizard.
3. Enter a database name, e.g. "Demo Spectra".
4. Click <***Next***>.

A new dialog box pops up, asking whether to create a new relational database for data storage or to use an existing one.

5. Leave the default option ***Create new*** enabled and press <***Next***>.

The next dialog asks which database engine should be used for storing data.

6. Select the default option and press <***Finish***>.

The *Main* window opens with an empty database.

3.2 Creating a spectrum type experiment

Before importing spectrum data, we will first create a spectrum experiment type.

7. In the *Main* window, click on + in the toolbar of the *Experiment types* panel and select ***Spectrum type*** from the list (see Figure 1). Press <***OK***>.

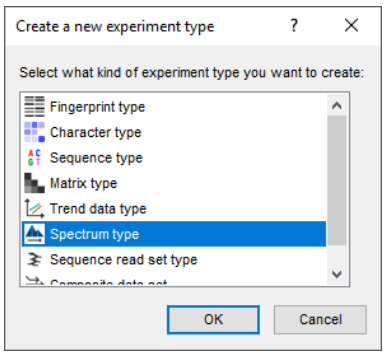

Figure 1: Create a new Spectrum type.

8. Enter a name, for example **Maldi**, leave the units for the horizontal and vertical axis at their defaults and press <***Next***> (see Figure 2).

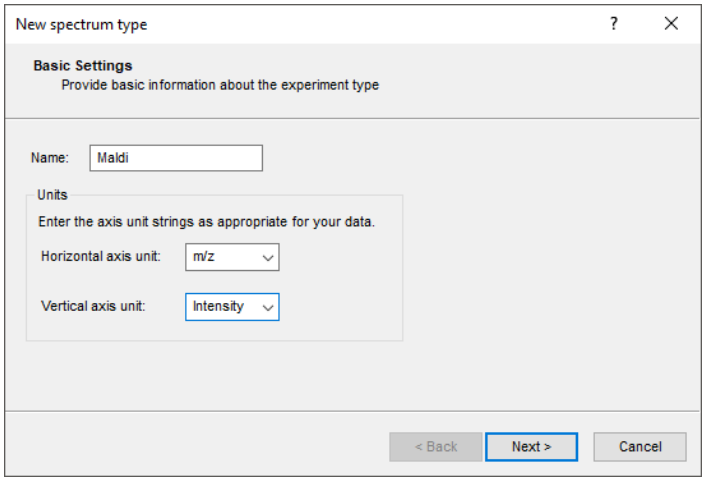

Figure 2: Basic settings.

Three predefined preprocessing templates are included: ***Preprocessing (Default)***, ***Preprocessing (Relaxed)***, and ***Preprocessing (Strict)***. The settings of each template can be changed in the *Spectrum Preprocessing* window and saved to the database. Since we will import already preprocessed spectrum data in this tutorial, the choice of a preprocessing template is irrelevant here.

9. Press <***Finish***> to complete the creation of the new spectrum type experiment.

The *Experiment types* panel now lists the spectrum type **Maldi** (see Figure 3).

4 Importing spectra

1. Select ***File*** > ***Import...*** (, **Ctrl+I**) to call the *Import* dialog box (see Figure 4).

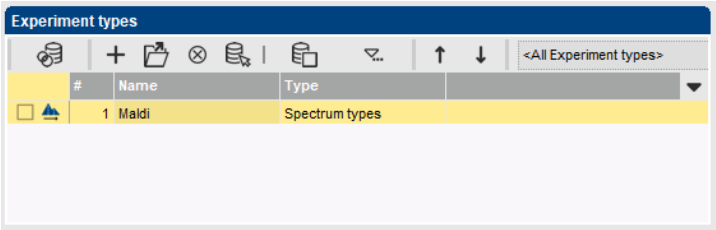

Figure 3: The *Experiment types* panel.

In this section we will import mzML files containing peak lists (see 2) in our BIONUMERICS database. mzML is a standardized format for exchange of spectrum type data.

2. Select the ***Import mzML data*** option, listed under the topic ***Spectrum type data*** and press <***Import***>.

More peak list import routines can be found under the topic ***Spectrum type data***.

