BIONUMERICS Tutorial:

Importing spectrum data: raw files

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 raw spectrum data is illustrated with a sample data set.

2 Sample data

As an exercise, we will import a set of MALDI-TOF spectra 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 raw spectra". 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***>.

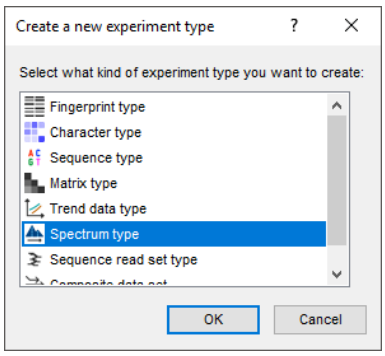

Figure 1: Create a new Spectrum type.

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).

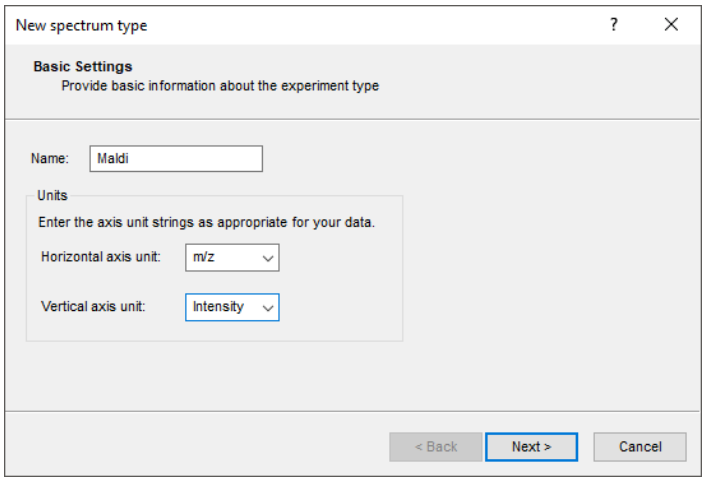

Figure 2: Basic settings.

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.

9. Select the template *Preprocessing (strict)* and 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.

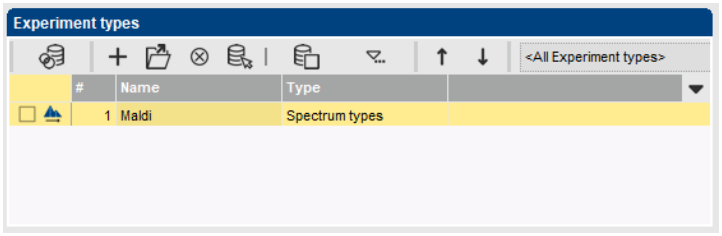

Figure 3: The *Experiment types* panel.

In this section we will import text files containing raw spectrum data (see 2).

2. Select the ***Import spectrum data*** option, listed under the topic ***Spectrum type data*** and press <***Import***> (see Figure 4).

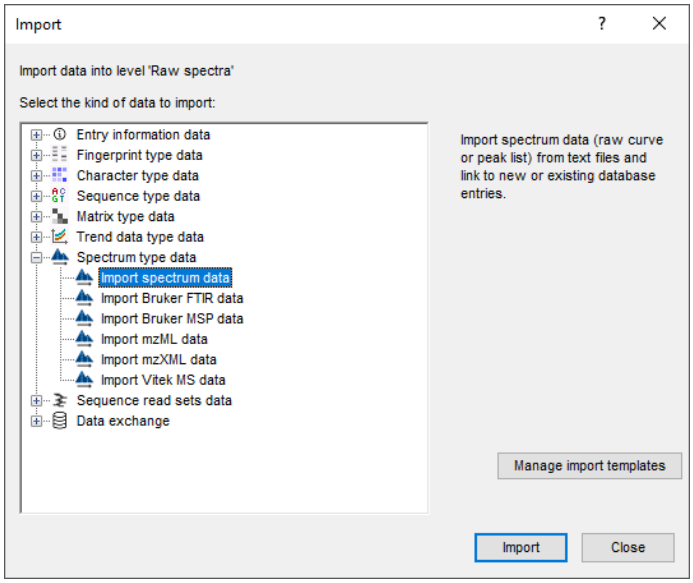

Figure 4: The Import tree.

