

## Automatic/Nightly Update of Corporate Mass Spectral/Structural Databases in NIST Format 2/11/02

### Introduction

The ability to combine libraries automatically is a new feature in the NIST search software. Their library utilities, Lib2Nist.exe and strdbld.exe, can be controlled externally by a very command lines. The utilities can then be called with a user-written DOS batch file to control the merging and distribution of databases. The batch files are executed as desired with the standard Scheduler function found in the Windows Operating system or JIT Scheduler (<http://www.gibinsoft.com/shareware/jit/>). I like the JIT (Version 4 is free) better than Windows Scheduler since no password or password updating is associated with the tasks.

Databases in binary format are converted to MSP (ASCII) files with Lib2Nist.exe. They can then be merged and converted back to a binary format for searching. Strdbld.exe, updates indices for user structures. The indexed databases can then be searched by structure to find similar structures, which are ranked in similarity between 1-1000. We are currently testing these capabilities in our Company and it is working very. If you try this approach, please share your experiences with us.

Users add spectra or make corrections to their individual databases. One person serves as a Librarian for users who need spectral interpretation or do not want to enter spectra into the database. The users and Librarian's databases are merged automatically nightly and distributed to all users. In order to minimize network traffic and transfer times, the bulk of our spectra (~33,000 currently) are kept on the users' computers and only new entries (~100-1000 in "New" Library) are sent daily. Occasionally, the existing "New" Library entries are combined with the "bulk" library named "ECC" and automatically distributed to users. The "ECC" library is only copied when the batch file, Get\_Lib.bat, notes changes.

We also use Get\_Lib.bat to update our "PM," "TSCA," and IonTrap libraries. The first two "libraries" only contain MW, MF, name, and CAS information. We find them useful for finding compounds by MW or MF when their spectra are not in any of the EI databases. The "PM" library is a listing of all purchased and manufactured chemicals at Eastman Chemical Company. The "TSCA" library is a listing of all the TSCA chemicals (polymers and inorganic salts excluded) obtained from a commercial CD purchased twice per year. The IonTrap library is only distributed to people with iontraps. We have found the iontrap spectra to often be significantly different than the spectra of magnetic, TOF, and quadrupole mass spectrometers. The batch file only copies the updated IonTrap library if the user had originally installed the IonTrap library on their computer. This approach can also be used to distribute updates to the NIST and Wiley Commercial Databases.

The NIST search software searches multiple libraries. Thus, the user can search their personal user library, the "ECC" Corporate Library, the "New" library, the NIST Main Library, the NIST Replicate Library, and the Wiley Library. The results of the multiple library search are merged into one report.

### Automated Batch Files

The batch files used to automatically update and distribute a merged database of user libraries are discussed below and outlined in block diagrams in Figures 1 and 2. This document was written to demonstrate an approach and the batch files will need to be modified to meet specific needs. Furthermore, these exact batch files were not extensively tested and might need "debugging" before they are used.

**Mrg\_Libs.bat:** The Librarian runs a batch file *Mrg\_Libs.bat*. This batch file merges the Librarian's library with all other user databases to create a library named "New" and indexes all the structures in user libraries to enable structure-similarity searching. This "New" library is then placed on the server for downloading by users. The merging of libraries is done automatically nightly on the Librarian's PC employing the standard Scheduler software distributed with the Window operating systems or JIT Scheduler (<http://www.gibinsoft.com/shareware/jit/>). I like the JIT (Version 4 is free) better than Windows Scheduler since no password or password updating is associated with the tasks. We don't really know how many libraries can be merged. The upper number of entries in a merged library is around 65,000. If there

is a limit on the number of libraries that can be merged, you could merge in multiple steps.

A copy of the Mrg\_Libs.bat file is shown in Figure 3. The Lib2Nist.exe is called by the “start” command in the batch file. The “start” command also calls an initialization (.ini) files, Mrg\_Lib.ini and Mrg\_lib2.ini, which are shown in Figures 4a and 4b. Detailed instructions (Cmdline.wri) for using the command line in Lib2Nist.exe are included in the distribution WinZip file from NIST. Strdbld.exe, a utility to index user structures, and associated documentation are available from NIST.

Mrg\_libs.bat also checks to make sure the lib2nist.exe and strdbld.exe are present and found in the correct location. The user is warned if changes are needed.

**Send\_Lib.bat:** This batch file is used to send a user’s personal library to the server. The Librarian then merges it with the Mrg\_Libs.bat file. The Send\_Lib.bat file is run automatically by the Windows Scheduler program on the user’s computer or or JIT Scheduler (<http://www.gibinsoft.com/shareware/jit/>). It doesn’t seem to be a problem to copy a library when the NIST Search Program is open and the library is being accessed. However, you cannot properly overwrite a library when the NIST search program is open and the library is being accessed (see Get\_Lib.bat Section).

A copy of the Send\_Lib.bat file is shown in Figure 5. The Lib2Nist.exe is called by the “start” command in the batch file. The “start” command also calls Send\_Lib.ini, which is shown in Figure 6. Detail instructions (Cmdline.wri) on using the command line in Lib2Nist.exe are included in the distribution WinZip file from NIST. The user must allow the librarian to have full access to the C:\NIST98 directory. The Sen\_lib.bat file could have copied the user's library to the server, but we had some trouble with delete privileges even though the server security was set for full access for all users.

**Get\_Lib.bat:** *Libraries are only updated if a newer version is present on the server.* The Get\_Lib.bat program is run on any user’s computer who wants to use the “New”, “ECC”, “TSCA”, “PM”, and “Iontrap” libraries. The “Iontrap” library is only useful to people using iontraps because the spectra are often much different than standard EI spectra obtained on quadrupoles and magnetic instruments. Get\_lib.bat can be run automatically nightly using the Windows Scheduler, or JIT Scheduler (<http://www.gibinsoft.com/shareware/jit/>), or run out of the Startup Folder when the user’s computer is booted, or starting manually by “double-clicking” on the Get\_Lib.bat icon. The instructions to the user for using Get\_Lib.bat are shown in Attachment 1.

If the NIST search is open and any user library is being accessed, a user cannot properly replace the current version of that user library on their system with the updated version from the server. To avoid this problem, the Batch file automatically closes the NIST sear program using a program named closeprog.exe written by program filestat.exe written by Dmitrii Tchekhovskoi [Dmitrii.Tchekhovskoi@nist.gov].

