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Libraries

# Libraries

## *Library Setup*

*Select Libraries*

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## *Search Results*

*Region Search*

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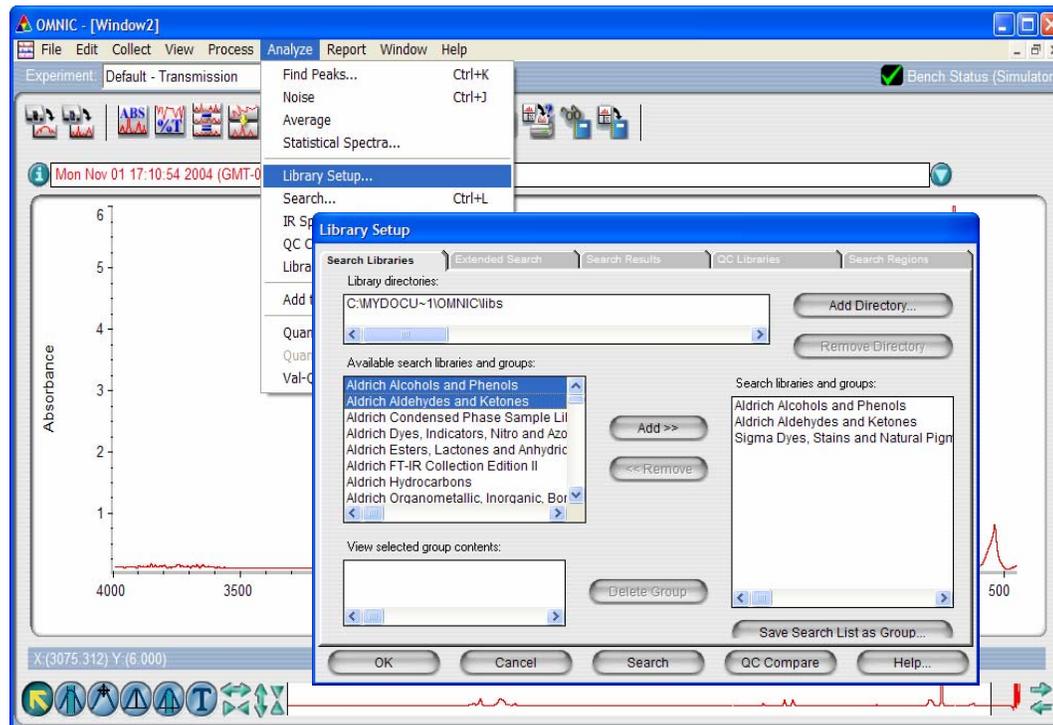
*Building a User Search Library*

*Building a QC Library*

*Library Setup for QC Libraries*

*QC Compare*

# Library Setup Select Libraries



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Performing commercial and user library searches is an important part of qualitative analysis.

To setup a library search, first select Analyze | Library Setup. Like most dialogues in OMNIC, several tabs run across the Library Setup Dialogue box. Under the Search Libraries Tab select meaningful libraries to search against. To do this, simply highlight the preferred libraries on the left hand side and click the Add button. To remove a library, highlight the library from the right side list and click Remove.

You may save a set of libraries that are used on a repetitive basis or with a specific experiment as a group by clicking the Save Search List as Group button located beneath the right hand pane. You will be prompted to type a title for the group. You may save several different groups.

# Library Setup - Configure Search

The screenshot shows the 'Library Setup' dialog box with the 'Search Results' tab selected. The 'Configure search results' radio button is chosen. The 'Search type' is set to 'Correlation'. The 'Offset negative values' checkbox is unchecked. In the 'List of Matches' section, 'List compounds with match values above:' is set to 0 and 'Maximum number of compounds in list:' is set to 10. In the 'Spectral Display' section, 'Number of library spectra to display:' is set to 5. The 'Show match values' checkbox is checked. At the bottom, there are buttons for 'OK', 'Cancel', 'Search', 'QC Compare', and 'Help...'.

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If you turn on Configure Search Results, the Search Type drop-down list box and the features in the List Of Matches box become available.

Specify the search type, or "algorithm," for the search by selecting an option from the Search Type drop-down list box. The types are described below.

**Correlation** - Normally gives the best results and is recommended for most applications. The algorithm removes any effect of offset in the unknown spectrum, thus eliminating the effects of baseline variation.

**Absolute Difference** - Puts more weight on the small differences between the unknown spectrum and library spectra. This means that impurities will have a larger effect on the search results.

**Squared Difference** - Emphasizes the large peaks in the unknown spectrum. Use this algorithm if you are identifying a noisy spectrum.

**Absolute Derivative** - Gives small peaks and peak shifts an increased effect on the search results. The algorithm removes any differences between the unknown and library spectra caused by an offset in the unknown spectrum. This algorithm is useful when you want to emphasize peak positions rather than peak intensities. Use this algorithm if you are identifying a spectrum with a tilted baseline (and you don't want to correct the baseline before the search).

**Squared Derivative** - Emphasizes large peaks as well as peak shape. The algorithm removes any differences between the unknown and library spectra caused by an offset in the unknown spectrum. This algorithm works well with spectra of poor quality.

## Library Setup - Configure Search Regions

Library Setup

Search Libraries | Extended Search | Search Results | QC Libraries | Search Regions

Use full spectral range  
 Use spectral regions

Region:(0.000,0.000) Baseline:0.000

Absorbance

Wavenumbers (cm-1)

<Back Next> Add Delete Full Scale

Index	Start	End
1	0.00	0.00

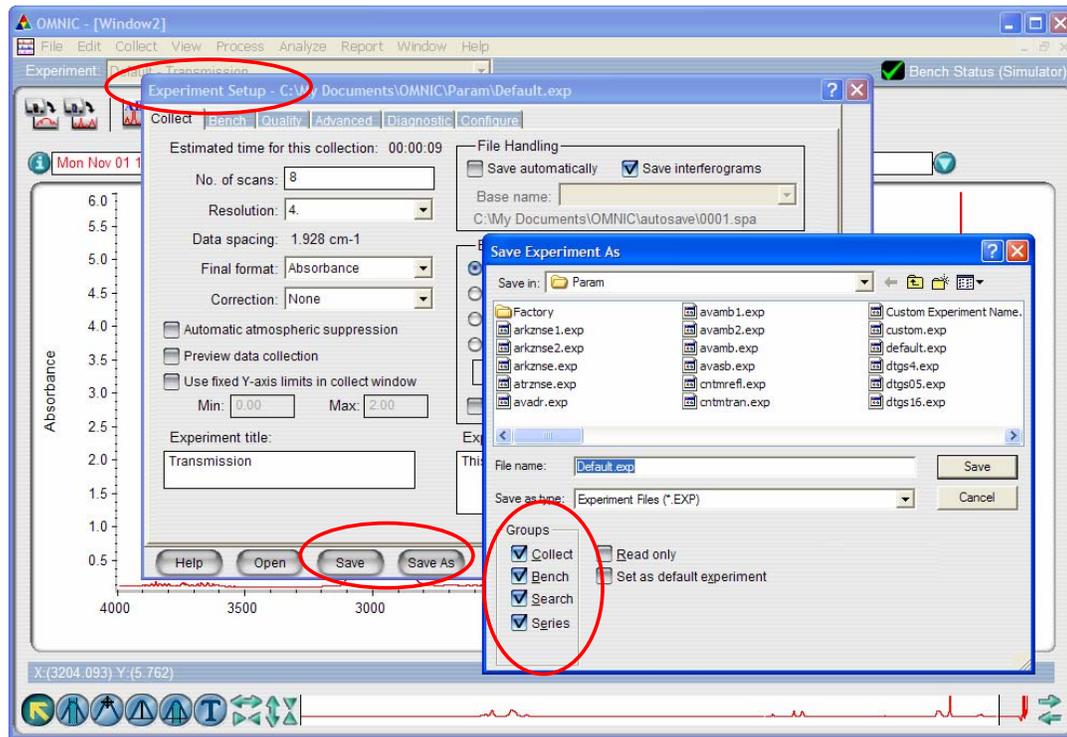
OK Cancel Search QC Compare Help...

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You may select an entire spectrum, or specific regions. If you decide to search only a region, be sure to enable Use Spectral Region. Then, select the regions to search by clicking in the spectrum and setting the area. More than one region may be searched by selecting the Add button and adding additional regions. The selected regions are indicated in the table on the bottom left corner as well as in the spectral window. When you perform the search, the spectral regions you specify will be used.