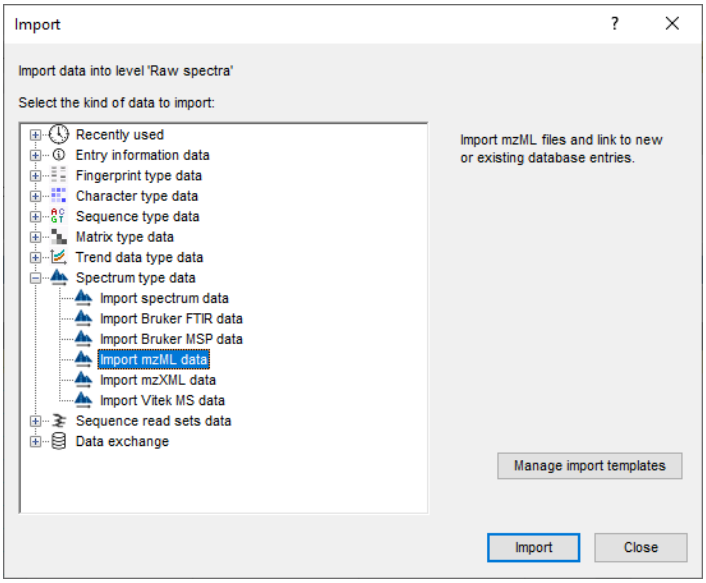

Figure 4: The ***Import mzML data*** option in the *Import* dialog box.

3. Browse to the folder, select all mzml files in this folder and press <***Open***> and <***Next***> (see Figure 5).

4. In the *Import template* wizard page of the wizard, press <***Create new***>.

As an exercise, we will link the file name to the BIONUMERICS ***Key*** field.

5. Double-click on the last row available in the grid or press <***Edit Destination***>.

6. Select ***Key*** in the *Edit data destination* dialog box (see Figure 6).

7. Press <***OK***>.

The grid is updated.

8. In the *Import template* dialog box, press <***Preview***> and verify the preview of the import (see Figure 7). Close the preview and press <***Next***> and <***Finish***>.

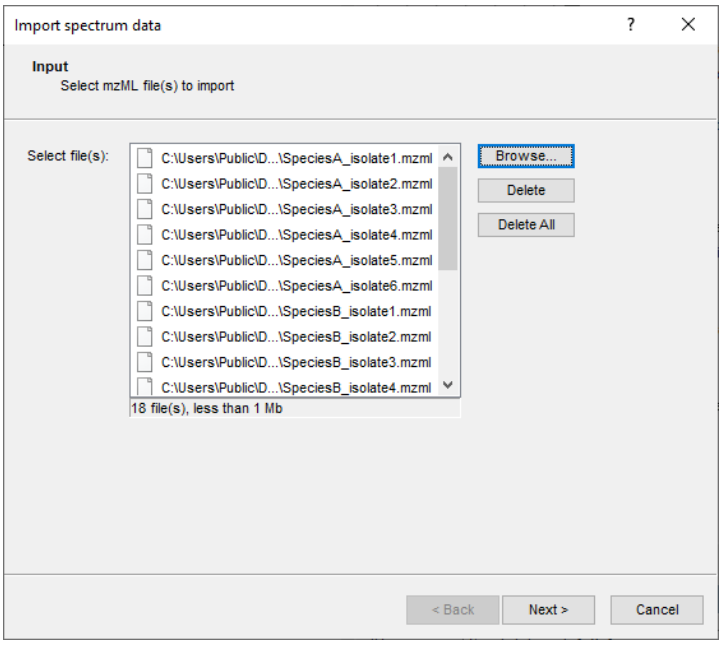

Figure 5: Select mzml files.

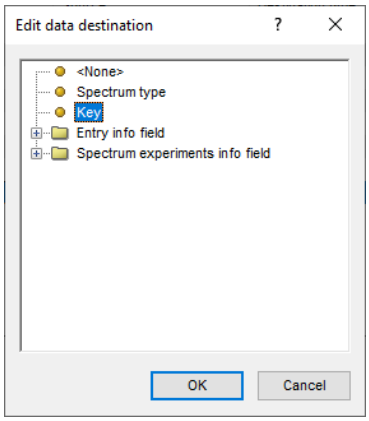

Figure 6: Select data destination.

9. Name the import template (e.g. ”Import peak lists”) and optionally give it a description. Press <***OK***>.

10. With the new import template highlighted, and the ***Maldi*** experiment selected (see Figure 8) press <***Next***> to go the next step where an overview of the actions that will be performed during the import is displayed (see Figure 9).

11. Press <***Next***> to go to the final step (see Figure 10).

Since we are importing peak lists (= processed peak data) in this tutorial, the option ***Input files contain processed peak data*** is automatically checked, and no options concerning the preprocessing need to be defined.

When importing raw spectrum data, the option ***Input files contain raw spectrum data*** is automatically checked, and options concerning the preprocessing can be defined.

12. Keep the option ***Input files contain processed peak data*** checked for our example files and press <***Finish***>.