A copy of several different Get\_Libs.bat files are shown in Figures 7a, 7b and 7c. I had to have several different ones depending on the Windows operating system present on the user’s computer. The DOS batch file switches attached to commands vary in Windows operating systems.

**Backup\_lib.bat:** This batch file automatically creates a copy of the “New” library every night with the creation date appended to the name. It is stored on the server. This allows us retrieve user entries if a user loses entries in their library or has a disk drive crash. An executable, filecopy.exe, was written for us by Paul Wehner at Eastman Chemical Company.

**Update\_structures.bat:** A batch file was written to automatically update user's structures. The batch file can be automatically scheduled to run by the user. Also, we find it useful to place on the first level of the Start menu in the Windows operating system. The user can then run the batch file after an entry is added to the library. Version 2 of the NIST search does not need to be closed in order to update a user's structural database. An example of Update\_structures.bat for jl\_user is shown in Figure 9.

## Sequencing Batch Files

The Librarian schedules the merging of files with Mrg\_Libs.bat to run at 5:00 AM. All users with personal libraries transfer them to the server at around 4:30 AM using Send\_lib.bat. Users can then Schedule Get\_Lib.bat to run at 5:30 AM or use another approach such as the Start Folder when booting, or manually running the batch file. Backup\_lib.bat is run at 6:00 AM every day.

### **Known Limitations**

Some DOS commands used in batch files were not the same in Windows NT 4.0 as they were in previous versions of Windows 95, 98, etc. Often the commands have different modifiers or switches (/ followed by various ASCII characters). The first time a batch file is run, the user will often be requested to determine if a file to be copied is a file or a directory. In all our batch files, the "file" would be the correct answer. After responding to this query the first time, the user is no longer prompted when using the batch file in subsequent uses.

Furthermore, DOS windows would not close in Windows 95 unless the user selected "Close On Exit" from properties the first time the batch file was executed. When you check the "Close on exit" box, the MSDOS creates a Get\_lib.pif file that is placed in the same directory as Get\_lib.bat. This is not a problem unless if the Get\_lib.bat file is located in your startup folder. In this case, the program will run twice on boot-up. Thus it is best to place only a shortcut to Get\_lib.bat in your startup folder. If you add "echo off" and "cls" as the last two commands in a batch file, the MSDOS window will close automatically in even Windows 95. No problem with exiting windows was noted in Windows NT 4.0.

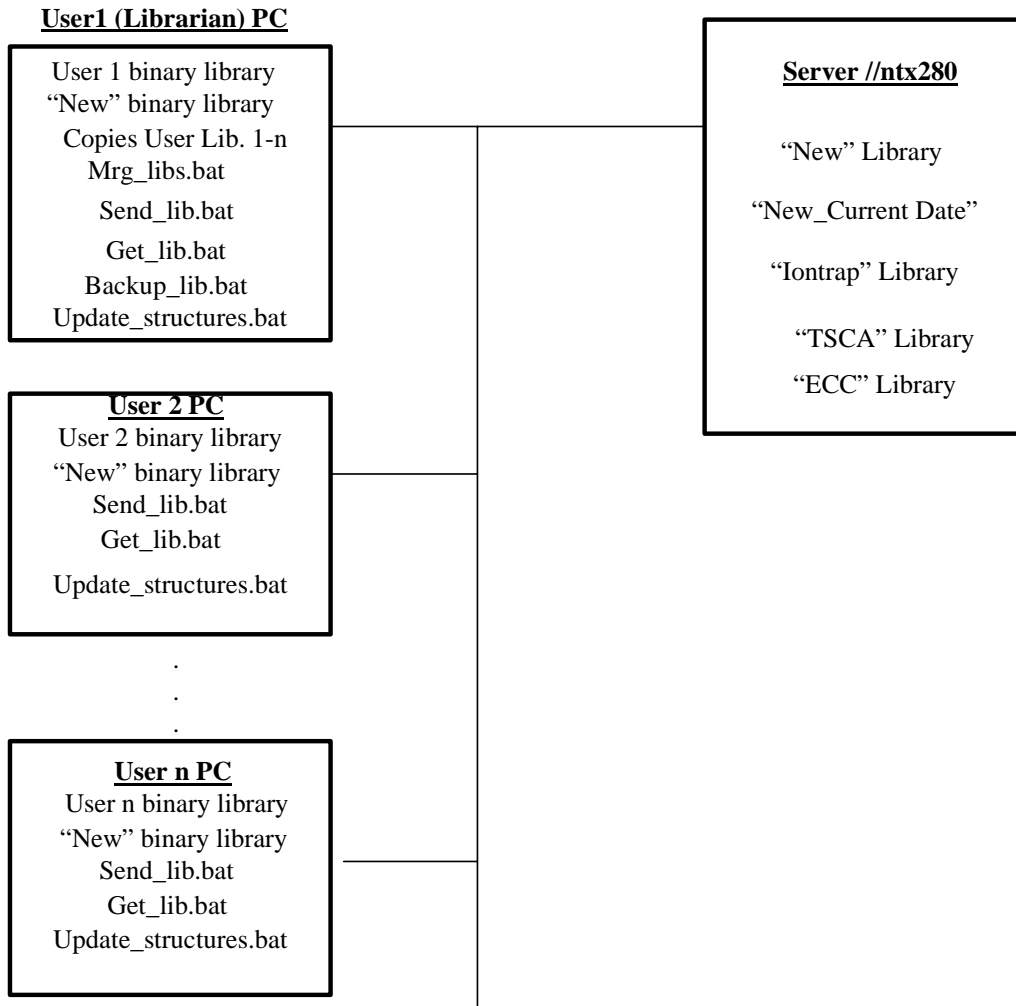
We put variables in programs for the location of the NIS user libraries and the server directory. This made it very easy to make changes in these directories in a batch file. Instead of multiple changes, only one change needed to be made at the first of the batch file using the "set name=variable" command. However, this caused some problems on Windows 95 systems. No problems were noted on Windows 98 and Windows NT 4.0 systems. Some Windows 95 machines would show "out of environment space" error when running and the libraries would not copy.