More raw spectrum data import routines can be found under the topic ***Spectrum type data***.

3. Browse to the folder, select all files in this folder and press <***Open***> and <***Next***>.

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

The only source of information available in the newly created import template is the file name. As an exercise, we will link the file name to the BIONUMERICS ***Key*** field.

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

6. Select ***Key*** in the *Edit data destination* dialog box and press <***OK***>.

The grid is updated.

7. In the *Import template* dialog box, press <***Preview***> and verify the preview of the import (see Figure 6). Close the preview and press <***Next***> and <***Finish***>.

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

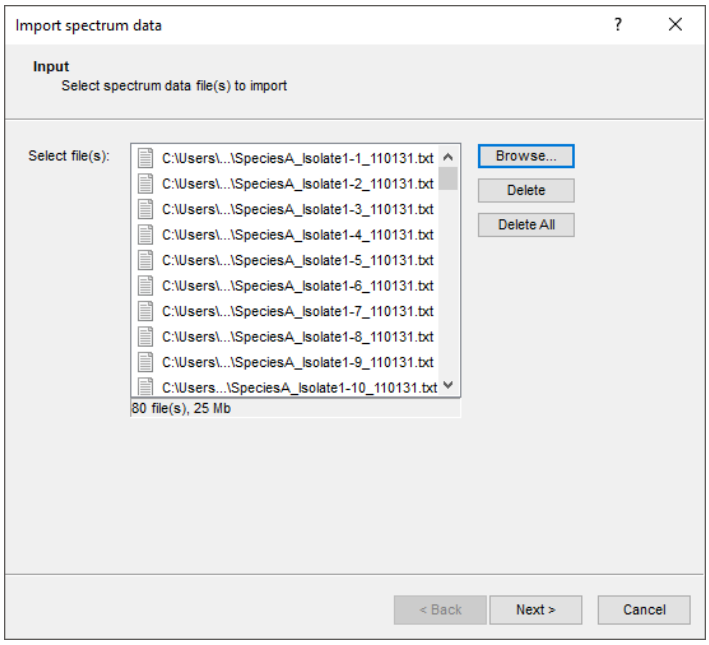

Figure 5: Select files.

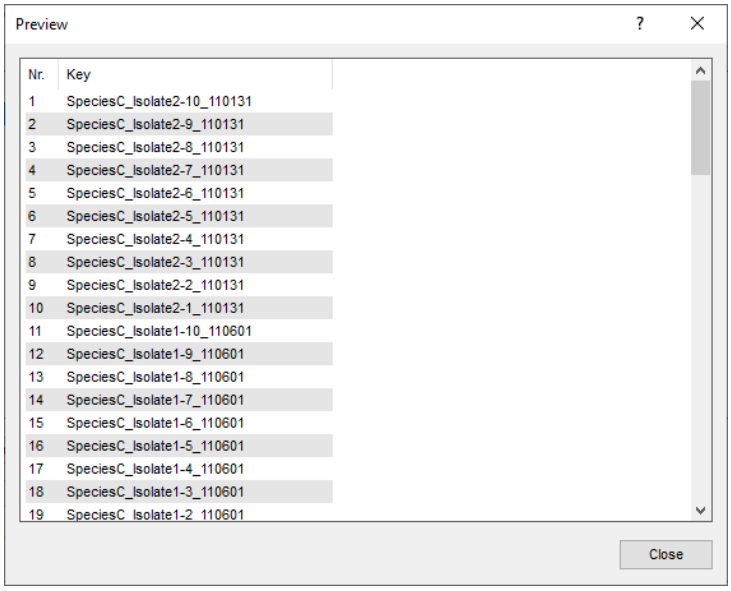

Figure 6: Preview.

9. With the new import template highlighted, and the ***Maldi*** experiment selected (see Figure 7) press <***Next***> to go the next step where an overview of the actions that will be performed during the import is displayed (see Figure 8).

