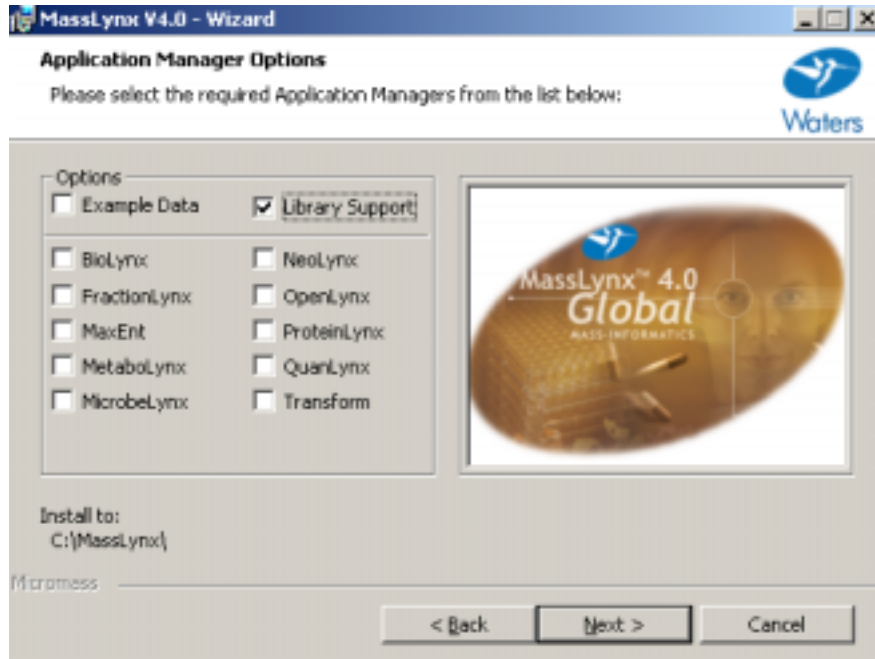


**Tips for Using MassLynx Version 4 Beta Version
with NIST Search Software**
(J Little, Feb 15, 2002)

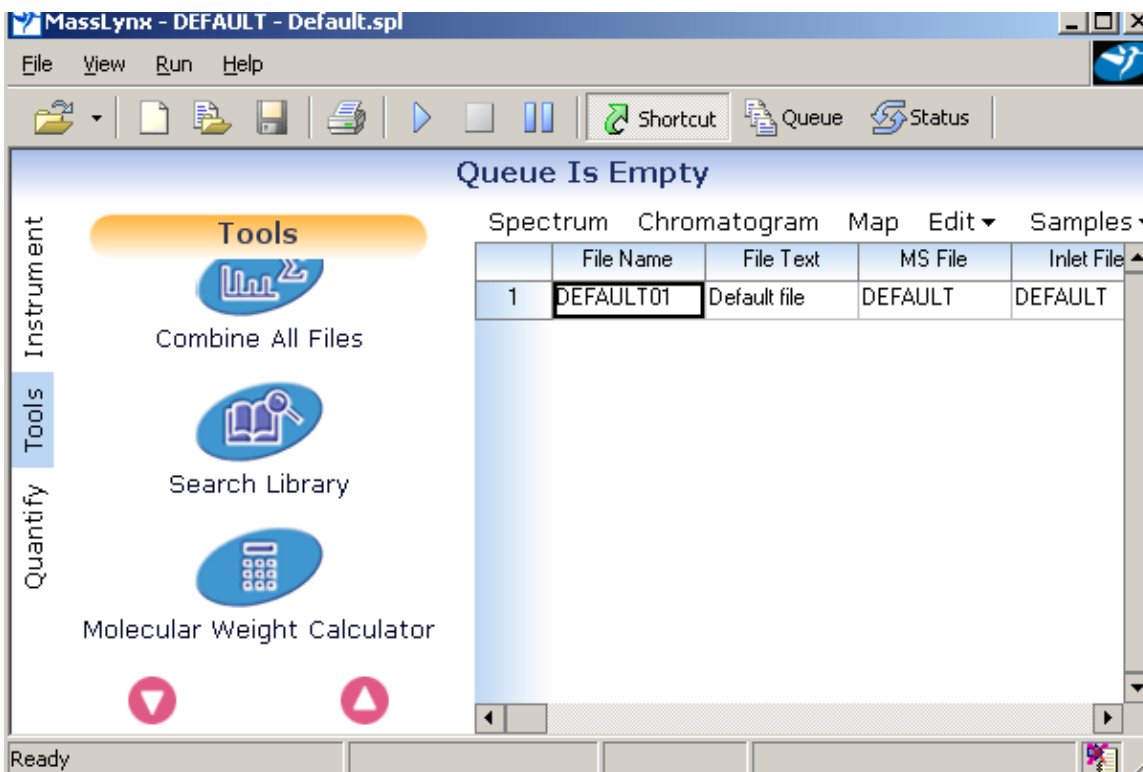
Earlier versions of MassLynx will not automatically transfer spectra from MassLynx to the NIST search. This capability was added to version 4 in early 2002.