This can be corrected by "right-clicking" on the banner at the top of the MSDOS window when the program fails. The "Program" tab is selected and the "initial environment" setting is changed from "Auto" to "1280." When you make this change, the MSDOS creates a Get\_lib.pif file that is placed in the same directory as Get\_lib.bat. This is not a problem unless if the Get\_lib.bat file is located in your startup folder. In this case, the program will run twice on boot-up. Thus it is best to place only a shortcut to Get\_lib.bat in your startup folder. To avoid this problem, just remove the "set name=variable" command and define explicitly in all commands the location of the server (%server%) and NIST user libraries (%nist%).

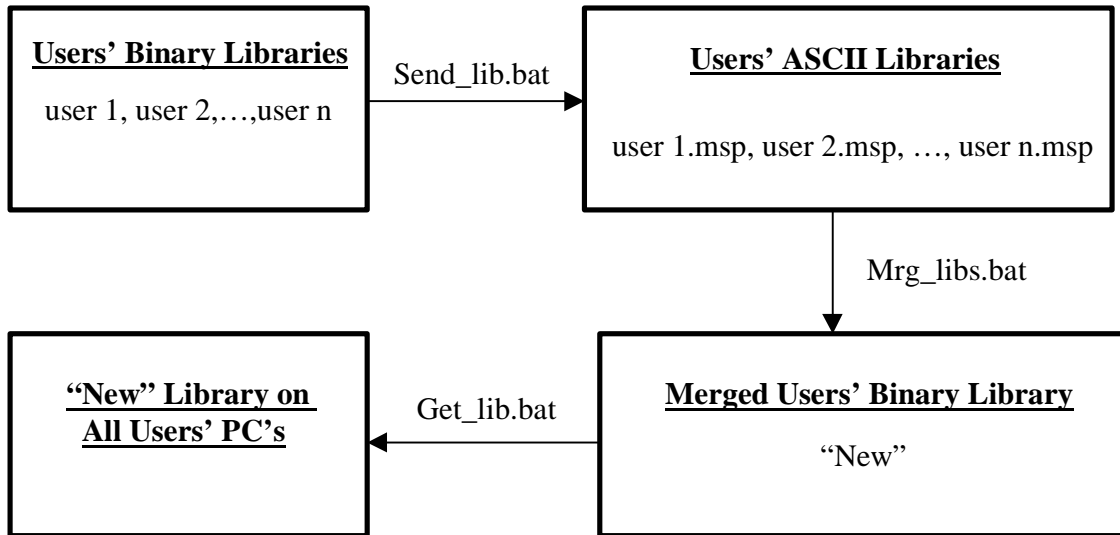
**Other Possible Approaches:** The whole process could be driven by the Librarian's PC including the Get\_Lib.bat and the Send\_Lib.bat functions. The status of the Library Search Program on the remote user computer could be checked with the filestat.exe program. Unfortunately, there is no easy way to inform the user that he is leaving his library search program open in a Batch file. That is why we decided to run the Get\_Lib.bat function under control of the users' computers.

The Snd\_Lib.bat function could be performed by the Librarian. As far as we can tell, a proper copy of the user's library can be obtained even if the NIST Library Search Program is open and the user library is being accessed.

**Fig. 1:** Block Diagram of User Computers 1 through n and Server on Corporate Network Showing Libraries and Batch Files



**Figure 2:** Block Diagram of Batch (.bat) File Conversions of Users' Libraries into Merged Library "New"



**Figure 3.** Example of Mrg\_lib.bat

```
@echo off
:      **Program written to automatically update Corporate Library
:      for Eastman Chemical Company. The program is capable of
:      of Combining entries from the all user libraries into a library
:      named "New." The program also updates all structure indexes for
:      user libraries and copies an ASCII file in HP JCAMP to a server.
:      The server JCAMP file is used to transfer spectra to a Micromass
:      OPUS data system for sharing and searching.
:
:      Written by James Little
:      7/12/2000
:
:
:      **Making sure all executables needed to run this program exist
:      and are found at the correct location

if not exist c:\mrg_lib\lib2nist.exe goto lib2nist_error
if not exist c:\nist98\strdbld.exe goto strdbld_error
if not exist c:\mrg_lib\mrg_lib.ini goto mrg_lib_ini_error
if not exist c:\mrg_lib\mrg_lib2.ini goto mrg_lib_ini_error

:
:
:      *Copying All User Libraries to Librarian's Directory
:      Must have 3 lines of commands for every user library copied
:      and the user must open the security on C:\nist98 directory
:      in order that the Librarian can copy them with this batch file.

del/q/s C:\mrg_lib\jl_user.mol\*. *
xcopy \\ntresapp03\mspec2\nist98\up_lib\drop\jl_user.msp C:\mrg_lib\jl_user.msp /s /h /f /r /c /y
xcopy \\ntresapp03\mspec2\nist98\up_lib\drop\jl_user.mol\*. * C:\mrg_lib\jl_user.mol\*. * /s /h /f /r /c /y
del/q/s C:\mrg_lib\gh_user.mol\*. *
del/q/s C:\mrg_lib\gh2_user.mol\*. *
xcopy \\ntresapp03\mspec2\nist98\up_lib\drop\gh_user.msp C:\mrg_lib\gh_user.msp /s /h /f /r /c /y
xcopy \\ntresapp03\mspec2\nist98\up_lib\drop\gh2_user.msp C:\mrg_lib\gh2_user.msp /s /h /f /r /c /y
xcopy \\ntresapp03\mspec2\nist98\up_lib\drop\gh_user.mol\*. * C:\mrg_lib\gh_user.mol\*. * /s /h /f /r /c /y
xcopy \\ntresapp03\mspec2\nist98\up_lib\drop\gh2_user.mol\*. * C:\mrg_lib\gh2_user.mol\*. * /s /h /f /r /c /y
del/q/s C:\mrg_lib\cc_user.mol\*. *
xcopy \\ntresapp03\mspec2\nist98\up_lib\drop\cc_user.msp C:\mrg_lib\cc_user.msp /s /h /f /r /c /y
xcopy \\ntresapp03\mspec2\nist98\up_lib\drop\cc_user.mol\*. * C:\mrg_lib\cc_user.mol\*. * /s /h /f /r /c /y
del/q/s C:\mrg_lib\dn_user.mol\*. *
xcopy \\ntresapp03\mspec2\nist98\up_lib\drop\dn_user.msp C:\mrg_lib\dn_user.msp /s /h /f /r /c /y
xcopy \\ntresapp03\mspec2\nist98\up_lib\drop\dn_user.mol\*. * C:\mrg_lib\dn_user.mol\*. * /s /h /f /r /c /y
del/q/s C:\mrg_lib\rd_user.mol\*. *
xcopy \\ntresapp03\mspec2\nist98\up_lib\drop\rd_user.msp C:\mrg_lib\rd_user.msp /s /h /f /r /c /y
xcopy \\ntresapp03\mspec2\nist98\up_lib\drop\rd_user.mol\*. * C:\mrg_lib\rd_user.mol\*. * /s /h /f /r /c /y
del/q/s C:\mrg_lib\km_user.mol\*. *
xcopy \\ntresapp03\mspec2\nist98\up_lib\drop\km_user.msp C:\mrg_lib\km_user.msp /s /h /f /r /c /y
xcopy \\ntresapp03\mspec2\nist98\up_lib\drop\km_user.mol\*. * C:\mrg_lib\km_user.mol\*. * /s /h /f /r /c /y

:
:
:      **Combining all user libraries. In this example, the user libraries are
:      named jl_user and gh_user. You can combine as many as you want
:      by just separating the user libraries by spaces. The created library
```