10. Press <***Next***> to go to the final step.

11. Press <***Next***>, check ***Do preprocessing***, select ***Preprocessing (strict)*** as ***Preprocessing*** option, leave all other settings at default and press <***Finish***> (see Figure 9).

The raw spectra will be imported. Depending on the performance of your computer, this may take a few minutes.

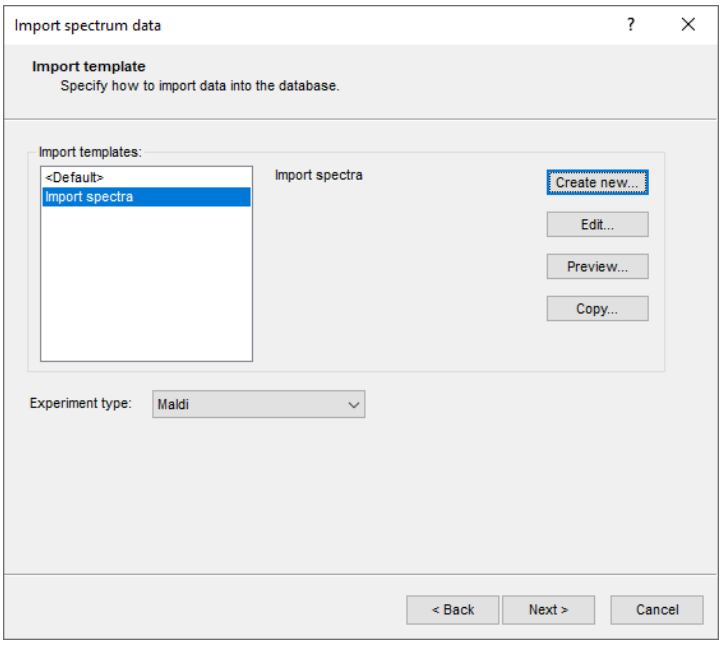

Figure 7: Import template.

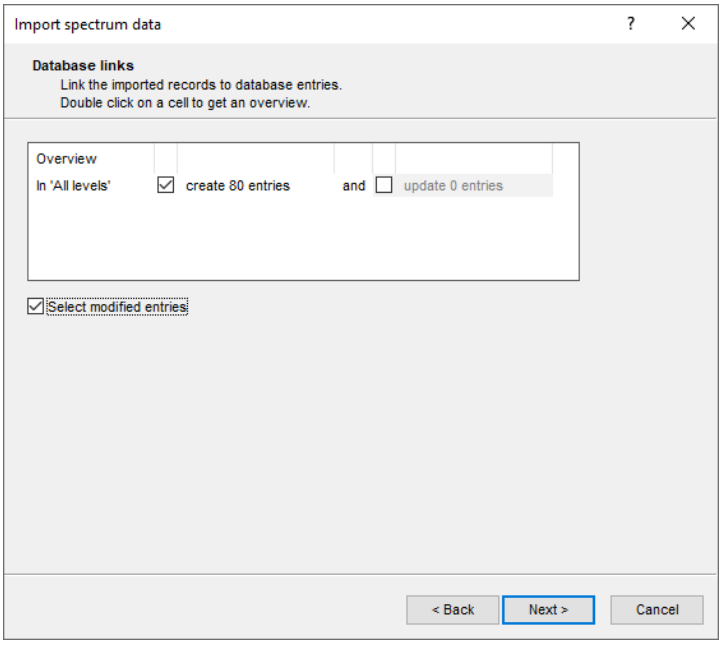

Figure 8: Import actions.

5 Preprocessing of spectra

Upon completion of the import, the *Spectrum Preprocessing* window will open automatically. If it does not open automatically, you can select all entries and use ***Analysis*** > ***Spectrum types*** > ***Open preprocessing window...*** to open the *Spectrum Preprocessing* window.

All the imported spectra are loaded in the *Spectrum Preprocessing* window with the preprocessing template selected in the last step of the *Import spectrum data* wizard (see Figure 10).