# Library Setup - Tie Library Setup to Experiment

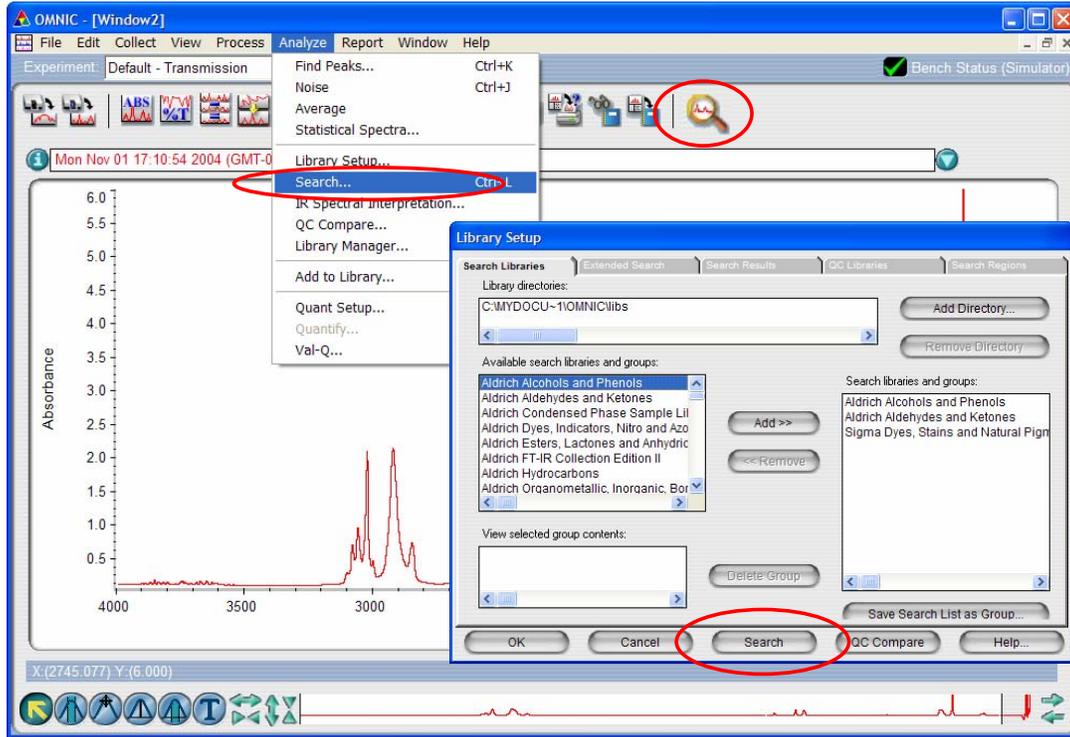


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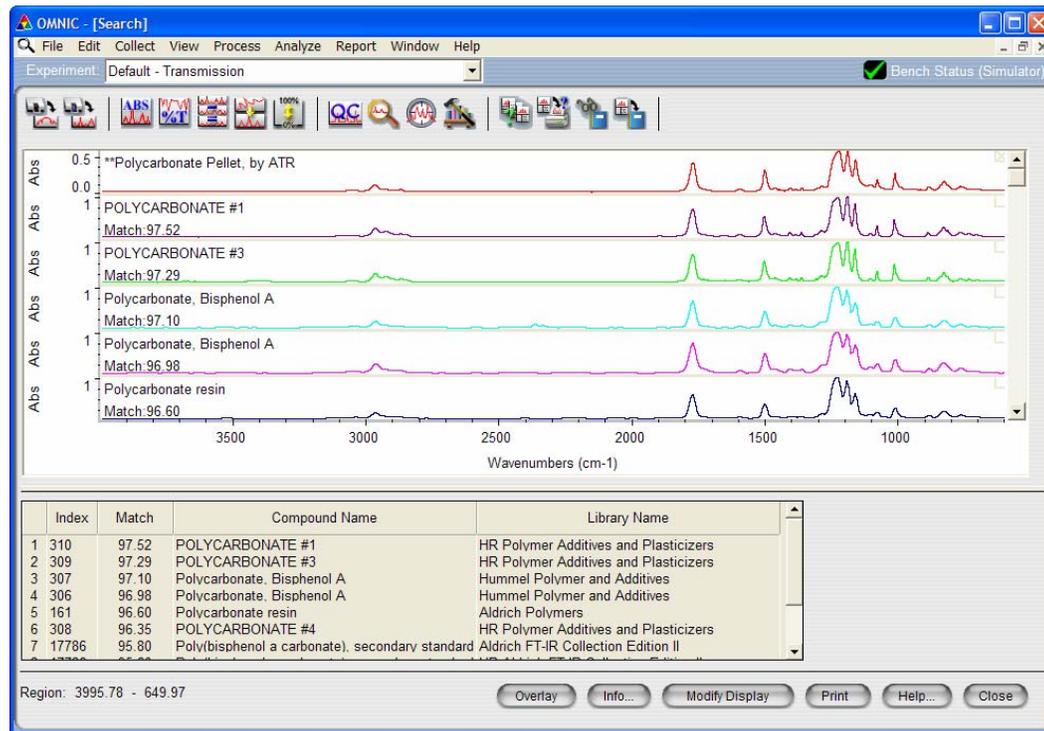
Library setups may be tied to specific experiment files in OMNIC. This means that as each experiment file is loaded in OMNIC, the associated Library list will also load. In order to tie the library setup to an experiment you must save the experiment again. Note that the "search" group is enabled, lower left hand corner of the Save Experiment As dialog box.

# Library Search Command



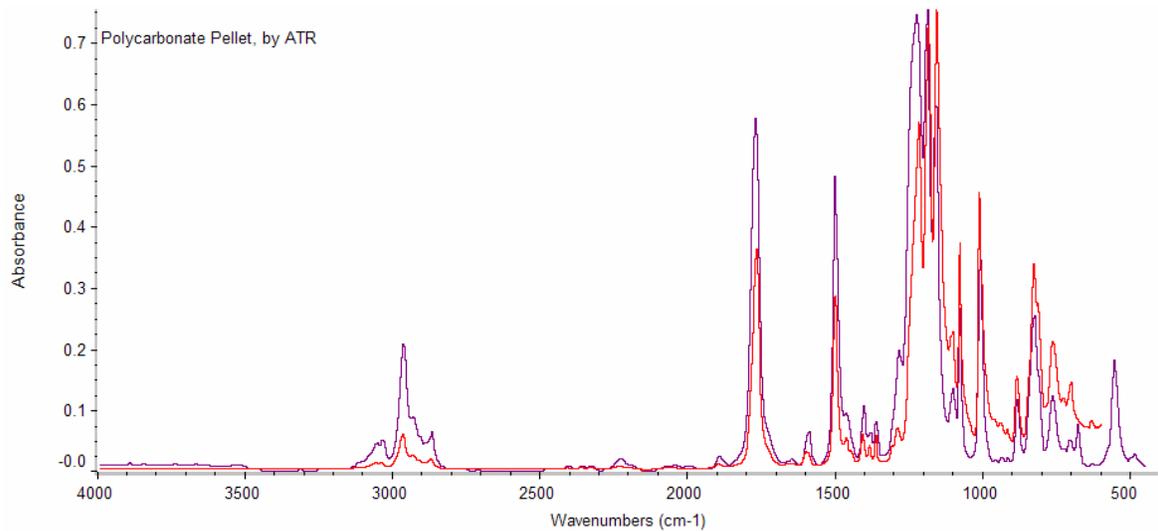
You may search either directly from OMNIC by selecting the Analyze drop down menu, and Search. Or, you may search directly from Library Setup by selecting Search button at the bottom of the Library setup dialogue box.

# Library Search Results Window



Search Results are displayed above. You may gain access to the spectra associated with the library hit by using the scroll bar on the right side of the spectral display. Note that you may also see any information specific to a listed hit by highlighting the hit in the list and the selecting the Info button located at the bottom of the screen. You may also modify the search window display by selecting Modify display.

# Examining Search Results



## ***Possible Reasons for differences:***

- Experimental technique
- Resolution
- Corrections applied or Library spectra were normalized

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Most commonly, the selected hit from the library is copied from the Search Result Window to an OMNIC window to compare results between a commercial library spectrum and the sample spectrum.

It is important that you make the final judgment as to the matching of the library spectrum to your sample. The search results can be in error and should not be taken as the absolute answer.

It is important to note that many of the older commercial libraries lack information regarding experimental conditions. These differences may impact the quality of the match value. Because of this, always use caution when reviewing the match value.