: is called "New".

C:

cd \Mrg\_Lib

del Mrg\_Lib.log

del/q/s \\ntresapp03\mspec2\nist98\up\_lib\new\\*.\*

start /wait lib2nist.exe /1stid=1 /log9 Mrg\_Lib.log Mrg\_Lib.ini jl\_user.msp gh\_user.msp gh2\_user.msp

cc\_user.msp dn\_user.msp rd\_user.msp km\_user.msp =new

:

: \*\*Finished combining libraries, copying them to server for users to access

:

xcopy new \\ntresapp03\mspec2\nist98\up\_lib\new\ /s /h /f /r /d /y

: \*\*Updating User Structural Links for all libraries having structures, in this

: case libraries iontrap and new. Usually new is the only one routinely

: needing updating.

C:\nist98\strdbld.exe /D:\\ntresapp03\mspec2\nist98\up\_lib\ iontrap /L:C:\mrg\_lib\strdbld\_iontrap.log

C:\nist98\strdbld.exe /D:\\ntresapp03\mspec2\nist98\up\_lib\ new /L:C:\mrg\_lib\strdbld\_new.log

: \*\*Updating User Structural Links for ECC library. Normally this not need

: routine updates, since infrequently are structures added. Therefore,

: the command is normally not run (rem placed before command).

C:\nist98\strdbld.exe /D:\\ntresapp03\mspec2\nist98\up\_lib\ ecc /L:C:\nist98\strdbld\_ecc.log

echo.

echo Current Entries in NIST New library combined with user entries and structure links updated

echo and placed on Server..

echo.

:

: \*\*Created hpj file to send to VAX for updating OPUS library using C\_lib.com on sta150

:

start /wait c:\mrg\_lib\lib2nist.exe /log9 Send\_Lib.log c:\mrg\_lib\mrg\_lib2.ini new

copy c:\mrg\_lib\new.hpj \\ntresapp03\mspec\libraries\opus.hpj

:

goto close\_screen

:lib2nist\_error

cls

echo.

echo \*\*WARNING: Exit this window and install lib2nist.exe at

echo c:\mrg\_lib\lib2nist.exe. It is a utility needed to

echo convert libraries between ASCII to binary

echo and binary to ASCII, etc.

echo.

pause

goto close\_screen

:strdbld\_error

cls

echo.

echo \*\*WARNING: Exit this window and install strdbld.exe at

echo c:\nist98\strdbld.exe. It is a utility needed to

echo link structures in user libraries to allow searching

echo of user databases/libraries by structure

```
echo.  
pause  
goto close_screen
```

```
:mrg_lib_ini_error  
cls  
echo.  
echo  **WARNING: Exit this window and install mrg_lib.ini and mrg_lib2.ini  
echo      at c:\mrg_lib\mrg_lib.ini and c:\mrg_lib2.ini! They are  
echo      needed to merge and distribute the Eastman "New" library.  
echo.  
echo.  
pause  
goto close_screen
```

```
:close_screen  
echo.  
echo off  
cls  
exit
```

**Figure 4a:** Mrg\_lib.ini

```
[directory]
NIST=<None>
input=c:\Mrg_lib
output=c:\Mrg_lib
type=0
[output]
Text=0
TextFileType=0
DB=1
CalcMW=0
IncludeSynonyms=1
KeepIDs=0
LinkMOLfile=0
MzAdd=0
MzMpy=1
NeedSubset=0
[subset]
```

**Figure 4b:** Mrg\_lib2.ini

```
[directory]
nist=C:\NIST98
input=c:\mrg_lib
output=C:\mrg_lib
type=0
[output]
Text=1
TextFileType=1
DB=0
CalcMW=0
IncludeSynonyms=1
KeepIDs=0
LinkMOLfile=0
MzAdd=0
MzMpy=1
NeedSubset=0
[subset]
```

**Figure 5:** Send\_lib.bat

```
@echo off
:
:   **Program written to automatically convert user library
:   from binary format to MSP (ASCII) format. It is then placed
:   on the server for merging into an updated "New" library
:   by Mrg_Libs.bat. Users can then get a copy for their computers
:   using Get_Lib.bat. The user's library should be named with their
:   initials followed by _user. In this example, the library was named
:   jl_user since the user's name is James Little. The user will
:   need to use the find and replace option in Notepad to replace
:   jl_user with their library name.
:
:
:   Written by James Little
:   3/18/2000
:
:   **Creating a MSP ASCII file of users entries. Lib2Nist.exe
:   and associated files are in C:\Nist98\utility folder
:
:
if not exist c:\mrg_lib\lib2nist.exe goto lib2nist_error
if not exist c:\mrg_lib\send_lib.ini goto send_lib_error
:
c:
cd \Nist98
del/q/s C:\nist98\jl_user.mo\*. *
del/q/s \\ntresapp03\mspec2\nist98\up_lib\drop\jl_user.mo\*. *
start /wait c:\mrg_lib\lib2nist.exe /log9 Send_Lib.log c:\mrg_lib\Send_lib.ini jl_user
xcopy C:\nist98\jl_user.mo\*. * \\ntresapp03\mspec2\nist98\up_lib\drop\jl_user.mo\*. * /s /h /f /r /c /y
xcopy C:\nist98\jl_user.msp \\ntresapp03\mspec2\nist98\up_lib\drop\jl_user.msp /s /h /f /r /c /y
:
:   **Commands needed to automatically close Windows in Windows 95
:   Not needed in Windows NT 4.0
:
goto close_window

:lib2nist_error

cls
echo.
echo   **WARNING: Exit this window and install lib2nist.exe and associated
echo       files at c:\mrg_lib\. They are needed to export your
echo       library to the server!
echo.
pause
goto close_screen

:send_lib_error

cls
echo.
echo   **WARNING: Exit this window and install send_lib.ini! It is needed
echo       to export your library to the server!
```

```
echo.  
pause  
goto close_screen
```

```
:close_window
```

```
echo off  
cls  
exit
```

