

## Use of NIST Library with Finnigan Xcalibur Software

### Table of Contents

- 1.0. Introduction
- 2.0. Installing Software
  - 2.1. Initial Install of Software
  - 2.2. Installing NIST, Wiley6 or 7, User, and Xcalibur Demo Libraries
  - 2.3. Updating to NIST Version 1.7 or 2.0
- 3.0. Using the Search Software
  - 3.1. Using Internal NIST-Xcalibur Search
  - 3.2. Using External NIST Search
- 4.0. Known Limitations, Variations from Standards, Bugs

### 1.0. Introduction

Xcalibur can use the NIST search in two ways. It can export the spectra to Version 1.7-2.1 of the NIST search program or it uses the NIST search software internally. In the export mode, the spectrum is automatically exported in ASCII format to the NIST search, the spectrum automatically searched, and the results displayed within the NIST search window. In the internal mode, Xcalibur uses the NIST dll (the guts of the NIST search) to search the unknown and the results are displayed within an Xcalibur program window.

This has several advantages in my opinion. The user can either chose to use the Xcalibur software alone or use the NIST search software if they are already using the latter in other applications. Another approach is to use both. The NIST program has a wide variety of capabilities including creation of user libraries with structures, searching of libraries by structures (Version 2 only), synonym-name searches, etc. Another big advantage is that the Xcalibur and NIST programs use the same binary format for storing EI reference spectra.