Because there is a slight difference in the range of the different spectra, we will add a trimming

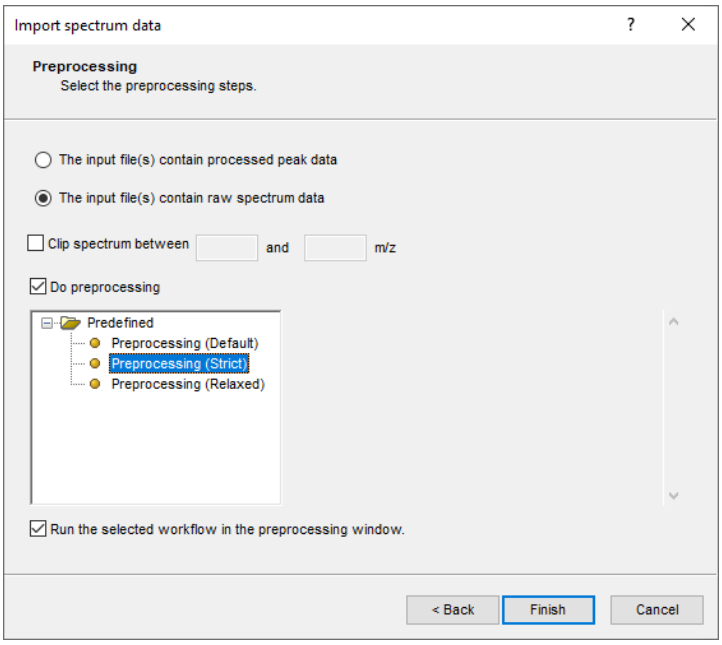

Figure 9: Preprocessing settings.

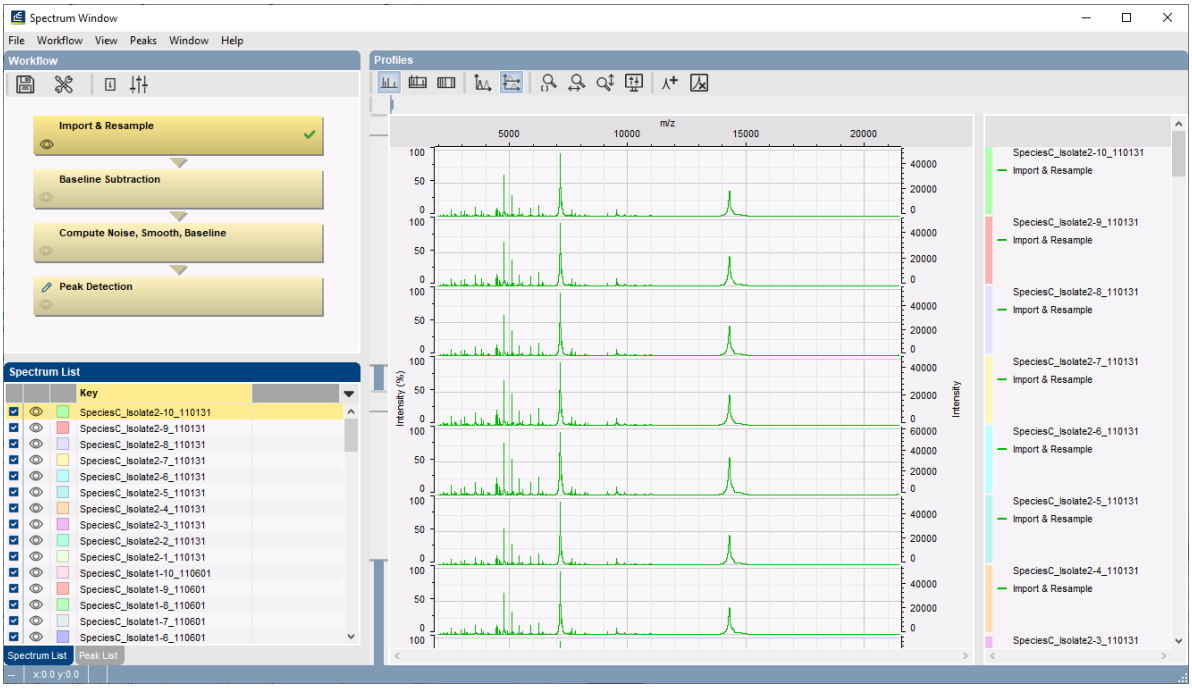

Figure 10: Spectrum window.

step to this template.