**Figure 6:** Send\_lib.ini

```
[directory]
nist=C:\nist98
input=c:\Nist98\
output=C:\Nist98
type=0
[output]
Text=1
TextFileType=0
DB=0
CalcMW=0
IncludeSynonyms=1
KeepIDs=0
LinkMOLfile=1
MzAdd=0
MzMpy=1
NeedSubset=0
[subset]
```

**Figure 7a:** Get\_lib.bat for Windows NT.

```
: Get_Bat Batch File written by James Little at Eastman
: Chemical Company, 1/14/2002 for Windows NT/2000
: Another version needed for Windows 95/98!
: Automatically closes
: NIST search if open! Program copies/updates user
: libraries ECC, NEW, TSCA, and PM. Also updates
: iontrap library if iontrap already exists on user system.
: Not everyone wants or needs the iontrap library.

cls

@echo off

: **Setting default directory for NIST98 Software and libraries
: Change if different on your systems! Removed in this file
: because on Windows 95 systems gives "out of environment space"
: errors! Would be nice to include in future versions. Would
: need to use %nist% in the place of the path for NIST98 in all
: copy commands!

: set nist=c:\nist98

: **Setting default location of server where libraries are stored
: Change if needed! Removed in this file because on Windows 95 systems
: gives "out of environment space" errors! Would be nice to include
: in future versions. Would need to use %server% in the place of the
: path for server in all copy commands!

: set server=\\ntresapp03\mspec2\NIST98\up_lib

@echo off
:
: **This batch file needs closeprog.exe (program written by
: Dmitrii Tchekhovskoi [Dmitrii.Tchekhovskoi@nist.gov]. The
: program is expected to be found at c:\filestat\filestat.exe

if not exist c:\ms_utilities\closeprog.exe goto close_error

: **Checking to make sure network connection is good
: sometimes network connection is lost due to network problems
: or user didnot update their network password after 90 days
: and network connection is lost

if not exist \\ntresapp03\mspec2\nist98\up_lib\ecc\name.inu goto n_error

: **Batch file assumes libraries will be copied directly to directory
: in the NIST98 foler, if using aliases to remote to a remote
: location, will need to modify batch file

if exist c:\nist98\ecc\alias.msdc goto alias_error
if exist c:\nist98\new\alias.msdc goto alias_error
if exist c:\nist98\pm\alias.msdc goto alias_error
if exist c:\nist98\tsc\alias.msdc goto alias_error
if exist c:\nist98\iontrap\alias.msdc goto alias_error
```

```

if exist c:\nist98\wiley6\alias.msdx goto alias_error
if exist c:\nist98\wiley7\alias.msdx goto alias_error

:   **Closing NIST program so libraries can be updated!

start /b /wait c:\ms_utilities\CLOSEPROG "NIST MS 2.0" "" 10000

:   **Copying libraries from server to user's library directory
cls
xcopy \\ntresapp03\mspec2\NIST98\up_lib\PM\*. * c:\nist98\pm\*. * /s /h /f /r /d
xcopy \\ntresapp03\mspec2\NIST98\up_lib\ecc\*. * c:\nist98\ecc\*. * /s /h /f /r /d
xcopy \\ntresapp03\mspec2\NIST98\up_lib\TSCA\*. * c:\nist98\TSCA\*. * /s /h /f /r /d
xcopy \\ntresapp03\mspec2\NIST98\up_lib\new\*. * c:\nist98\new\*. * /s /h /f /r /d
rem xcopy \\ntresapp03\mspec2\NIST98\up_lib\wiley6\*. * c:\nist98\wiley6\*. * /s /h /f /r /d

:   **Not everyone wants iontrap libraries, batch file checks
:   to see if installed on system, if it is, then it will copy

if not exist c:\nist98\iontrap\user.dbu goto skip_iontrap
xcopy \\ntresapp03\mspec2\NIST98\up_lib\iontrap\*. * c:\nist98\iontrap\*. * /s /h /f /r /d

:skip_iontrap

echo.
echo   **THIS PROCEDURE UPDATED YOUR USER LIBRARIES
echo.
echo   **If (0) files were copied, no library updates were needed
echo.
echo   **If you get tired of always having to close this window, edit
echo   Get_Lib.bat text file with Notepad program or Word and place
echo   a ":" before the "pause" command below.
echo.

:pause

:   **If you want to start the NIST search program automatically after
:   running this program, remove the ":" in front of the start command
:   below.  Might have to change the name of the program depending
:   on the version of NIST software employed.

:start c:\nist98\nist$.exe

goto close_screen

:alias_error
cls
echo.
echo   **WARNING: Batch Program needs to be modified, your libraries
echo           are stored on a remote disk and aliases are being used.
echo           Contact James Little
echo.
pause
goto close_screen

:n_error
cls

```

```
echo.
echo  **WARNING: Couldn't read network drive!
echo      Error caused by one of two problems:
echo      -network connection lost, reboot computer
echo      -password expired, change network password, then reboot
echo.
pause
goto close_screen

:close_error
cls
echo.
echo  **WARNING: Close.exe program not found at c:\ms_utilities\close.exe!
echo      c:\ms_utilities\closeprog.exe! This program closes NIST Search
echo      so that libraries can be updated. Call you mass spec program
echo      administrator!
echo.
pause
goto close_screen

:  **Command needed to automatically close Windows in Windows 95
:  Not needed in Windows NT 4.0

:close_screen
echo.
echo off
cls
exit
```