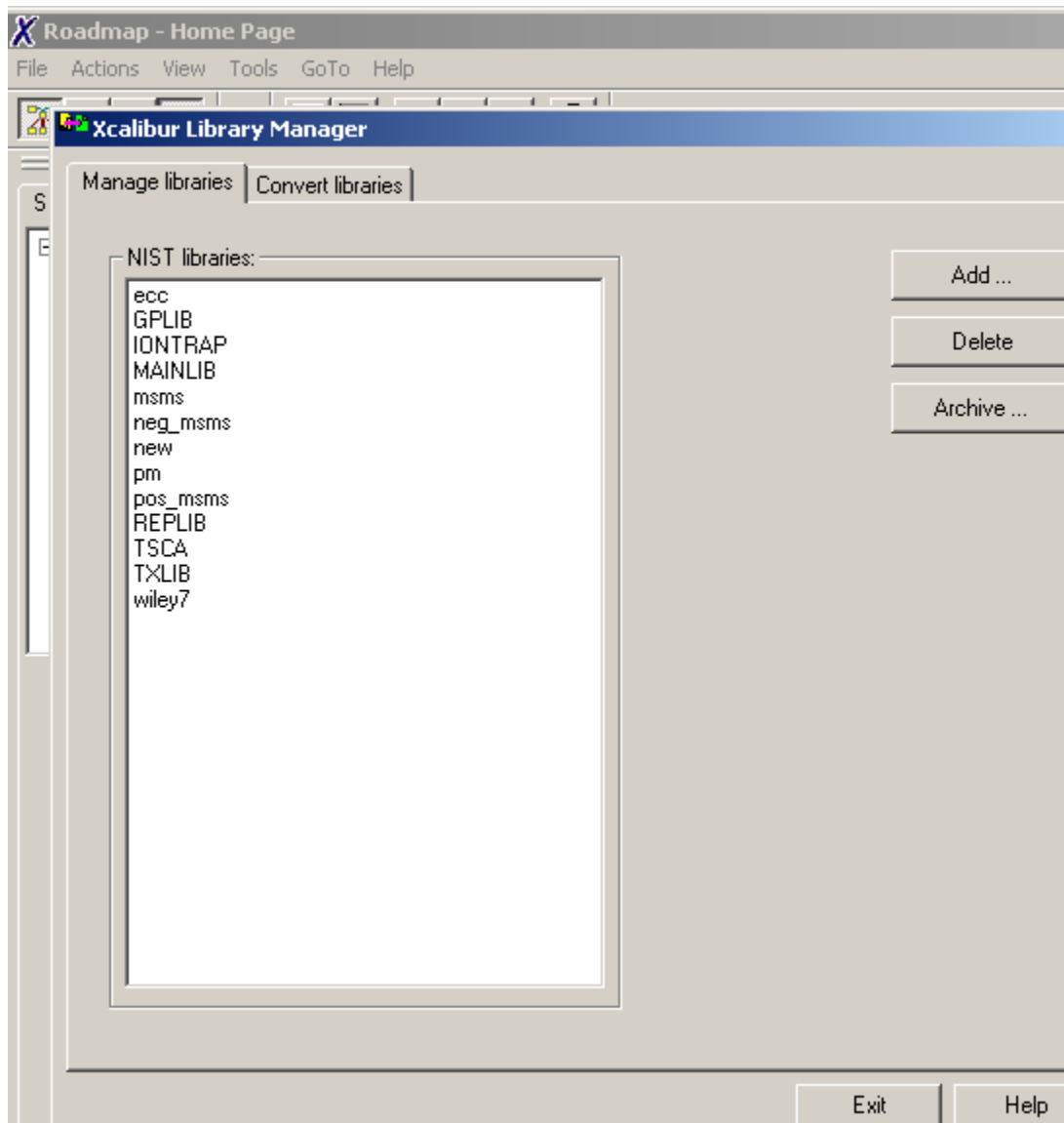
### 2.0. Installing Software

**2.1. Initial Install of Software:** The Xcalibur software (I've only used Version 1.0) is very easy to install. In addition, the NIST Version 1.6 is installed as a part of the Xcalibur install. The NIST software is installed in the C:\Program Files\NISTMS\MSSEARCH directory.

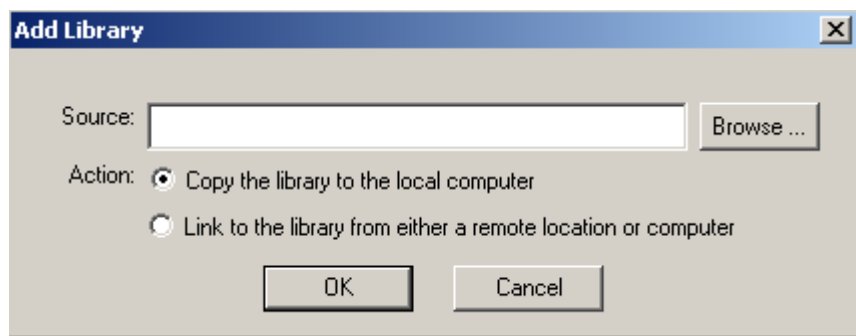
**2.2. Installing NIST, Wiley6 or 7, User, and Xcalibur Demo Libraries:** After installing the software, the user will have to install the NIST MAINLIB and the REPLIB. The MAINLIB contains the best (in NIST's opinion) spectrum for each compound. The REPLIB contains duplicates of many of the spectra in the MAINLIB. The latter library is very useful since spectra can vary from instrument to instrument and NIST sometimes "guesses" incorrectly which spectrum is the correct one. You'll need to purchase a copy of these libraries in NIST binary format and install these libraries in the C:\Program

Files\NISTMS\MSSEARCH directory. Copies of the Wiley6 and Wiley7 are also commercially available.

If you have user libraries, copy them (folder will contain up to 28 different subfiles) to the C:\Program Files\NISTMS\MSSEARCH by “right clicking-moving or copying them” from their current directory. Another way to copy libraries is to go to Xcalibur Roadmap Homepage to the tools/library manager option.



This will then allow you to Browse for the library of interest.



The program will then copy the library to the local computer or create a link. In the latter case, the library is left in its initial location and a link is created. Look inside the library folder and you will see a file named `alias.msd`, which contains the location of the library. I prefer having a copy locally if possible instead of a link through an alias for speed of access and control.

There are three libraries supplied on the Xcalibur CD named GPLIB (5826 compounds, variety of structure types), TXLIB (2211 drug components), and TRLIB (570 compounds, variety of structure types) to explore the capabilities of the NIST/Xcalibur search software.