The peak lists are imported and linked to the newly created samples. The file names are displayed

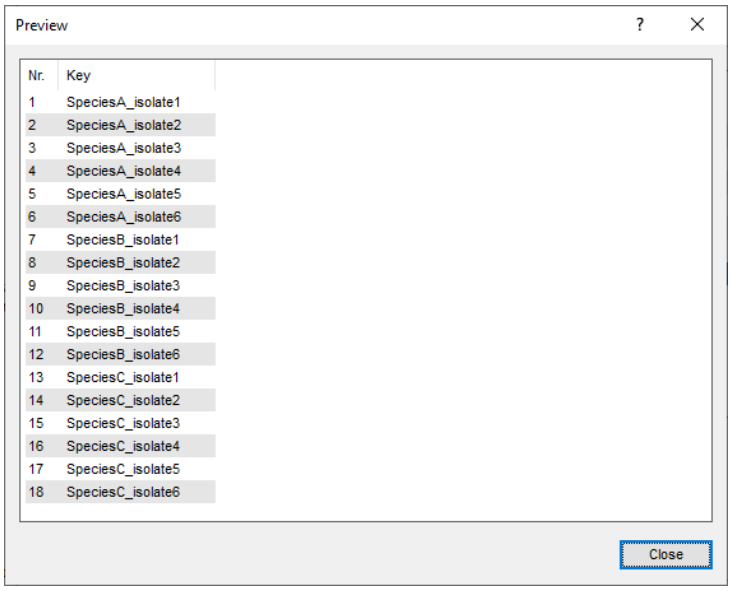

Figure 7: Preview.

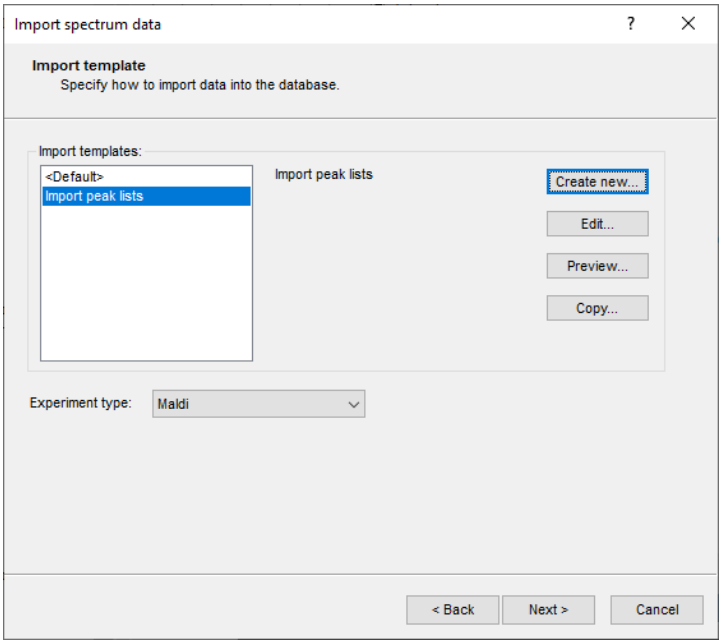

Figure 8: Import template.

in the ***Key*** field in the *Database entries* panel.

13. Click on a green colored dot for one of the entries in the *Experiment presence* panel to open the spectrum in the *Spectrum* window (see Figure 11).

14. Click on the spectrum in the *Profiles* panel to make it the active spectrum in the window.

15. Click on the *Peak List* panel to display the Peak List table.

16. Double-click on a peak in the *Peak List* panel: the peak is highlighted in *Profiles* panel and the view is updated.

17. Use the zoom sliders in the *Profiles* panel to obtain the best view.

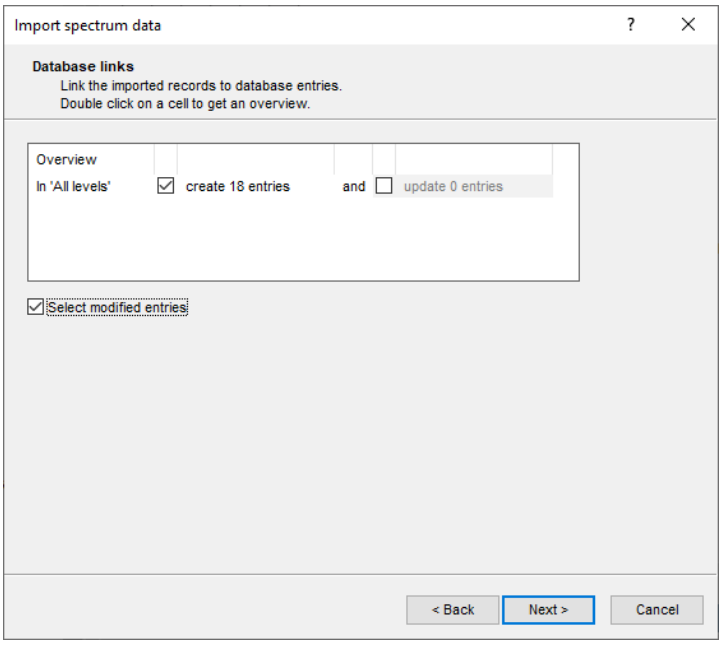

Figure 9: Import actions.

