

TM016 - Database searching and creation

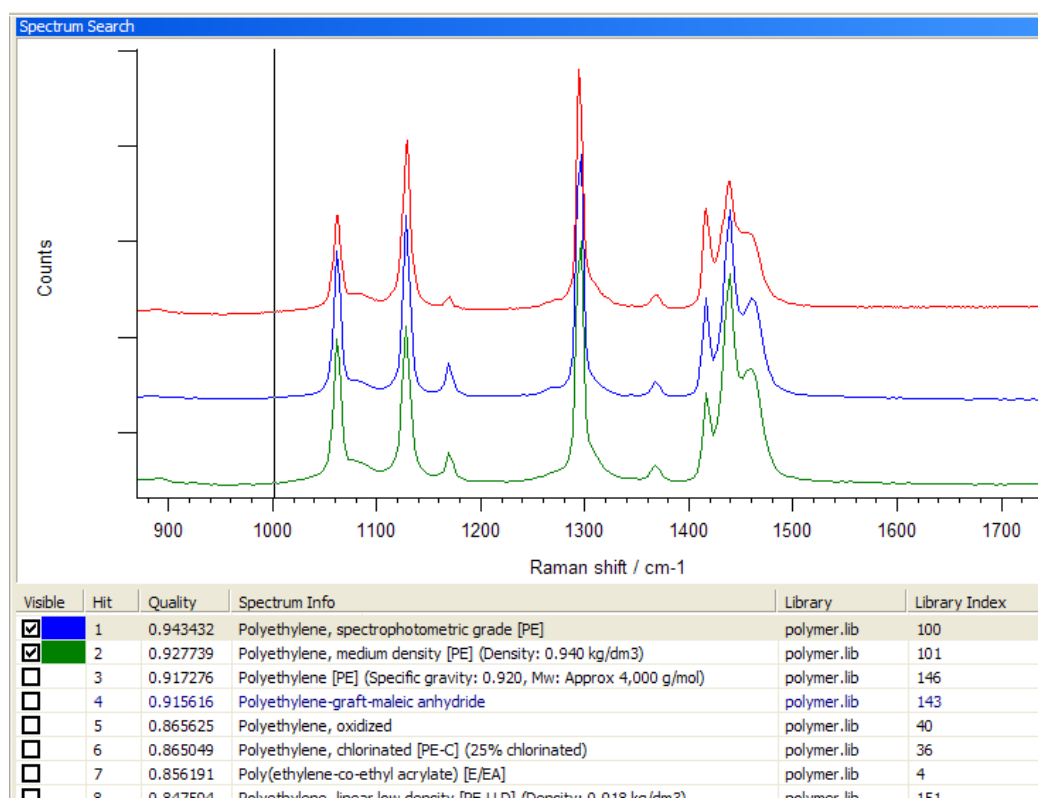
WiRE™ 5

This document aims to show the WiRE™ 5 user how to search their spectra against Raman spectral databases, and how to create their own databases. It assumes that the WiRE™ 4 software and the GRAMS package Spectral ID have been installed correctly.

Searching against databases

1 – With a spectrum open in WiRE 5, select either *Analysis/Spectrum Search* from the toolbar or right-click in the viewer and select *Tools/Spectrum Search*. If any library files are available, then a search will automatically be performed on opening. If no library file is currently selected, then a message will be displayed. To change, add or remove libraries to be searched against, right-click in the Spectrum Search window and select *Properties*. Select the *Libraries* tab and use the 'Add' button to browse for *.lib files. These should be stored locally on the computer.

With a library (or libraries) selected, you can search your spectrum against it by right-clicking in the window and selecting *Search now*. The closest ranked 'hit' will be shown at the top of the list. Use the *Properties* tabs to select the parameters that are shown, the display method and the method of searching (i.e. First derivative correlation algorithm). The sample spectrum can also be searched using the *Text* rather than the data. For example, if you have some knowledge of the sample species, using the text search function can be used to narrow down the search.



- Display – *Single* shows only the sample spectrum and the selected library entry. Use the mouse to select other library matches.
- Overlaid – The sample spectrum is displayed with *n* spectra from the library, where *n* is the value entered in “Initial number of spectra visible”. Other spectra can be added to the view, or spectra removed, by checking or unchecking the check boxes in the ‘Visible’ column.
- Stacked – The number of spectra to be shown are divided equally in the available ‘height’ of the Spectrum Search window.
- Offset – The vertical ‘distance’ between spectra can be defined using the “Offset between spectra as proportion of available area”. This will resemble the ‘Stacked’ or ‘Overlaid’ displays depending on the number of spectra and % value set.