**2.3. Updating to NIST Version 1.7 or 2.0:** After the initial install, you can update to either Version 1.7 or Version 2 of the NIST search. I will only discuss the latter since it allows the user to search the NIST database and user databases by structure. Obtain a copy of the Version 2.0 search software from NIST or a distributor. Install the software making sure it finds the current version (should find automatically) and select option to overwrite the existing version. This will place all the new NIST software in `C:\Program Files\NISTMS\MSSEARCH`. This is the location required by Xcalibur to link to the NIST software.

After the update to Version 2.0 is complete, you must make a copy of `nistms.exe`, rename it to `nist$.exe`, and place it in the `C:\Program Files\NISTMS\MSSEARCH` directory. `Nistms.exe` is the executable for calling/running the NIST search. Leaving the original copy of `nistms.exe` in addition to `nist$.exe` allows AMDIS (another data processing program installed with NIST search) to access the NIST search. You might find AMDIS useful for automatically deconvoluting components in complex GC-MS analyses.

If the NIST software was already installed before Xcalibur, I *think* Xcalibur will detect the location and change its internal pointer, but I've not thoroughly tested this approach. If you had version 2.0 installed, it might not since Xcalibur is looking for `nist$.exe` and the Version 2 executable is named `nistms.exe`.

### 3.0. Using the Search Software

**3.1. Using Internal NIST-Xcalibur Search:** The NIST search can be employed within Xcalibur very easily. However, personally I prefer the NIST search (*see next section*) external search because of its abilities to search with constraints, search by structure, etc.

To use the internal search, open the Qual Browser from the RoadMap Homepage. Open a GC-MS file to process. When I installed Xcalibur, the default was to display only a total chromatogram. To see a spectrum, single left click the “insert cell above” icon (if you leave the cursor over an icon, it displays its function) on the Qual Browser toolbar.



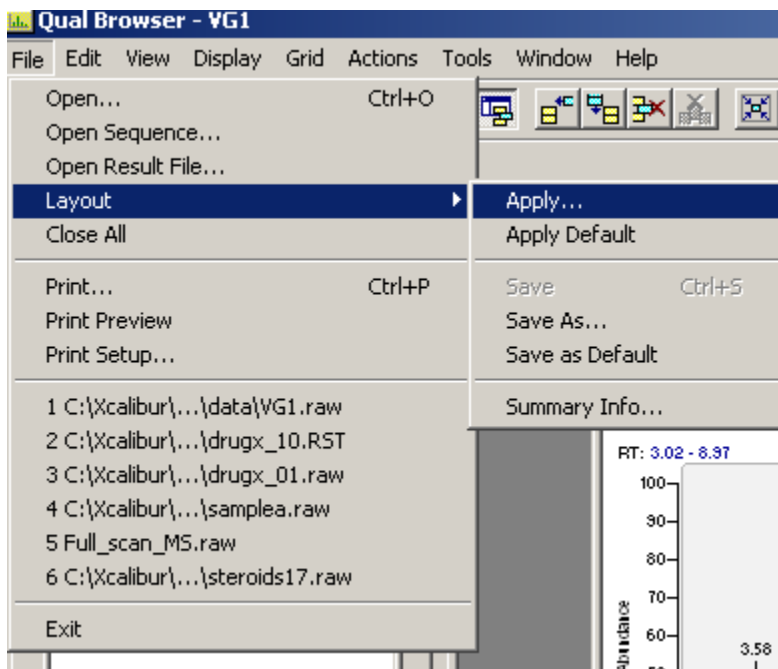
This will insert another cell. Select the bottom cell by single left clicking on the “tack” icon (should turn green),



then single left click the “view spectrum” icon on the toolbar.