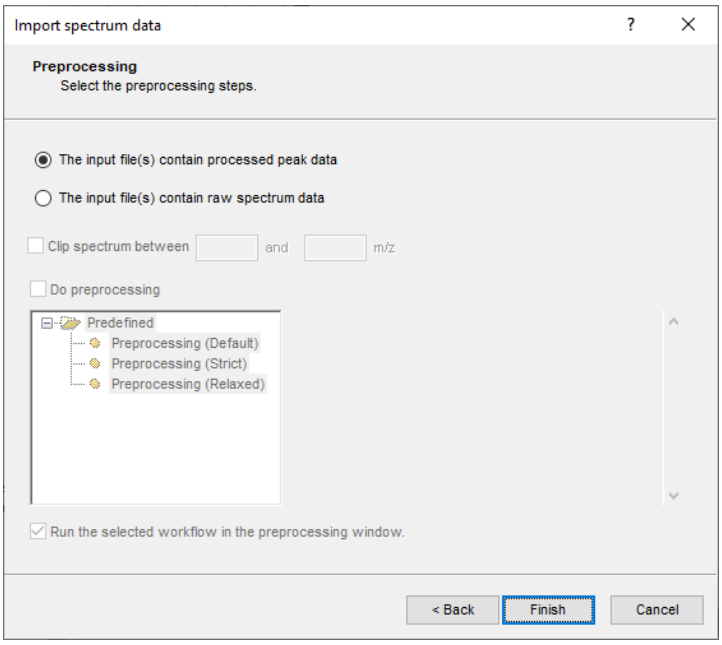

Figure 10: Select preprocessing action.

18. Close the *Spectrum* window with ***File*** > ***Exit***.

Since we have imported peak lists (= processed peak data) no preprocessing is required.

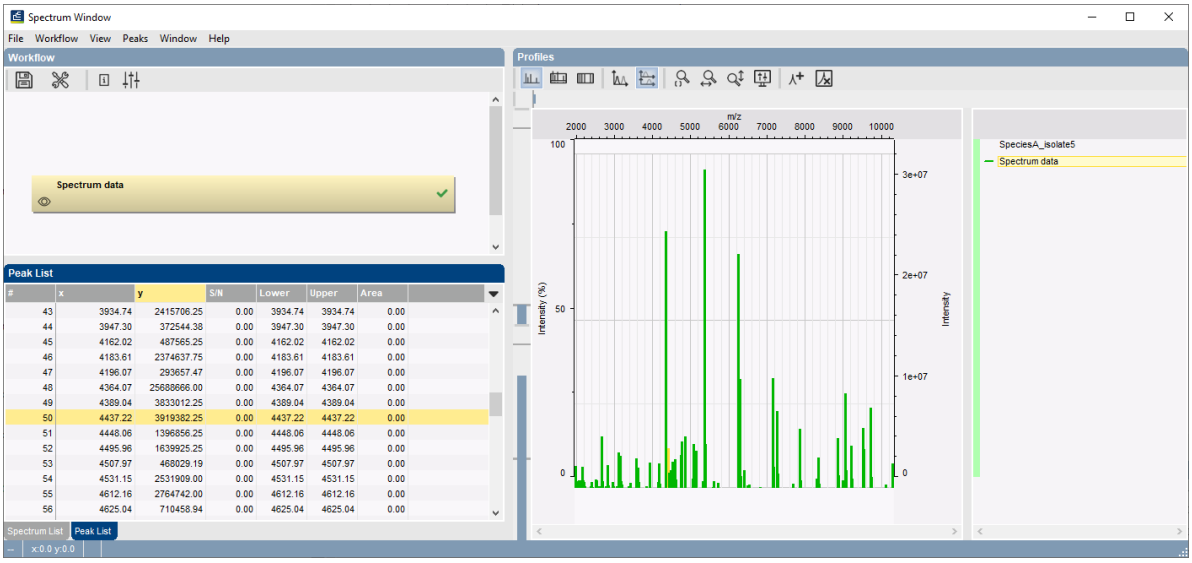

Figure 11: Spectrum with peak list.