**Figure 7b:** Get\_lib.bat for Windows 95 and 98.

```
: Get_Bat Batch File written by James Little at Eastman
: Chemical Company, 1/14/2002 for Windows 95/98
: Another version needed for Windows nt/2000!
: Automatically closes
: NIST search if open! Program copies/updates user
: libraries ECC, NEW, TSCA, and PM. Also updates
: iontrap library if iontrap already exists on user system.
: Not everyone wants or needs the iontrap library.

cls

@echo off

: **Setting default directory for NIST98 Software and libraries
: Change if different on your systems! Removed in this file
: because on Windows 95 systems gives "out of environment space"
: errors! Would be nice to include in future versions. Would
: need to use %nist% in the place of the path for NIST98 in all
: copy commands!

: set nist=c:\nist98

: **Setting default location of server where libraries are stored
: Change if needed! Removed in this file because on Windows 95 systems
: gives "out of environment space" errors! Would be nice to include
: in future versions. Would need to use %server% in the place of the
: path for server in all copy commands!

: set server=\\ntresapp03\mspec2\NIST98\up_lib

@echo off
:
: **This batch file needs closeprog.exe (program written by
: Dmitrii Tchekhovskoi [Dmitrii.Tchekhovskoi@nist.gov]. The
: program is expected to be found at c:\filestat\filestat.exe

if not exist c:\ms_utilities\closeprog.exe goto close_error

: **Checking to make sure network connection is good
: sometimes network connection is lost due to network problems
: or user didnot update their network password after 90 days
: and network connection is lost

if not exist \\ntresapp03\mspec2\nist98\up_lib\ecc\name.inu goto n_error

: **Batch file assumes libraries will be copied directly to directory
: in the NIST98 folder, if using aliases to remote to a remote
: location, will need to modify batch file

if exist c:\nist98\ecc\alias.msdc goto alias_error
if exist c:\nist98\new\alias.msdc goto alias_error
if exist c:\nist98\pm\alias.msdc goto alias_error
if exist c:\nist98\tsc\alias.msdc goto alias_error
if exist c:\nist98\iontrap\alias.msdc goto alias_error
```

```
if exist c:\nist98\wiley6\alias.msdx goto alias_error
if exist c:\nist98\wiley7\alias.msdx goto alias_error
```

```
:    **Closing NIST program so libraries can be updated!
```

```
start /m /w c:\ms_utilities\CLOSEPROG "NIST MS 2.0" "" 10000
```

```
:    **Copying libraries from server to user's library directory
```

```
cls
```

```
xcopy \\ntresapp03\mspec2\NIST98\up_lib\PM\*. * c:\nist98\pm\*. * /s /h /f /r /d /y
```

```
xcopy \\ntresapp03\mspec2\NIST98\up_lib\ecc\*. * c:\nist98\ecc\*. * /s /h /f /r /d /y
```

```
xcopy \\ntresapp03\mspec2\NIST98\up_lib\TSCA\*. * c:\nist98\TSCA\*. * /s /h /f /r /d /y
```

```
xcopy \\ntresapp03\mspec2\NIST98\up_lib\new\*. * c:\nist98\new\*. * /s /h /f /r /d /y
```

```
rem xcopy \\ntresapp03\mspec2\NIST98\up_lib\wiley6\*. * c:\nist98\wiley6\*. * /s /h /f /r /d /y
```

```
:    **Not everyone wants iontrap libraries, batch file checks
```

```
:    to see if installed on system, if it is, then it will copy
```

```
if not exist c:\nist98\iontrap\user.dbu goto skip_iontrap
```

```
xcopy \\ntresapp03\mspec2\NIST98\up_lib\iontrap\*. * c:\nist98\iontrap\*. * /s /h /f /r /d /y
```

```
:skip_iontrap
```

```
echo.
```

```
echo    **THIS PROCEDURE UPDATED YOUR USER LIBRARIES
```

```
echo.
```

```
echo    **If (0) files were copied, no library updates were needed
```

```
echo.
```

```
echo    **If you get tired of always having to close this window, edit
```

```
echo    Get_Lib.bat text file with Notepad program or Word and place
```

```
echo    a ":" before the "pause" command below.
```

```
echo.
```

```
:pause
```

```
:    **If you want to start the NIST search program automatically after
```

```
:    running this program, remove the ":" in front of the start command
```

```
:    below. Might have to change the name of the program depending
```

```
:    on the version of NIST software employed.
```

```
:start c:\nist98\nist$.exe
```

```
goto close_screen
```

```
:alias_error
```

```
cls
```

```
echo.
```

```
echo    **WARNING: Batch Program needs to be modified, your libraries
```

```
echo    are stored on a remote disk and aliases are being used.
```

```
echo    Contact James Little
```

```
echo.
```

```
pause
```

```
goto close_screen
```

```
:n_error
```

```
cls
```

```
echo.
echo  **WARNING: Couldn't read network drive!
echo      Error caused by one of two problems:
echo      -network connection lost, reboot computer
echo      -password expired, change network password, then reboot
echo.
pause
goto close_screen

:close_error
cls
echo.
echo  **WARNING: Close.exe program not found at c:\ms_utilities\close.exe!
echo      c:\ms_utilities\closeprog.exe! This program closes NIST Search
echo      so that libraries can be updated. Call you mass spec program
echo      administrator!
echo.
pause
goto close_screen

:  **Command needed to automatically close Windows in Windows 95
:  Not needed in Windows NT 4.0

:close_screen
echo.
echo off
cls
exit
```