# Search Expert Results

The screenshot displays the OMNIC software interface. The main window shows an IR spectrum plot with the following text: "Polycarbonate Pellet, by ATR", "Use for Advanced ATR Corrector. Correction parameters: Diamond crystal, RI = 2.40, Angle of incidence = 45 degrees", "Poly(bisphenol a carbonate), average MW ca. 64", "Match 89.38", "Aldrich Catalog No: 18162-5", "CAS Number: 25037-45-0", "Molecular Formula:", "Volume & Page Number: 3.4619A". The x-axis is labeled "Region: 2600.00 - 450.00". The y-axis is labeled "Absorbance".

The "Library Setup" dialog box is open, showing the "Extended Search" tab. The "Use search expert" option is selected and circled in red. Other options include "Configure search results". The "Search type" is set to "Correlation". The "List of Matches" section has "List compounds with match values above:" set to 10 and "Maximum number of compounds in list:" set to 10. The "Spectral Display" section has "Number of library spectra to display:" set to 5. The "Show match values" checkbox is checked. Buttons at the bottom of the dialog include "OK", "Cancel", "Search", "QC Compare", and "Help...".

 **The best match is very good, but the second best match is also similar.**

Buttons at the bottom of the main window include "Info...", "View Match List", "Print", "Help...", and "Close".

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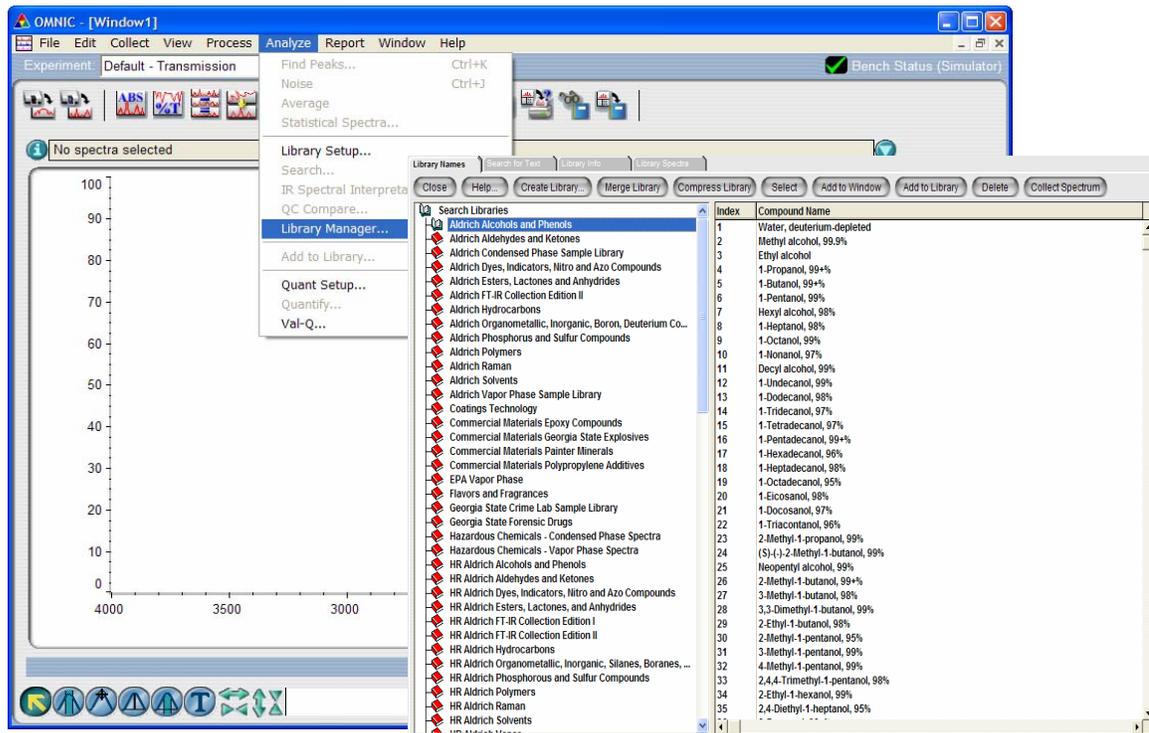
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Search Expert examines the spectral data from 2600 to 450  $\text{cm}^{-1}$ . When a match is found, it comments on the quality. In this example it found the first match to be excellent.

To use Search Expert be sure to enable it in the Library Setup Dialogue box, Search Results Tab.

Search Expert is great for inexperienced users who want more reassurance about the quality of the result.

# Library Manager - Library Name Tab



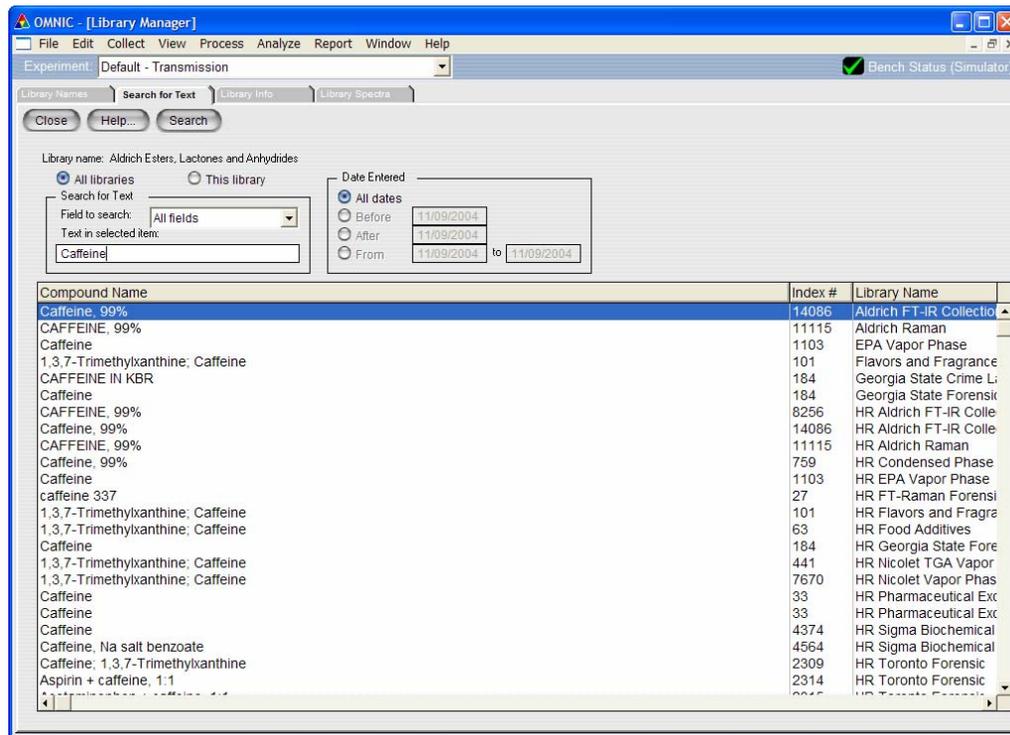
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Commercial and User libraries may be managed using Library Manager. Select Analyze | Library Manager. Like many other OMNIC Dialogue boxes, there are several tabs across the top. The first tab lists all the libraries available. By selecting a library from the left hand list, all the spectra contained in the library appear on the right hand side. You may sort the spectra by index number or by name by selecting Compound Name title bar.

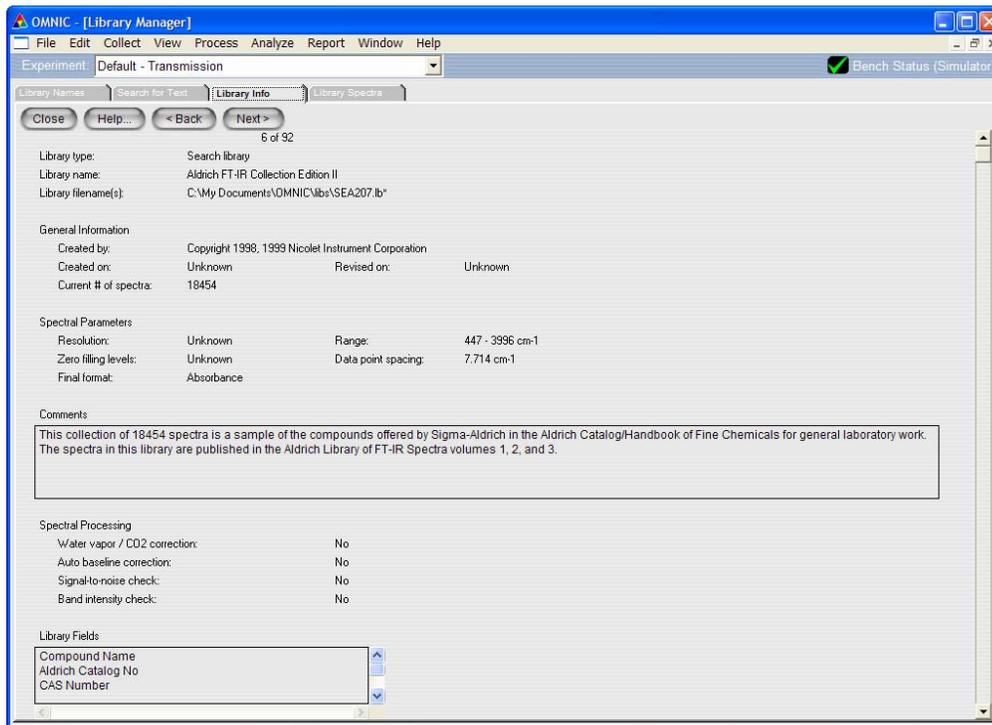
Note the buttons running across the top of the display are used with User Libraries and will be discussed later.