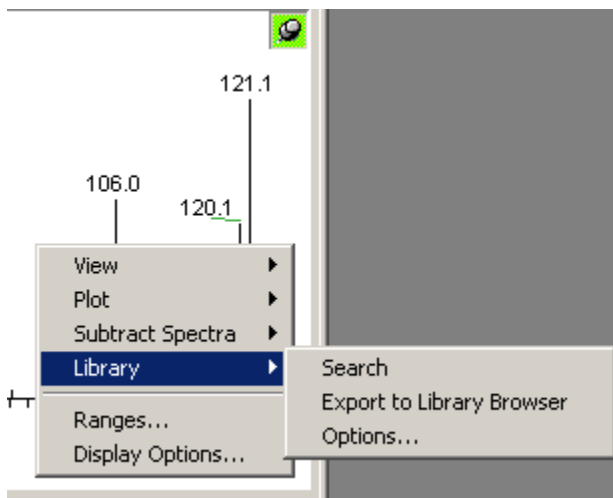


Now after you have everything setup, be sure to go to the file/layout option on the menu at the top left corner of the Qual Browser window. Either “save as” the layout or I just saved as the default layout. You can then recall the default layout or a particular configuration you find useful.

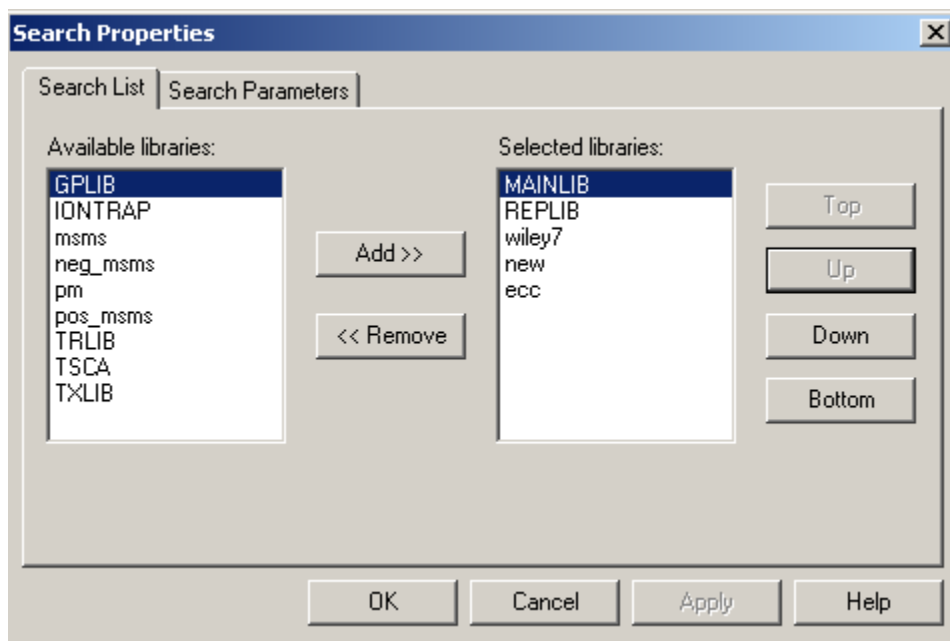


Now we're ready to do a search. Get a spectrum by making sure the "tack" on the spectrum window is selected (green tack) and left single click on the component of interest in the chromatogram window.

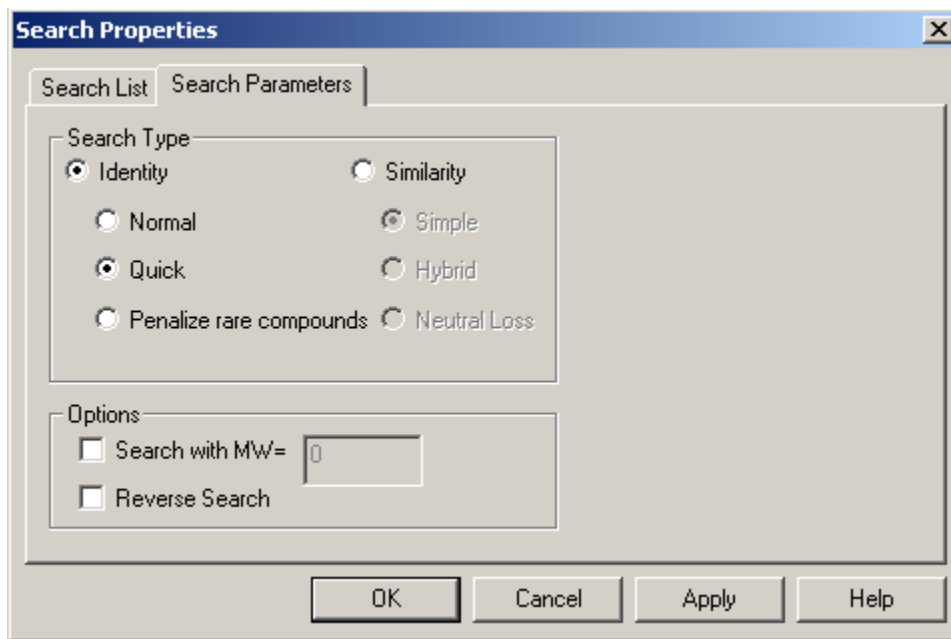
Then "right-click" (Not left click!) within the spectrum window and the following menu will be displayed:



The first time you select this menu, you will need to select the Options... tool. This will allow you to select which libraries to search and their order of search. Add all the libraries of interest to be searched and select their search order by moving them around in the list with the up, down, bottom keys. Sometimes order can be important, but usefully not a significant consideration. I would suggest the mainlib and replib be the first on the list since they are the highest quality and more diverse in my opinion.



You should also select the Search Parameters tab in the above window:



The most common setup is the identity with the quick presearch. The Normal presearch is a little more inclusive, but I find a Quick presearch to work in most cases and it saves time. The “Search with MW” option can yield much better results in some cases (partial spectrum of component in library, noisy user spectrum, etc) if the MW of the component is known. There are several other interesting options. See documentation including

-NIST Version 2.0 Users’ Manual

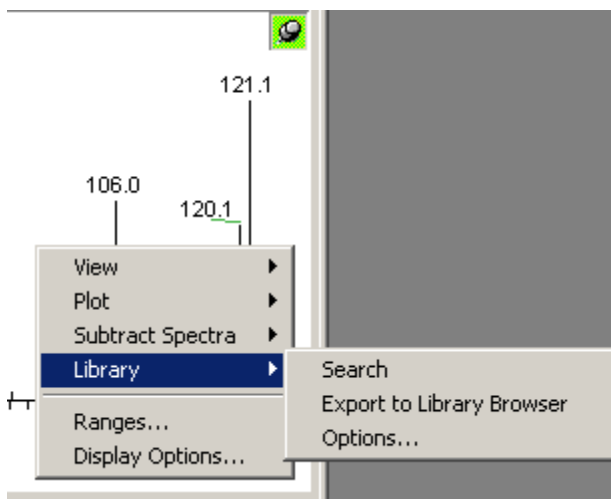
-Help tabs within Xcalibur

-“Users’s Manual for Using NIST” on my Web site, <http://users.chartertn.net/slittle/>

You are now ready to search the library by “right-clicking” on the spectrum window and selecting the library/search option. The library will be searched and the results displayed in an Xcalibur window. To see the structures/spectral information, just left click on the library result of interest. Unfortunately, the up and down keys on the keyboard do not move the user through the displayed results.

**3.2. Using External NIST Search:** I prefer this option since the NIST program allows more options for the user including window presentation, structure searching, variety in the comparison of the unknown to library fits, ability to easily create user libraries, etc.

The approach is similar (*see previous section*). Obtain a spectrum, “right click” (not left!) on the spectrum to be searched and select the