1. With the **Import & Resample** step of the preprocessing template highlighted in the *Workflow* panel, select ***Workflow*** > ***Show flow chart...***. This will open the *Workflow* window for this step of the template.

2. In the left panel, highlight the operator ***Processing*** > ***X-axis*** > ***Trimming*** and select ***File*** > ***Add operator...*** ( ).

3. In the resulting dialog box (see Figure 11), fill in **2000** as X-axis minimum, do not use an upper limit and press <***Next***>.

The trimming operator is added to the end of the workflow, resulting in the workflow shown in Figure 12.

4. Close the *Workflow* window.

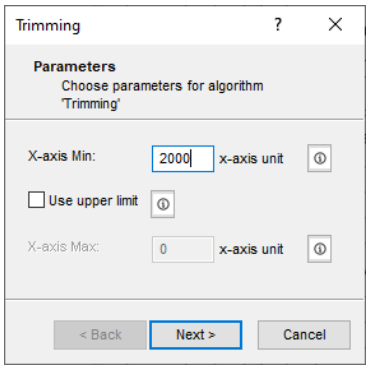

Figure 11: Parameters of the trimming operator.

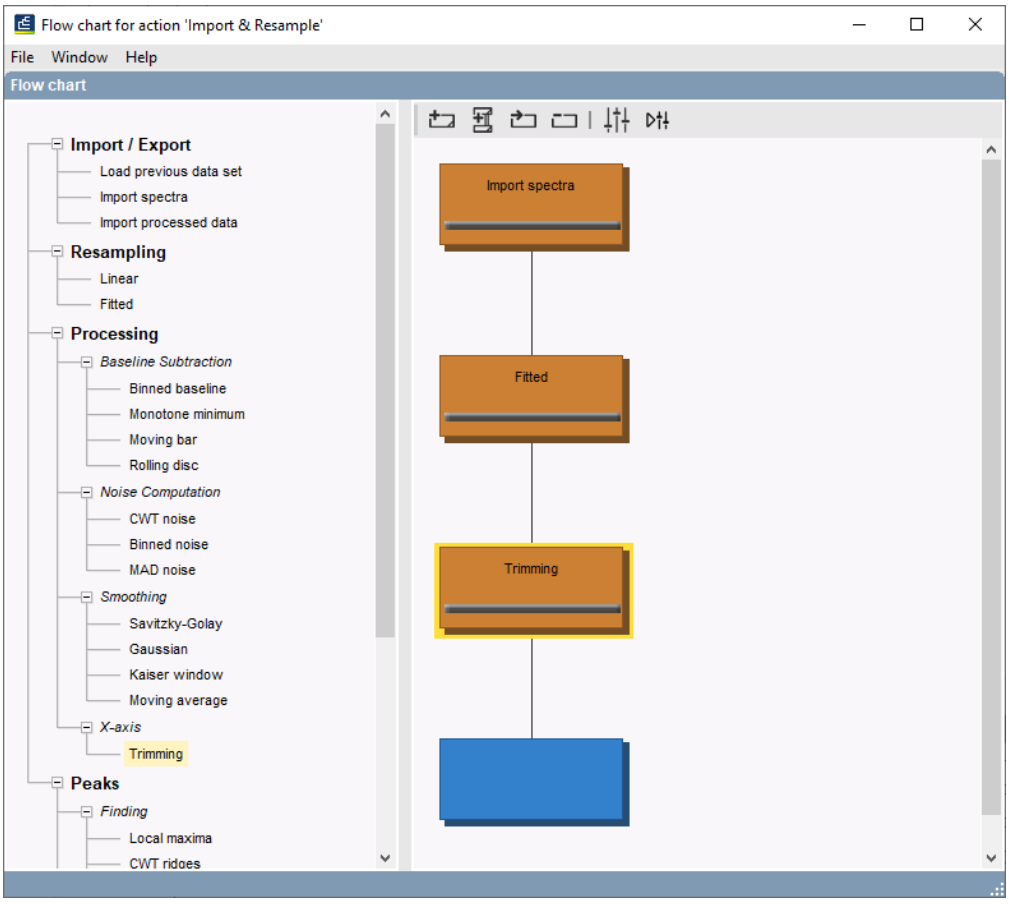

Figure 12: Final workflow with trimming operator.

5. Select ***File*** > ***Save workflow as template...***, enter a name for the new template (e.g. ”Strict with trimming”) and press <***OK***>.

This template will now be available for future import and preprocessing of spectra.