# Library Manager - Search for Text Tab



You may search a library for text by selecting the Search for Text tab. You may search all the libraries available, or a single library selected under the Library Names tab. You may search all available fields in a library or just the compound name. In this example we searched for all spectra containing the word Nujol in all fields looking for a representative spectrum prepared as a Nujol Mull.

# Library Manager - Library Info Tab



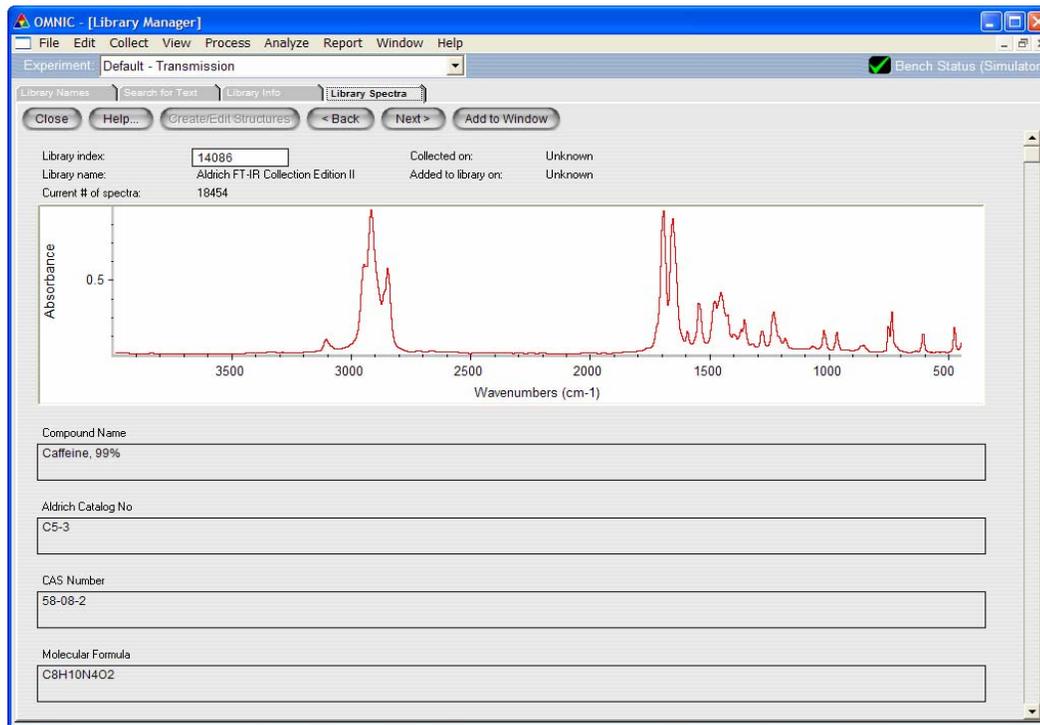
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Selecting the Library Info Tab gives all information available about a selected library. Note that many of the older commercial libraries have very little information, especially the experimental conditions used to collect data. This is one reason why we encourage you to develop your own user libraries.

You may cycle through all the libraries available by selecting the back and next buttons at the top of the display

# Library Manager - Library Spectra Tab

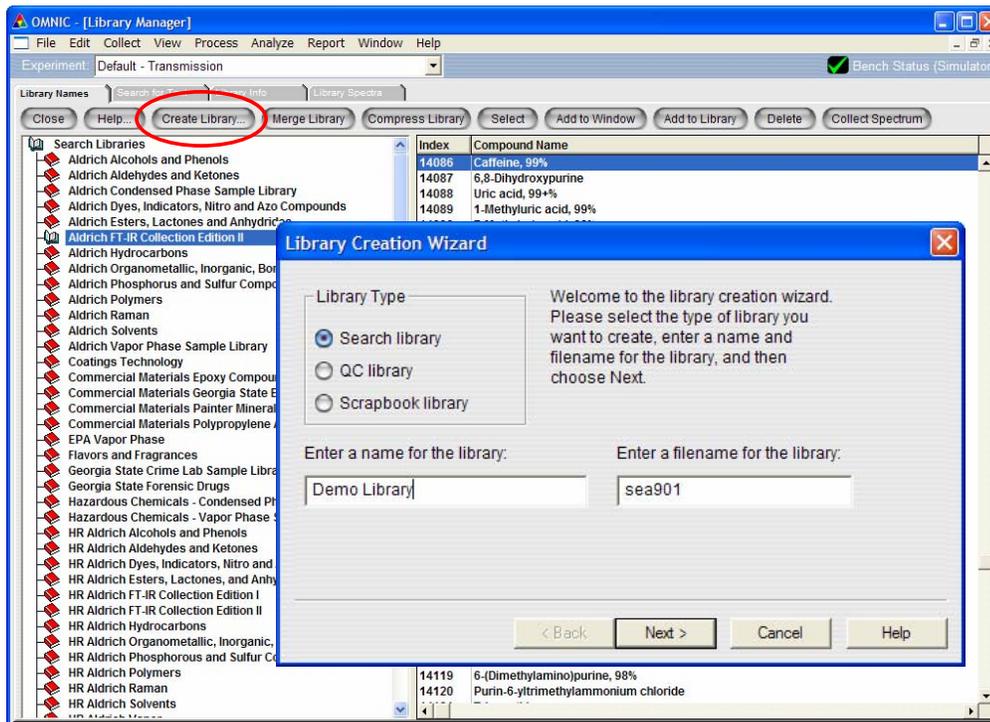


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Library Spectra Tab gives you access to individual spectra contained in the selected library, as well as any available information about the spectrum. You may copy the spectrum out to an OMNIC window by selecting the Add to Window button at the top of the display. This can be useful when preparing synthetic spectra or doing a visual comparison.

# Library Manager - Creating User Search Library



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Quite possibly the most important feature of Library Manager is the ability to create a new User Library. To do so, simply select the Library Names Tab and then select Create.

OMNIC provides a Library Creation Wizard to help you step through the process of creating a library. The first box that appears requires you to decide what type of library to create and to give the library a name.

Library Types:

Search Libraries -- this is the most commonly used User Library. It allows you to input reference spectra and to search against using any of OMNIC's search algorithms. It behaves just like a commercial library except that you can add and delete spectra.

QC Libraries – Discussed at the end of this section.

Scrapbook Libraries – A place to store unusual spectra. You may not search against a scrapbook library.

# Library Manager - Creating User Search Library

The image displays two screenshots of the 'Library Creation Wizard' dialog box. The first screenshot shows the 'Comments about this library' step, where the user has entered 'This is a demo library for training purposes' in the text area and 'Trainer name' in the name field. The second screenshot shows the 'Titles of custom information fields' step, where the user has entered 'CAS number:', 'Solid or Liquid', and 'BLANK' in the three text boxes. Both screenshots include 'Back' and 'Next' buttons.