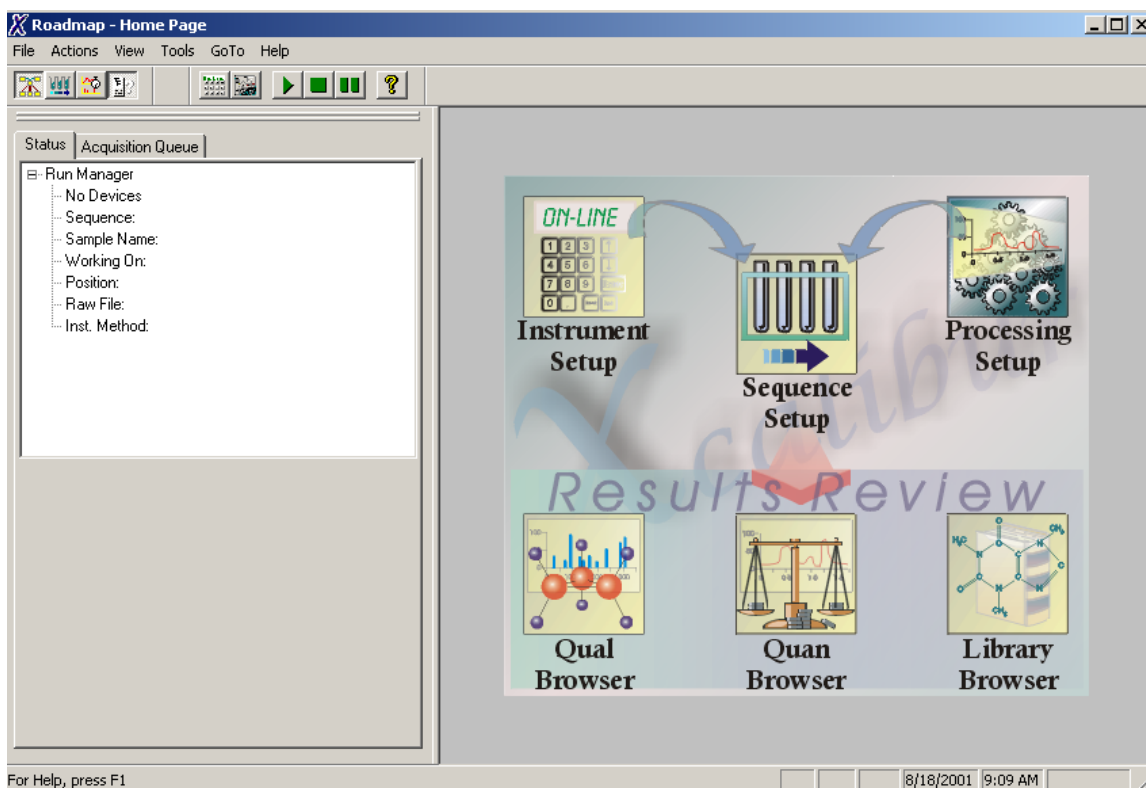


“Export to Library Browser” option. Xcalibur will then export the spectrum to a temporary ASCII file, open the NIST external search algorithm, and search the unknown if the automated search option in NIST software is selected. Tips for using the NIST software can be found in:

-NIST Version 2.0 Users’ Manual

-“Users’s Manual for Using NIST” on my Web site, <http://users.chartertn.net/slittle/>

The NIST has many useful searching capabilities besides spectral searches including structure, name, synonym, molecular formula, CAS number, etc. To open the NIST program from within Xcalibur, go to the Library Browser Icon on the Roadmap-Home page or click on GoTo/Library Browser on the Roadmap-Home Page toolbar.



#### 4.0. Known Limitations, Variations from Standards, Bugs

Very refreshing not to find any “Bugs” in the use of the Xcalibur software. We did note that if Xcalibur data files contained an unexpected character (e.g. a space) in the first 8 letters of the name, the spectrum would not be exported to the NIST external search.

The Xcalibur software exports spectra to the external NIST search by the following mechanism. The Xcalibur software copies the following txt information into C:\program file\nistms\mssearch\autoimp.msdc

C:\Xcalibur\LibSpecs\VG1.fil

Xcalibur created the following information in VG1.fil

C:\Xcalibur\LibSpecs\VG1.MSD

The VG1.MSD is the file containing the mass spectrum in ASCII format, which is pasted automatically into the NIST program for searching. The file extension for this ASCII file should have been .msp, but NIST seems to accept it anyway. The overwriting of the autoimp.msdc file by Xcalibur will cause problems if the user is using other programs such as the Agilent (HP) data processing with the NIST search. The Agilent software does not overwrite the autoimp.msdc file and it depends on the path normally found in that

file. Other programs such as ACD, Wsearch, etc. might have similar problems if used on the same computer.

For more details for the standard for connecting data processing programs such as Xcalibur, ACD, AMDIS, Wsearch see "Details" document on my web page, <http://users.chartertn.net/slittle/>.