6. Press the last step of the preprocessing template in the *Workflow* panel, i.e. <***Peak Detection***>, to execute the entire preprocessing workflow. Leave the limit for the signal to noise ratio at default and press <***Next***>.

Depending on the performance of your computer, the execution might take a few minutes.

With the ”Peak Detection” step still selected in the *Workflow* panel, the preprocessed spectra are displayed in the *Profiles* panel (see Figure 13). The detected peaks are indicated with circles on top of the peaks.

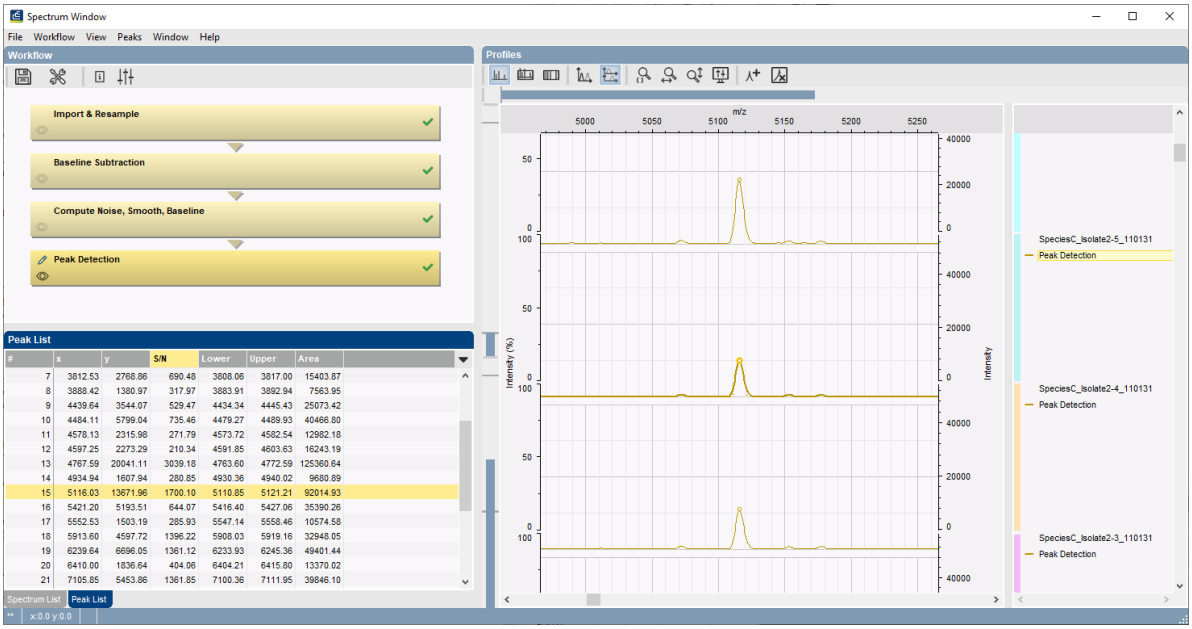

Figure 13: Spectrum window.

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

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

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

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

11. Save the results by selecting ***File*** > ***Save spectrum data*** ( ). Close the *Spectrum Preprocessing* window.

The preprocessed spectra are now available in the database and further analysis can be performed.