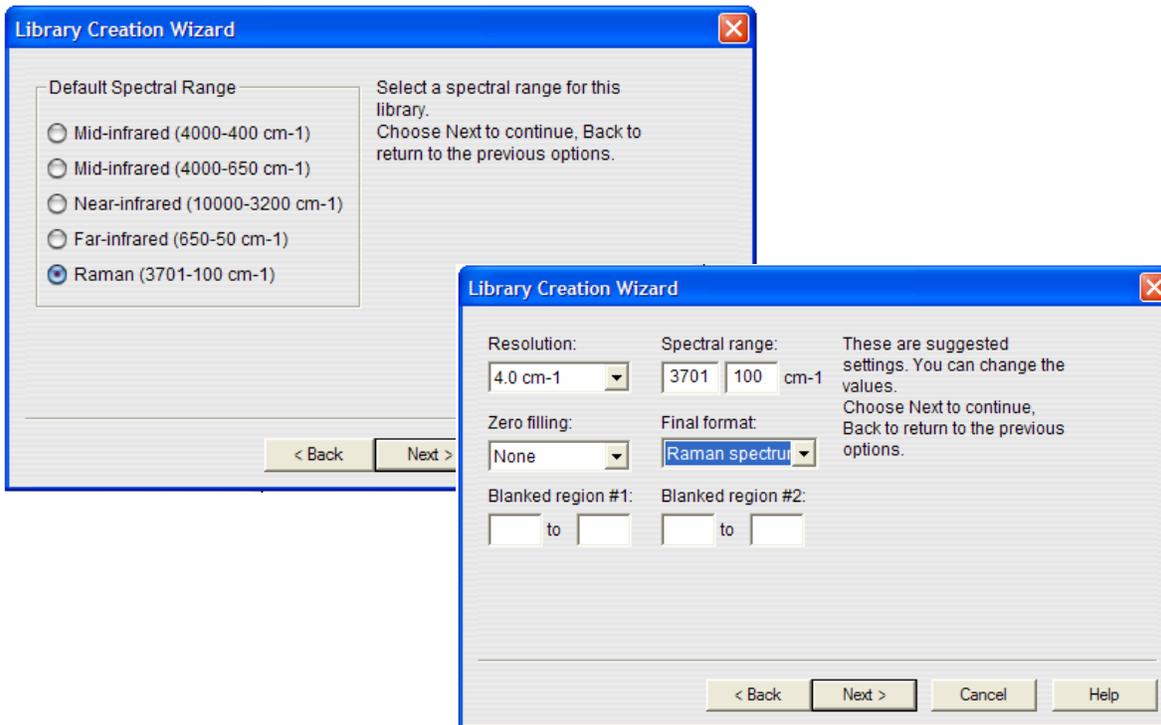
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The next two boxes request additional information to be stored as part of the header of the library. We encourage you to enter as much meaningful information as you can regarding the library. Information about how the spectra were collected can be particularly helpful.

You may also enter "custom information" into the header of each spectrum inserted into a library. The third wizard box provides a place for such an entry. This is reserved for anything other than the title of the spectrum. For example, if you were running standards with a known CAS number you would enter "CAS Number". When a spectrum is entered into this library you will be prompted to enter a title as well as CAS Number.

# Library Manager - Creating User Search Library



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When the first spectrum you attempt to add to a user search library or QC library has a lower resolution (higher numerical value) than that specified when the library was created, it will not be added. A message will appear indicating that the resolution is lower than expected.

When the first spectrum you attempt to add to a user search library or QC library has a higher resolution (lower numerical value) than that specified when the library was created, it will be added. However, the spectrum will be deresolved to match the resolution of the library. No message appears in this case. All subsequent spectra of any resolution that you attempt to add will be accepted by the library. When these spectra are added, the data point spacing (which determines the spectral resolution) is adjusted to match that of the library.

The first spectrum you add to a user search library or QC library determines the spectral range of the library. If the spectral range specified when you created the library is different from that of the first spectrum, the library's spectral range will be adjusted. After the first spectrum has been added and you attempt to add a spectrum with a narrower spectral range, the spectrum will not be accepted by the library. A message will appear indicating that the spectral range does not include the entire library range. If you attempt to add a spectrum with a broader spectral range after the first spectrum has been added, the spectrum will be accepted by the library. However, the spectral range will be decreased to match the spectral range of the library. No message appears in this case. This is why we suggest that you make user libraries specific to experimental techniques!

## Library Manager - Creating User Search Library

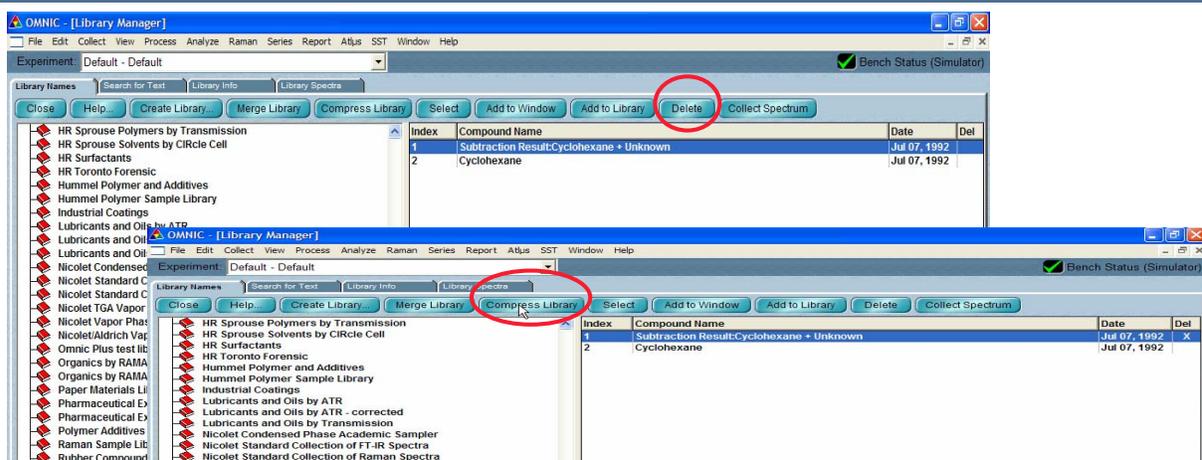


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The last wizard box asks whether you would like to correct or check the spectrum prior to putting in the library. Because the library is a permanent collection of reference spectra it is recommended that you manually perform corrections and checks on each spectrum prior to adding to a library. This will ensure that you approve of the quality of each spectrum before it becomes a permanent addition to a library

# Deleting Library Entries from User Libraries



- After deleting an entry, it is necessary to press the compress library button to remove it entirely
- Libraries that have not been compressed will display deleted entries with a red X in the del column at the far right of the screen.
- This extra step is necessary as some users leave the deleted entry as a place holder to preserve the index number system of their library.

After you delete one or more spectra from a user library, you can use the Compress Library button on the Library Names tab of Library Manager

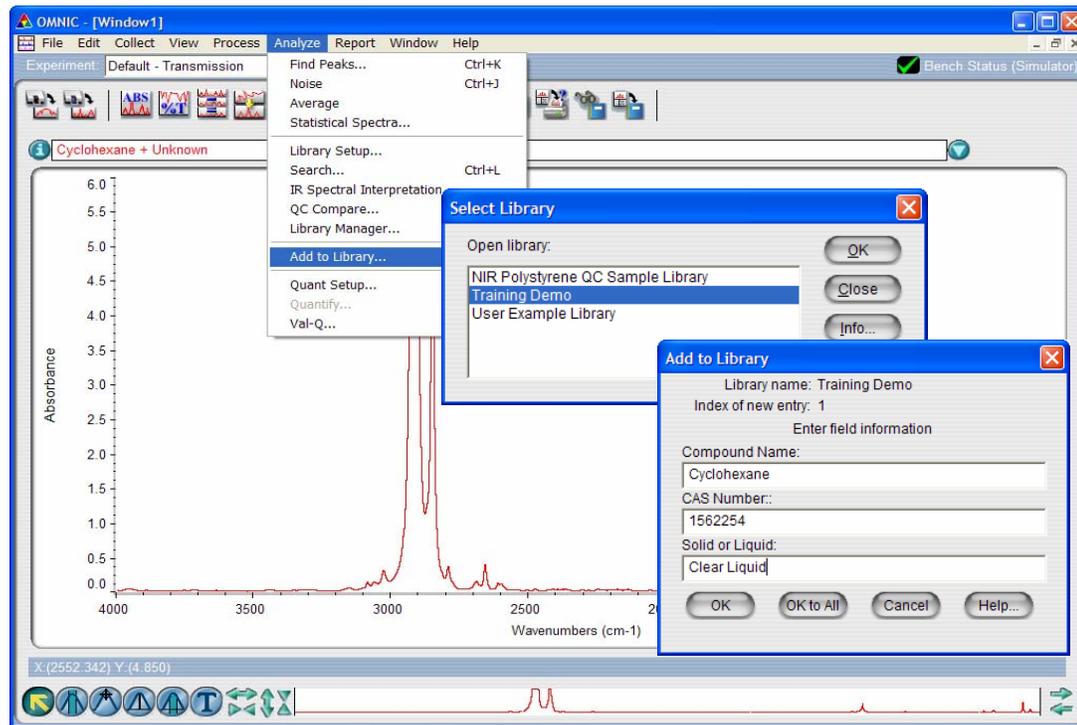
to remove the deleted spectra (including the "X" in the Del column) from the list of library spectra. The remaining spectra are then consecutively renumbered.