**Figure 7c:** Get\_lib.bat for Windows 2000.

```
: Get_Bat Batch File written by James Little at Eastman
: Chemical Company, 1/14/2002 for Windows NT/2000
: Another version needed for Windows 95/98!
: Automatically closes
: NIST search if open! Program copies/updates user
: libraries ECC, NEW, TSCA, and PM. Also updates
: iontrap library if iontrap already exists on user system.
: Not everyone wants or needs the iontrap library.

cls

@echo off

: **Setting default directory for NIST98 Software and libraries
: Change if different on your systems! Removed in this file
: because on Windows 95 systems gives "out of environment space"
: errors! Would be nice to include in future versions. Would
: need to use %nist% in the place of the path for NIST98 in all
: copy commands!

: set nist=c:\nist98

: **Setting default location of server where libraries are stored
: Change if needed! Removed in this file because on Windows 95 systems
: gives "out of environment space" errors! Would be nice to include
: in future versions. Would need to use %server% in the place of the
: path for server in all copy commands!

: set server=\\ntresapp03\mspec2\NIST98\up_lib

@echo off
:
: **This batch file needs closeprog.exe (program written by
: Dmitrii Tchekhovskoi [Dmitrii.Tchekhovskoi@nist.gov]. The
: program is expected to be found at c:\filestat\filestat.exe

if not exist c:\ms_utilities\closeprog.exe goto close_error

: **Checking to make sure network connection is good
: sometimes network connection is lost due to network problems
: or user didnot update their network password after 90 days
: and network connection is lost

if not exist \\ntresapp03\mspec2\nist98\up_lib\ecc\name.inu goto n_error

: **Batch file assumes libraries will be copied directly to directory
: in the NIST98 foler, if using aliases to remote to a remote
: location, will need to modify batch file

if exist c:\nist98\ecc\alias.msdc goto alias_error
if exist c:\nist98\new\alias.msdc goto alias_error
if exist c:\nist98\pm\alias.msdc goto alias_error
if exist c:\nist98\tsc\alias.msdc goto alias_error
if exist c:\nist98\iontrap\alias.msdc goto alias_error
```

```
if exist c:\nist98\wiley6\alias.ms8 goto alias_error
if exist c:\nist98\wiley7\alias.ms8 goto alias_error
```

```
:    **Closing NIST program so libraries can be updated!
```

```
start /b /wait c:\ms_utilities\CLOSEPROG "NIST MS 2.0" "" 10000
```

```
:    **Copying libraries from server to user's library directory
```

```
cls
```

```
xcopy \\ntresapp03\mspec2\NIST98\up_lib\PM\*. * c:\nist98\p m\*. * /s /h /f /r /d /y
```

```
xcopy \\ntresapp03\mspec2\NIST98\up_lib\ecc\*. * c:\nist98\ecc\*. * /s /h /f /r /d /y
```

```
xcopy \\ntresapp03\mspec2\NIST98\up_lib\TSCA\*. * c:\nist98\TSCA\*. * /s /h /f /r /d /y
```

```
xcopy \\ntresapp03\mspec2\NIST98\up_lib\new\*. * c:\nist98\new\*. * /s /h /f /r /d /y
```

```
rem xcopy \\ntresapp03\mspec2\NIST98\up_lib\wiley6\*. * c:\nist98\wiley6\*. * /s /h /f /r /d /y
```

```
:    **Not everyone wants iontrap libraries, batch file checks
```

```
:    to see if installed on system, if it is, then it will copy
```

```
if not exist c:\nist98\iontrap\user.dbu goto skip_iontrap
```

```
xcopy \\ntresapp03\mspec2\NIST98\up_lib\iontrap\*. * c:\nist98\iontrap\*. * /s /h /f /r /d /y
```

```
:skip_iontrap
```

```
echo.
```

```
echo    **THIS PROCEDURE UPDATED YOUR USER LIBRARIES
```

```
echo.
```

```
echo    **If (0) files were copied, no library updates were needed
```

```
echo.
```

```
echo    **If you get tired of always having to close this window, edit
```

```
echo    Get_Lib.bat text file with Notepad program or Word and place
```

```
echo    a ":" before the "pause" command below.
```

```
echo.
```

```
:pause
```

```
:    **If you want to start the NIST search program automatically after
```

```
:    running this program, remove the ":" in front of the start command
```

```
:    below. Might have to change the name of the program depending
```

```
:    on the version of NIST software employed.
```

```
:start c:\nist98\nist$.exe
```

```
goto close_screen
```

```
:alias_error
```

```
cls
```

```
echo.
```

```
echo    **WARNING: Batch Program needs to be modified, your libraries
```

```
echo    are stored on a remote disk and aliases are being used.
```

```
echo    Contact James Little
```

```
echo.
```

```
pause
```

```
goto close_screen
```

```
:n_error
```

```
cls
```

```
echo.
echo  **WARNING: Couldn't read network drive!
echo      Error caused by one of two problems:
echo      -network connection lost, reboot computer
echo      -password expired, change network password, then reboot
echo.
pause
goto close_screen

:close_error
cls
echo.
echo  **WARNING: Close.exe program not found at c:\ms_utilities\close.exe!
echo      c:\ms_utilities\closeprog.exe! This program closes NIST Search
echo      so that libraries can be updated. Call you mass spec program
echo      administrator!
echo.
pause
goto close_screen

:  **Command needed to automatically close Windows in Windows 95
:  Not needed in Windows NT 4.0

:close_screen
echo.
echo off
cls
exit
```

**Figure 8.** Backup\_lib.bat

```
:   **Program written to create a backup copy of a library
:   (in this particular case, "New") with the current date
:   appended to the folder name. It is placed on the server
:   for storage and automatic archival. These dated copies
:   of the library are useful for retrieving user entries
:   if necessary. Filecopy.exe allows the user to set the
:   desintation of the dated-created file.
:
:   James Little 7/14/00, filecopy.exe written by Paul Wehner
:
:   **Making sure filecopy exists and is in proper directory

if not exist c:\mrg_lib\filecopy.exe goto filecopy_error

c:\mrg_lib\filecopy.exe \\ntresapp03\mspec2\nist98\up_lib\new

goto close_screen

:filecopy_error
cls
@echo off
echo.
echo   **WARNING: Exit this window and install filecopy.exe at
echo       c:\mrg_lib\filecopy.exe. It is a utility needed to
echo       make a copy of "New" with the current date appended
echo       to the folder name. The created folder is stored
echo       on the server.
echo.
echo.
pause
goto close_screen

:close_screen
echo.
echo off
cls
exit
```

**Figure 9:** Update\_structures\_jl\_user.bat

```
rem    Written by James Little at Eastman
rem    Chemical Company, 7/8/2000; Runs program to update
rem    structure links in a user library. Will have to customize
rem    for every user. 7/11/00

cls

@echo off
rem
rem    **This batch file needs strdbld.exe (program written by
rem    NIST. The program is expected to be found at
rem    c:\nist98\strdbld.exe

if not exist c:\nist98\strdbld.exe goto strdbld_error
cls
echo.
echo.
echo    **THIS PROCEDURE AUTOMATICALLY UPDATES YOUR USER LIBRARY
echo    MUST BE CUSTOMIZED FOR EVERY USER AND RUN EVERYTIME
echo    A USER ADDS AN ENTRY WITH A STRUCTURE TO THEIR USER LIBRARY.
echo.

C:\nist98\strdbld.exe /D:C:\nist98_jl_user /L:C:\NIST98\strdbld.log

goto close_screen

:strdbld_error
cls
echo.
echo    **WARNING: Exit this window and install strdbld.exe at
echo        c:\nist98\strdbld.exe. It is needed to
echo        update your user library structures for
echo        structure searching.
echo.
pause
goto close_screen

rem    **Command needed to automatically close Windows in Windows 95
rem    Not needed in Windows NT 4.0

:close_screen
echo.
echo off
cls
exit
```

## **Addendum 1: Instructions to Users on Updating "New" Library**

### **Change in Method of Updating Libraries Searched with NIST Software**

We are updating the NIST searchable libraries daily. Libraries will only be replaced if newer versions are available. Libraries checked will include New, ECC, TSCA, PM, and Iontrap. This will replace new.exe file that I have been E-mailing you. We will be using a Windows bat file, Get\_Lib.bat, to perform the daily update of New entries.