Installation of MassLynx: When installing MassLynx version 4, the user needs to select Library option in the installation setup. You might also want to select Example Data under options.

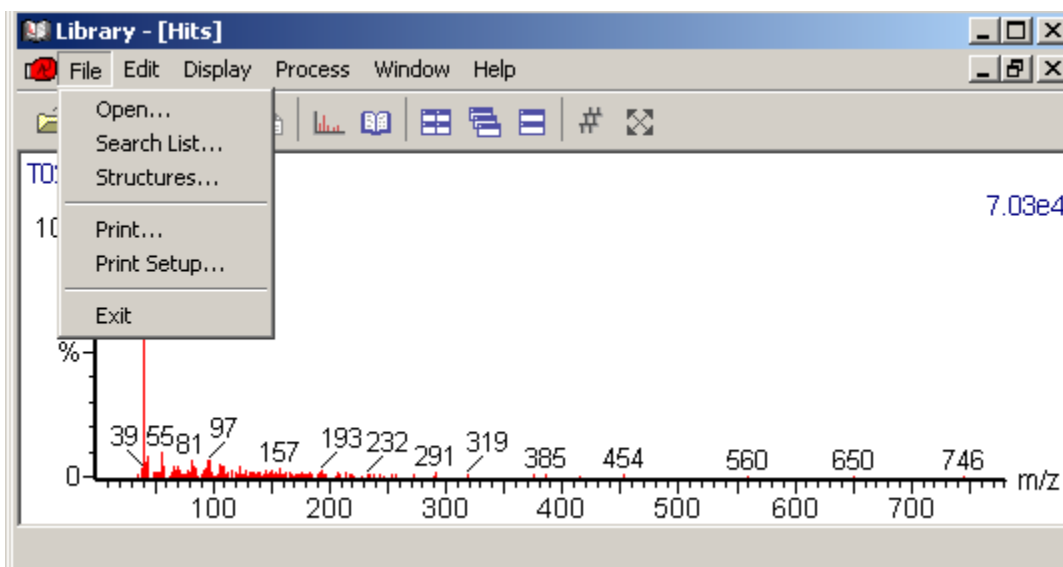


If you forget to do this during the installation, you should be able to turn on the library support by opening the win.ini file (in C:\Winnt on Windows NT), changing AppEnabled00=FALSE to AppEnabled00=TRUE in the [MassLynx] section and saving the file. It would be a good idea to make a backup copy of this file before editing in case something goes awry!

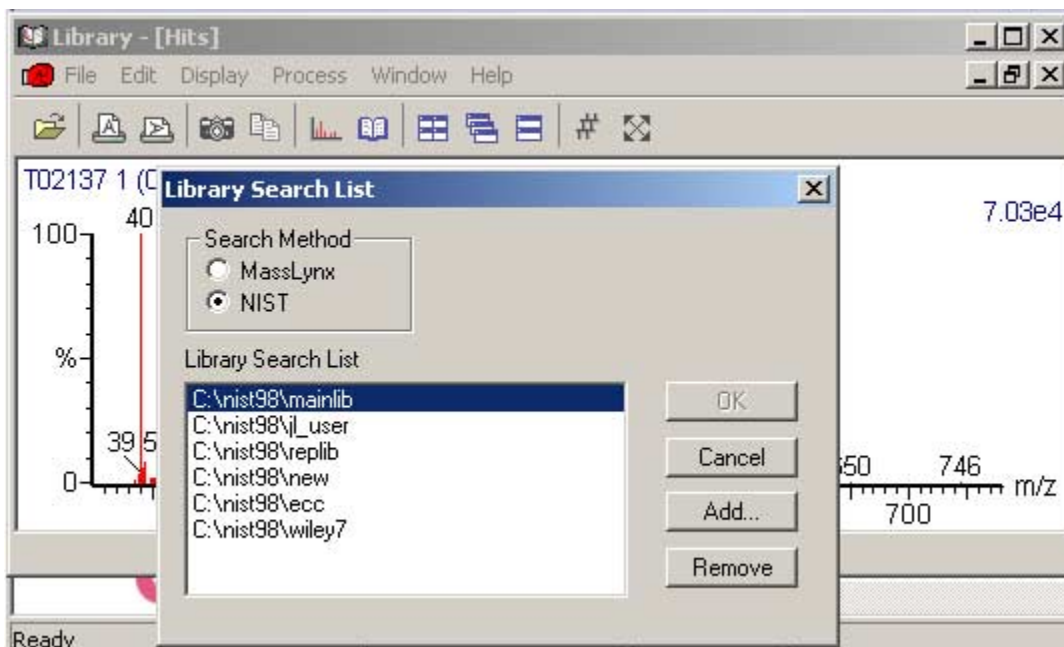
Selecting NIST Search: After opening MassLynx, the selection of the library is performed by selecting the tools and then the "Search Library" Icon on the main MassLynx Window.