## Library Manager

### Creating User Search Library Summary

- Consider making user libraries experiment specific
- Be explicit in comments about the library
- Consider Resolution - Higher Res data is deresolved, lower Res is hyper-resolved (data points added)
- Consider Spectral Range - 1st spectrum going in sets range of library forever after
- If you delete an entry from a library don't forget to COMPRESS library to eliminate "holes"

## Add a Spectrum to Search Library



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To add a spectrum to a User Created Search Library, select Add to Library from the Analyze drop down Menu. Select the library which you want to use and then enter compound name. Note that the Compound Name comes by default from the title of the spectrum. Also enter any additional information you may have placed into custom information fields. Additional information, in this example the CAS number, comes from the comments field of the spectrum.

## QC Libraries and QC Compare

- A QC library is a collection of known reference spectra with a similar characteristic. This collection is known as a compound type.
- A QC Library may have one or many compound types.
- QC Compare employs a QC Library to verify the composition of a sample as belonging to a compound type.
- It provides a calculated measure as to how well the material compares to the most similar reference within the compound type.
- It is NOT used to identify unknown materials.

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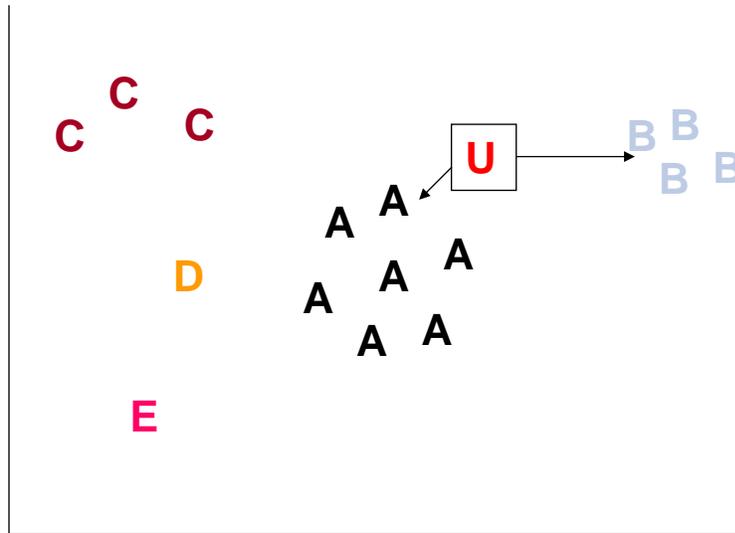
QC Libraries and QC Compare are used to characterize materials you already know something about by comparing the similarity between reference materials and sample material. A compound type is a collection of spectra which come from a larger population that represents some attribute or feature you wish to monitor. For example, you may develop a library which represents a component in your final product that may vary in concentration.

A QC Library may contain several compound types, or you may create several QC Libraries with a single compound type. The choice will depend on how you wish to search the QC library.

It is important to note that QC libraries are NOT used to identify unknown materials. In addition, the calculation algorithm used is not like that used for a simple correlation coefficient.

# Graphical Representation of QC Compare

- QC Compare utilizes the “nearest neighbor” classification.\*



Useful Link: <http://cgm.cs.mcgill.ca/~soss/cs644/projects/simard/>

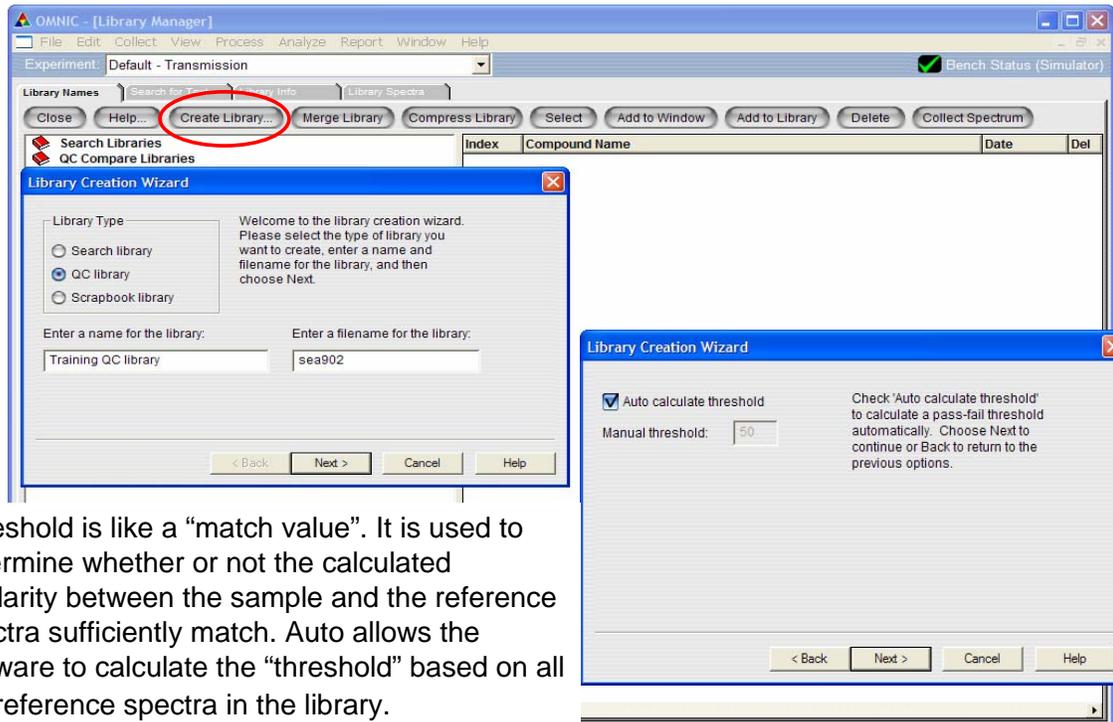
\* T. M. Cover and P. E. Hart, "Nearest Neighbor Pattern Classification," *IEEE Transactions on Information Theory*, Vol. IT-13(1), 1967, pp.21-27.

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This is a pictorial illustration of the Nearest-Neighbor algorithm.

# Library Manager - Creating QC Libraries



Threshold is like a “match value”. It is used to determine whether or not the calculated similarity between the sample and the reference spectra sufficiently match. Auto allows the software to calculate the “threshold” based on all the reference spectra in the library.

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Creating a QC library is just like creating a search library except you must define the library type as a QC library.

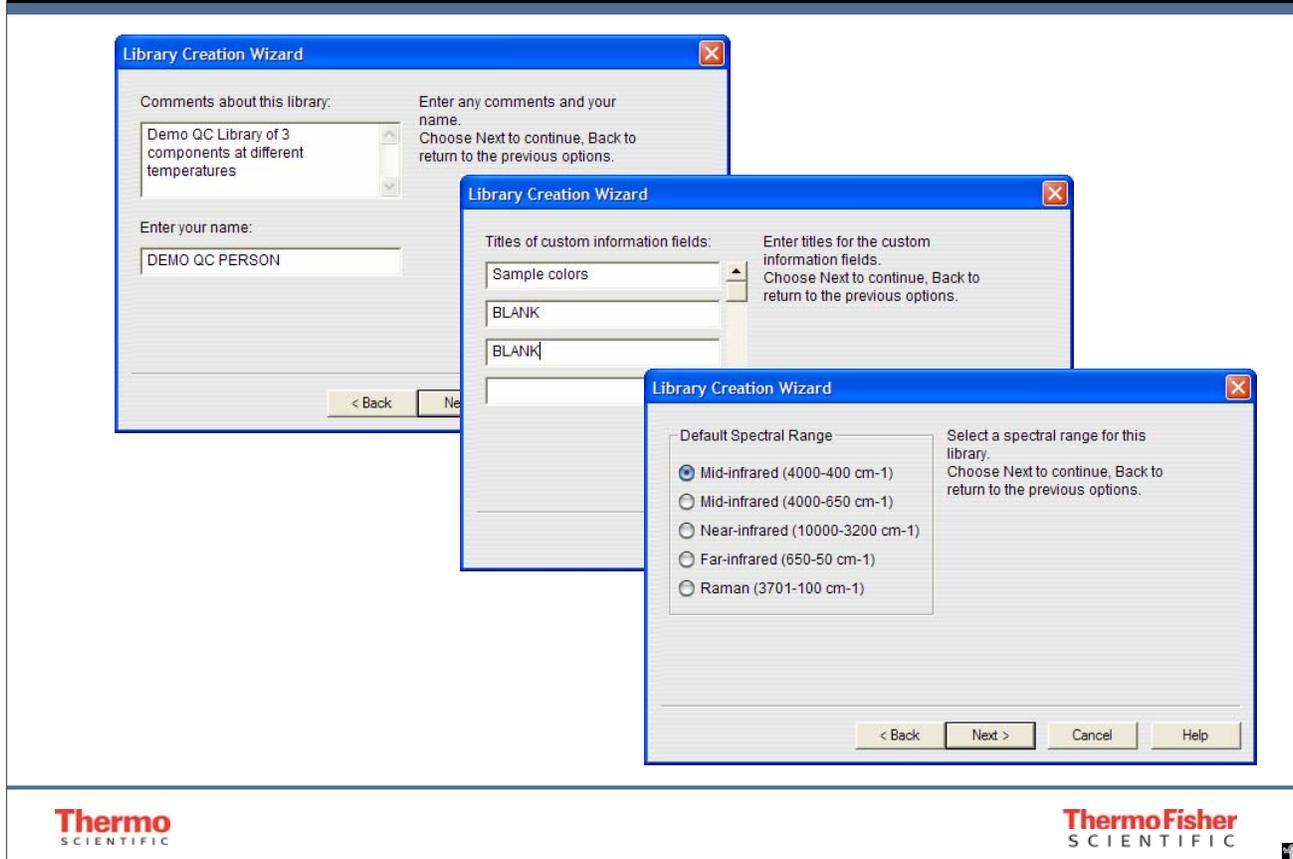
Select Library Manager from the Analyze drop down menu. Then select the create button. Select QC Library as Library Type. Enter a name and select next.