Right-clicking on a single entry in the ‘Spectrum Info’ column will allow you to view any additional information stored with the reference library spectra. Right-clicking in the results table allows the results table to be saved. It could then be pasted into a document, for example. Right-clicking in the spectrum viewer allows mask regions to be set and removed (*Add mask regions*, *Remove mask regions*). When *Add mask region* is selected, the cursor icon changes to the mask symbol. Left-click in the spectrum to add the mask and use the mouse to drag the upper and lower bounds of the mask region. Right-click in the mask region (*Remove mask region*) to remove them. Regions that are masked will not be searched against the database. Masks can also be added through *Properties/Pre-Processor*.

For help, use the Renishaw User Guide, or the Spectral ID Help.

Creating new databases from clones

The easiest way to create a new database is to clone an existing database. For example, the Renishaw Database of Polymeric Materials. **Important: All spectra that are to be used in a single database should be recorded with the same spectral range.** Using the Template function in WiRE 5 to collect reference spectra should ensure that the same range is used throughout. It is a good idea to use the common Galactic .spc format when acquiring spectra for a database. You will be able to search .wxd and many other formats of Raman data against the library this way. Either save the spectra as .spc while in WiRE 5 or perform a Batch Conversion on the whole set of .wxd files that will form the database. Always aim to acquire the best data you can (i.e. the best signal to noise ratio) when collecting reference spectra from **well-characterised** samples.

With the reference data collected (more spectra can be added later, if needed):

- Open Spectral ID and go to *Tools/Library Manager* and press ‘Create new’ and give the new database a name (the extension .lib will be added). Ideally, save in the same folder as other .lib files, if any.
- In the ‘New library’ window, select ‘Clone’ and select the library to be cloned. Change the range, if necessary, to match the spectral range of your data. Axes should be Raman shift/cm⁻¹ and Counts. Pressing ‘OK’ takes you to the ‘Edit library’ window. Press ‘Add entry’ and select the data to add to the library. Press ‘Next’ and in the ‘Add to Library Wizard’ insert a line of text that describes the sample in the ‘SPC Comment Line’. Add any useful additional text in the relevant text box and press ‘Finish’ to complete the addition.

- Search for and add the new library using the *Spectrum Search Properties/Libraries* tab in WiRE 5.

For help, use the Spectral ID Help.

Creating a new database from scratch

Prior to collecting the reference data it is prudent to establish carefully the desired spectral range for data collection. This value is important for database construction as the range, and number of data points, should be kept constant for a certain laser configuration, and may affect the ability to add data to the same database.

To ascertain the correct parameters to use when creating a new database it is advised that a 'dummy' trial on a single spectrum be first performed. Collect this spectrum over the desired range;

- The range is determined from the spectral acquisition set-up, where it is recommended that a standard measurement template be used to ensure the **same** spectral range is used for each spectrum.

Save this spectrum as a .spc file (or save as wxd file format and use Renishaw 'batch converter' for multi file conversion), close this file and reopen in Spectral ID (open unknown).

The number of data points is found from Spectral ID; *File/Information*.

The dialogue below should be used as a template for the correct fields and values to use for a new database. Of course the spectral range and data points number will be specific to any particular database.

New Library - [C:\GRAMSN\SAMPLIB\example.lib]

Library Data

Range: Begin: 200 End: 3500

Data Points: 826

X Axis: Raman Shift (cm-1)

Y Axis: Counts

Comment:

Resolution: ☐ 8-bit ☒ 16-bit ☐ 32-bit

Library Type

☒ Optical Spectra ☐ Mass Spectra

Library Processing

☐ Baseline Corrected

Peak Picking: ☒ Single ☐ Double

Clone Defaults OK Cancel Help

With the reference data collected (more spectra can be added later, if needed):

1. Open Spectral ID and go to *Tools/Library Manager* and press 'Create new' and give the new database a name (the extension .lib will be added). Ideally, save in the same folder as other .lib files, if any.
2. Edit the 'New library' parameters for the values specific to the new database. It is recommended that a spectral template be used to ensure consistency. Where laser power, acquisition time, and accumulations may vary from sample to sample.
3. In the 'New library' window, select 'Clone' and select the library to be cloned. Change the range, if necessary, to match the spectral range of your data. Axes should be Raman shift (cm^{-1}) and Counts. Pressing 'OK' takes you to the 'Edit library' window. Press 'Add entry' and select the data to add to the library. Press 'Next' and in the 'Add to Library Wizard' insert a line of text that describes the sample in the 'SPC Comment Line'. Add any useful additional text in the relevant text box and press 'Finish' to complete the addition.
4. Search for and add the new library using the *Spectrum Search Properties/Libraries* tab in WiRE 5.