The following window should appear and then select File/Search List option:

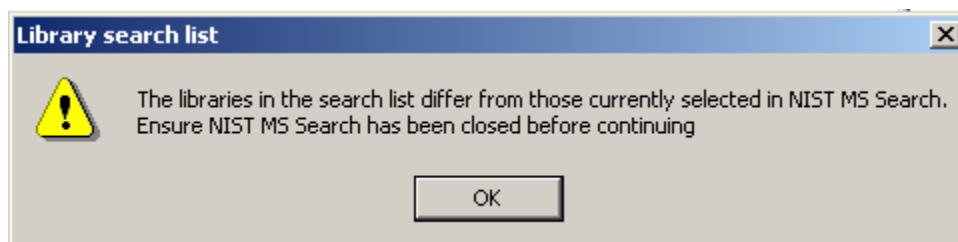


Toggle the NIST search button to the NIST setting and add whichever libraries you want to search in the NIST search to the list one at a time. The NIST libraries are folders found in the NIST98 or MSSEARCH folder. In the following example, I am searching the NIST library, the NSIT replicate, the Wiley7, and various user libraries.



MassLynx has done a good job of integrating the NIST search. They allow the user to select the libraries to search from MassLynx instead of from the Library Search Options window in the NIST program. This is done by the MassLynx software accessing the nistms.ini file used with the NIST search program and changing the libraries to be searched. However, if the NIST search program is already open, the libraries to be searched WILL NOT be updated. This is because the NIST search only checks the nistms.ini file to determine libraries to search when it is first opened.

Thus, the next time the user performs a search with the NIST library, the user is warned that the NIST program must be manually closed.

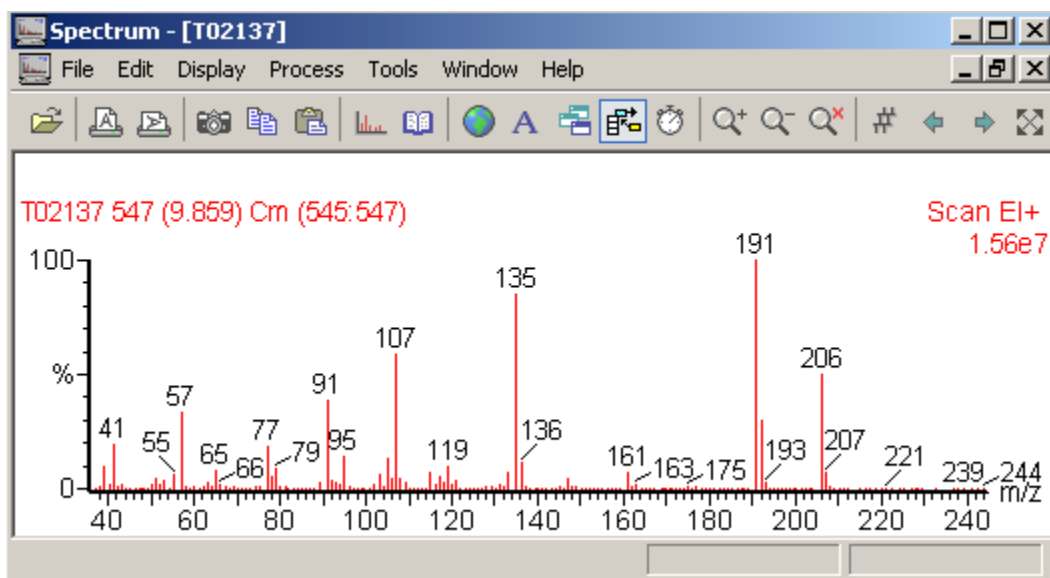


This warning is ONLY noted if the NIST library search software is open when a library is added or deleted from the list to search. MassLynx actually checks to see if the NIST program is running when a change is made. After the user selects OK in the above window, the search will continue with the OLD list of libraries selected. Close the NIST program and perform the search again from within MassLynx. The NIST program will be opened automatically and the search performed with the new list of libraries specified from within MassLynx.

You can still select the libraries to search using the Library Search Options Icon in the NIST search, however, every time you close the NIST search window and reopen the MassLynx program, it will revert back to libraries chosen under MassLynx. You must choose at least one library to search in MassLynx in order that the NIST Library Search Software can be used with MassLynx. Thus even if you want to specify the libraries to search using the NIST Library Search Options menu, you must have at least one library initially selected from MassLynx!

Searching the NIST Library: After the software is installed and the NIST library is selected, the search is normally initiated from the Spectrum window in MassLynx. Just select the spectrum of interest in Chromatogram using either the Combine icon (see Combine Spectra under MassLynx Chromatogram Help) or just select an individual scan. If you select the single scan, using the Refine button on the spectrum window will automatically remove background nicely (see Refine under MassLynx Spectrum Help Topics).

After you get the spectrum you want to search in the spectrum window by either using either the Combine or Refine approaches, then click on the library button (icon that looks like an open book) on the Spectrum bar.



The Library Icon also can be found on the MassLynx Library Menu Bar.

Switching Between NIST and MassLynx Library Searches: You can easily switch between the NIST and MassLynx Searches. Just change the Radio button in the Library window (File/Search List.. menu item) to whichever you want. However, the libraries are in different binary formats. Thus if you wanted to search the NIST library with both programs, you will need a copy of the NIST library in both NIST binary and MassLynx formats!