The next box which appears requires you to decide how to handle the “threshold”.

“Threshold” can be thought of as a match value, and in fact is referred to as the “critical match value” when looking at the results of QC Compare. A comparison that falls below the threshold value is said not to match.

When “Auto threshold” is selected the “threshold” is calculated as the similarity (and dissimilarity) between your all the spectra in your QC library, not just those spectra representing a single compound type. It is recalculated each time a new spectrum is added. For this reason, it is a good idea to for single QC Libraries to contain similar compound types.

# Library Manager - Creating QC Libraries



The following screens are identical to the ones that we reviewed in creating a search library. It is recommended to add QC to the title of any QC compare libraries that are created to easily differentiate them from standard search libraries.

Like a search library, you are encouraged to enter as much information as possible about the library. You may also enter custom information and finally select a default spectral range to populate the next Wizard box.

# Library Manager - Creating QC Libraries

**Library Creation Wizard**

Resolution: 4.0 cm-1      Spectral range: 4000 400 cm-1      These are suggested settings. You can change the values. Choose Next to continue, Back to return to the previous options.

Zero filling: None      Final format: Absorbance

Blanked region #1: | to |      Blanked region #2: | to |

< Back      Next >

**Library Creation Wizard**

Default Spectral Processing

- Water/CO2 correction
- Auto baseline correction
- Signal-to-noise check
- Intensity warning level

These are recommended processing options. Make changes as desired. Choose Finish to create the library or Back to return to the previous options.

< Back      Finish      Cancel      Help

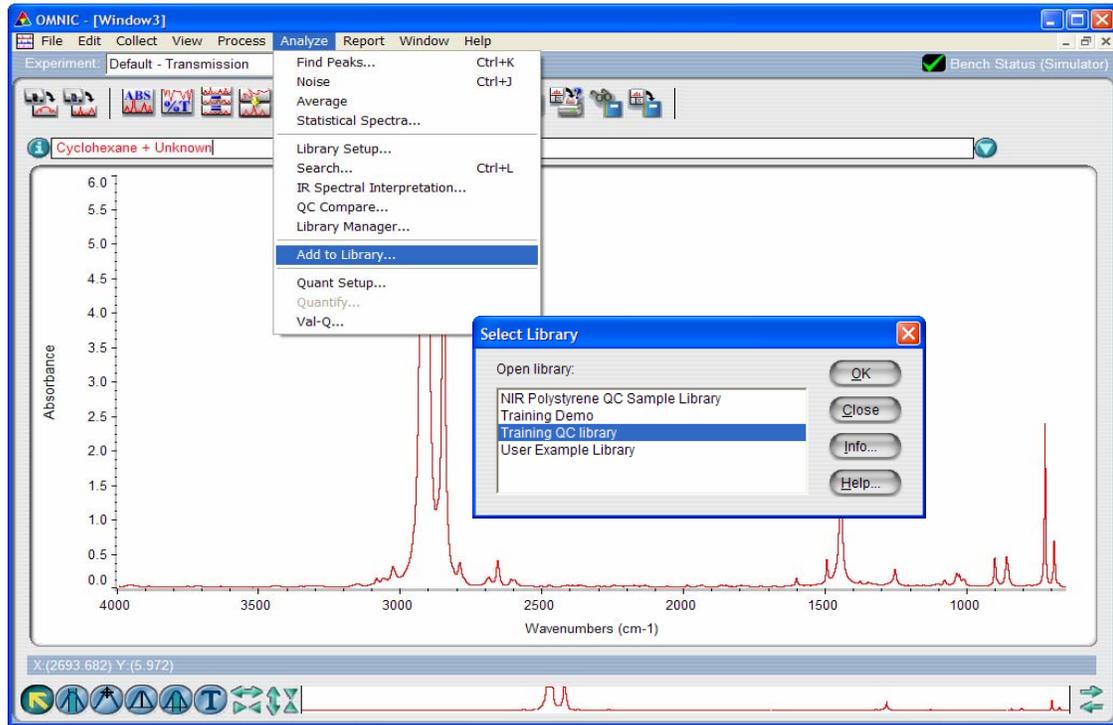
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Just as in search libraries, you must decide ahead of time the resolution of the library as once it is set it can not be changed. The spectral range is based on the spectral range of the first spectrum added to the library.

Any processing should be done outside of the library so that you know the quality of the spectra being added.

# Adding a Spectrum to QC Libraries



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## Adding a Spectrum to QC Libraries

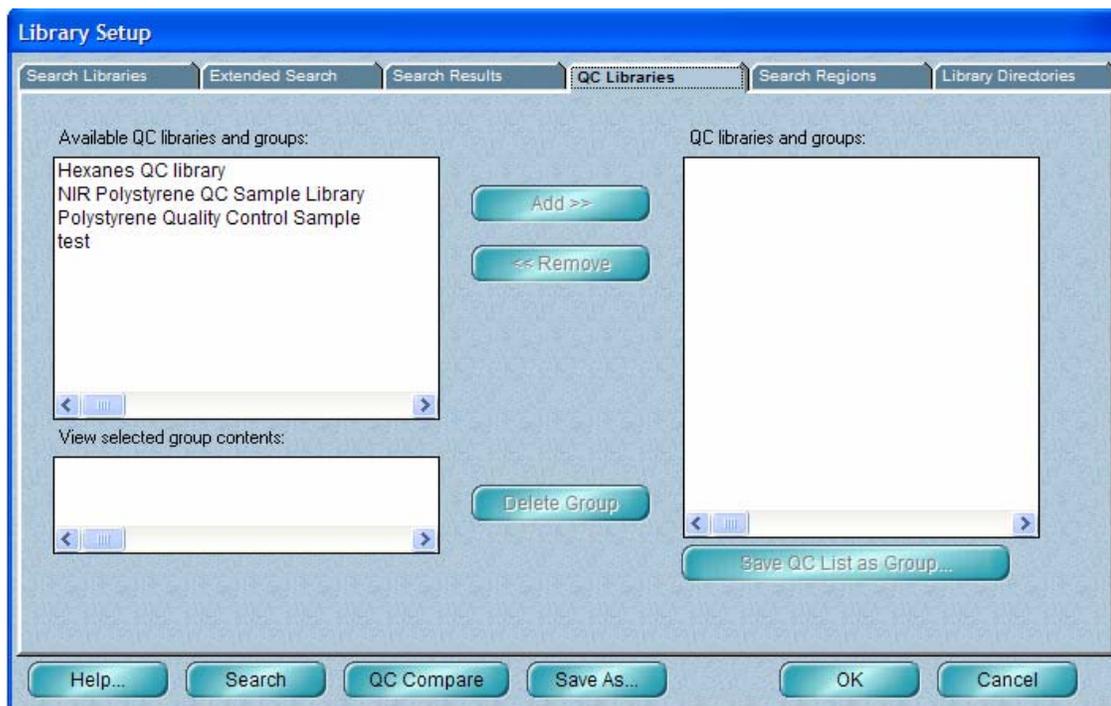
The image displays two sequential screenshots of the 'Add to Library' dialog box. Both windows have a blue title bar with a close button (X) in the top right corner. The left window shows the initial state: 'Library name: Hexanes QC library', 'Index of new entry: 1', 'Match threshold: 50.00', and 'Best match value:'. The 'Add to current compound type' radio button is unselected, and the 'Enter a compound type' radio button is selected. The 'Enter field information' section contains three empty text boxes for 'Compound Name:', 'Formula weight:', and 'LIMS number:'. The right window shows the state after the first entry: 'Index of new entry: 2', 'Match threshold: 50.00', and 'Best match value: 100.00'. The 'Add to current compound type' radio button is now selected. The 'Enter field information' section contains three text boxes: 'Compound Name:' with '10% hexane, 90% cyclohexane', 'Formula weight:', and 'LIMS number:'. Both windows have 'OK', 'OK to All', 'Cancel', and 'Help...' buttons at the bottom.

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Adding a spectrum to a QC library is similar to adding it to a search library except that you must define compound types. In this example, the first spectrum added into the QC library was cyclohexane, a new compound type was entered. The second spectrum was also a mixture of hexanes. So, Hexanes were selected under "Add to current compound type".

## Library Setup - Selecting QC Libraries

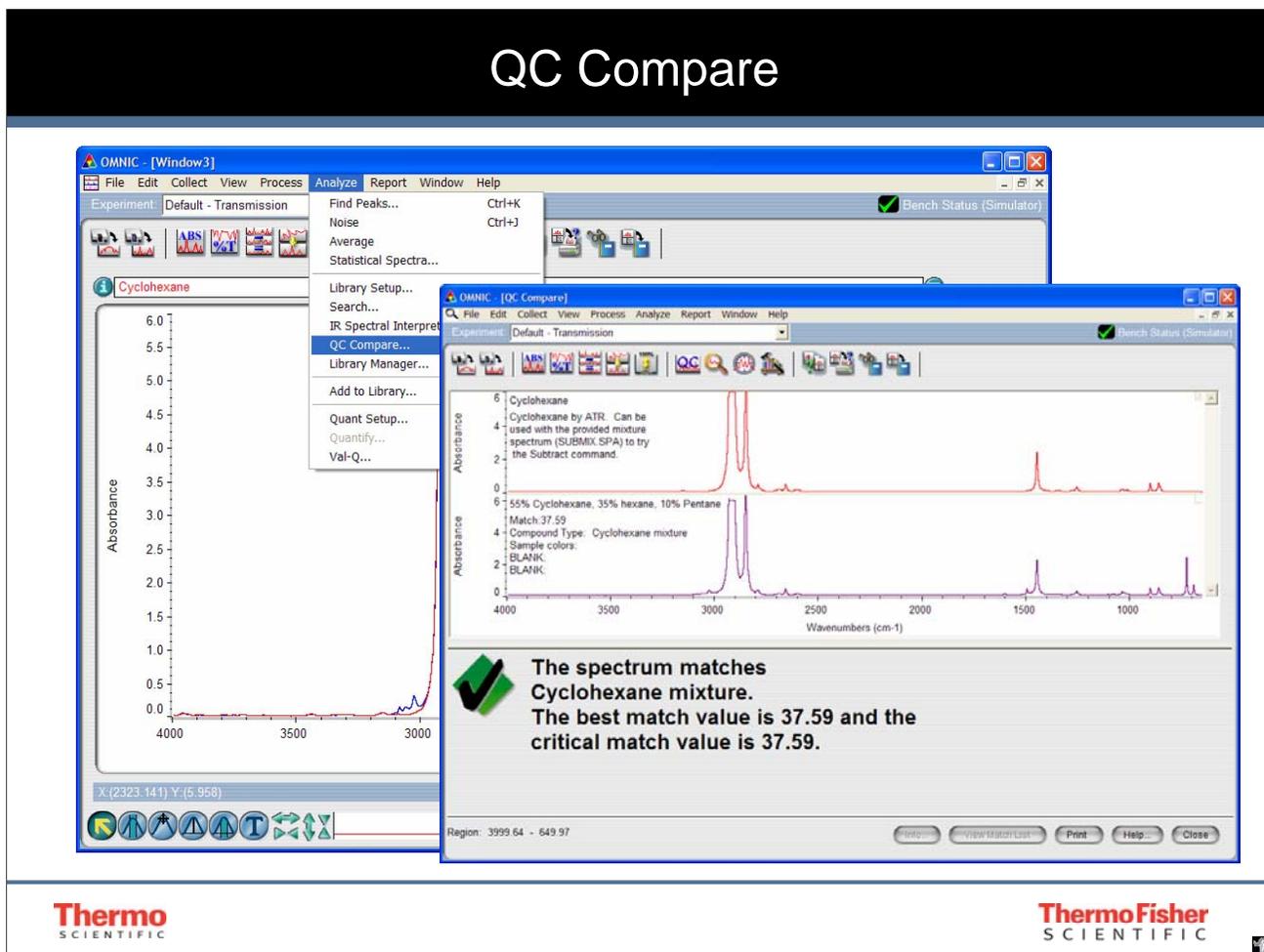


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Before you can use QC Compare you must select your newly created QC Library. Using the Analyze drop down menu select Library Setup. Then select the QC Libraries Tab. Highlight the new library and click Add to transfer it to the list on the right hand side of the screen. You may select QC Compare directly from this window or return to OMNIC window, select Analyze, select QC Compare.

# QC Compare

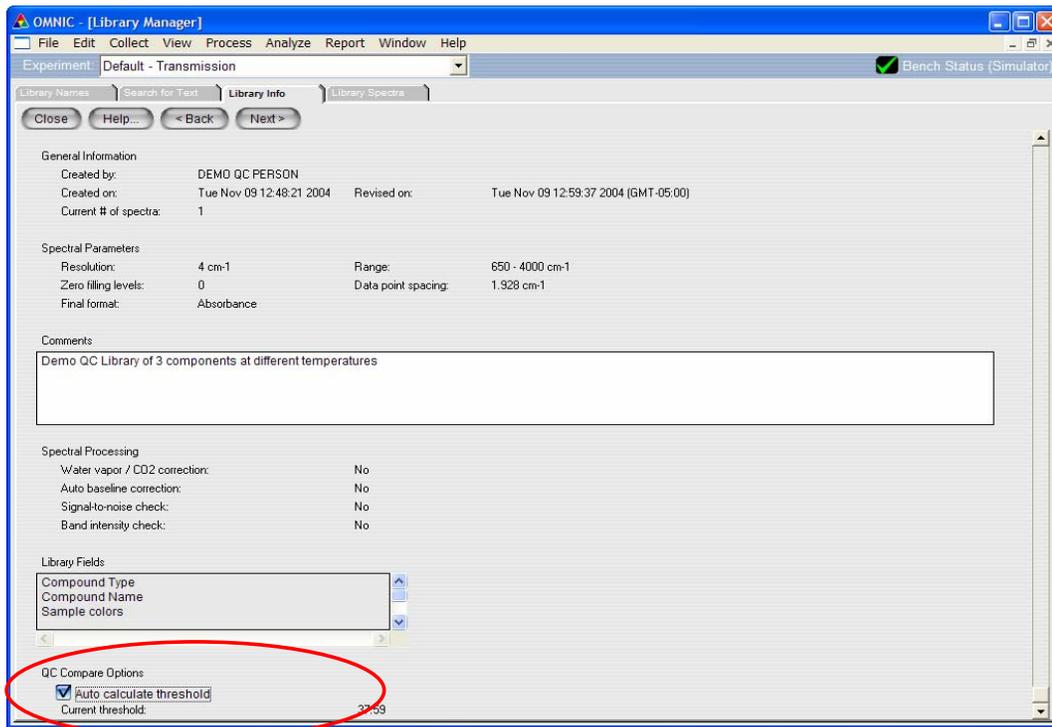


This screen shows the result of QC Compare. In this example, a xylene mixture of unknown concentration was analyzed. It compares favorably to the QC library of Hexanes. The top spectrum is the unknown Xylene. The bottom spectrum is the spectrum which matches best to the unknown. The software comments that the spectrum matches because it is above the critical match value. Recall that the critical match value is actually the threshold.

The best match value is calculated using a correlation coefficient with a scaling function applied.

If you prefer to use a correlation coefficient without the scaling function you can set up a classification method using TQ Analyst software.

# Manually Changing Threshold



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You may manually change the threshold by Selecting Analyze | Library Manager | Library Info Tab. Scroll to the bottom of the display to make changes.

## Library Manager - QC Library Summary

- Like Search Libraries, use the same Experimental Conditions including resolution and spectral range for reference spectra
- Keep similar compound types together in one QC library
- Use Auto threshold to allow OMNIC to calculate threshold value based on all reference spectra in QC Library
- Recall that the Critical Match Value is the same as the threshold value and is based on a “nearest neighbor” algorithm.
- The Best Match value calculated between your sample spectrum and the best library match is the familiar correlation coefficient *with a scaling function applied.*

# Libraries - Review

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*Select Libraries*

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*Choosing Regions*

*Tying Libraries to Experiment setup*

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