#### **Known Problems:**

-If your NIST Search Program is open, your library will not update properly. You will get a warning to close your NIST Search and run Get\_Bat.bat file manually.

-The DOS window will need to be closed every time the program runs. If you get tired of this, see information in the DOS window that tells you how to close automatically.

#### **NIST Libraries Stored on a Server or Remote Drive:**

The program will warn you if you are using aliases to store your user libraries on a remote disk (one other than C:). You will then have to edit the Get\_Lib.bat file using a text-editing program such as Word or Notepad. Just change the letter to that of the mapped letter where your libraries are located. If you need help with this, give me a call and I will send you a customized Batch file.

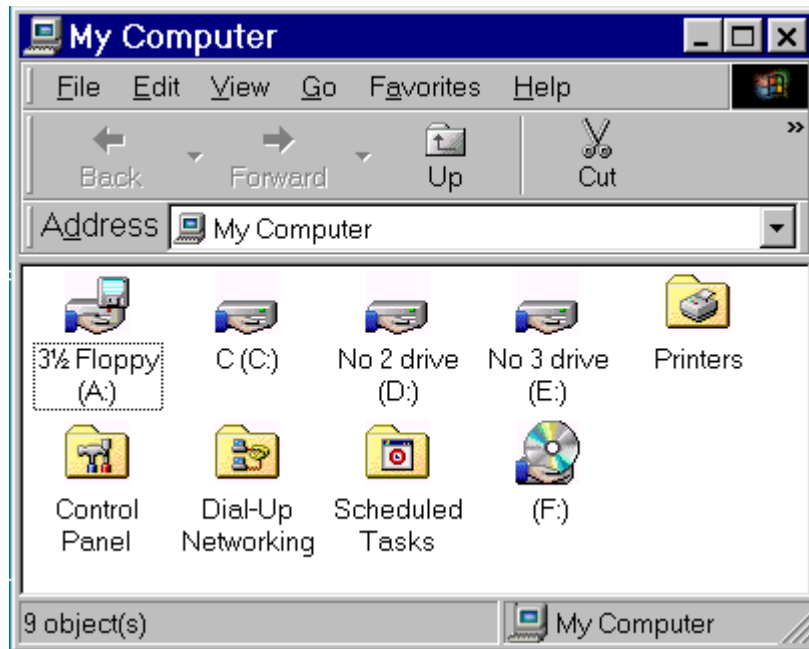
#### **Filestat Program:**

Get\_lib.bat needs a program named filestat.exe. It needs to be installed at c:\filestat\filestat.exe.

#### **Ways to Update:**

You can use this bat file in one of three different way. Pick whichever meets your needs:

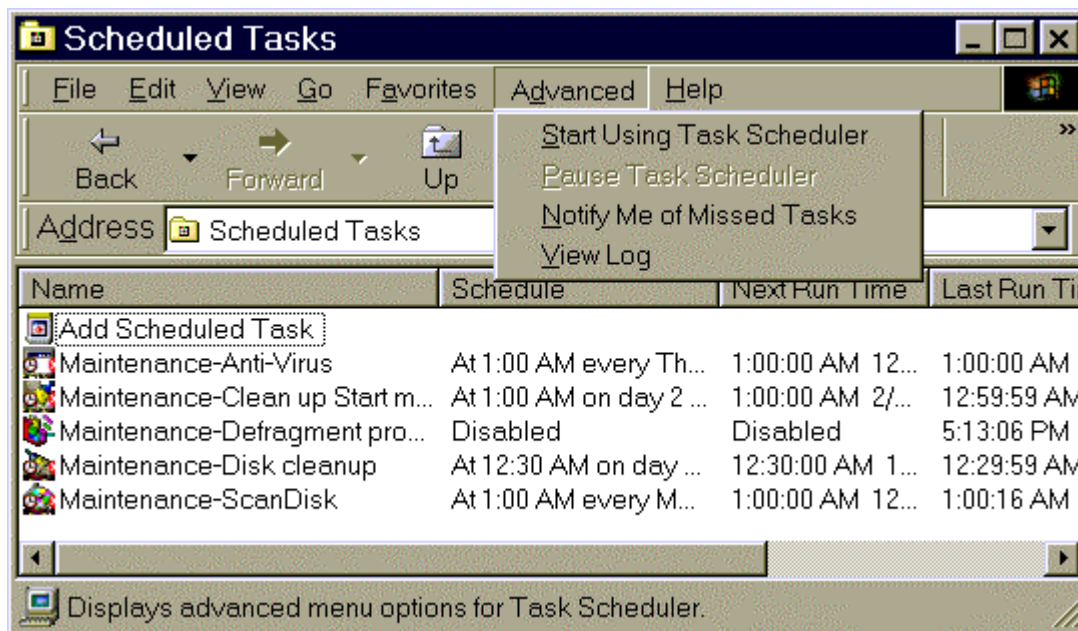
1. If you want to do it manually, just copy Get\_Lib.bat it to your desktop. Click on it whenever the urge hits you. You will also need to create a Folder named with the following name and path: C:\filestat and place filestat.exe in this folder.
2. If you boot every night, you can copy Get\_Lib.bat to your startup folder, which is probably located at C:\Windows\Start Menu\Programs\StartUp. It will update whenever you reboot your computer. You will also need to create a Folder named with the following name and path: C:\filestat and place filestat.exe in this folder.
3. The following instructions are used if you want to update automatically. Create a Folder named with the following name and path: C:\filestat and place filestat.exe in this folder. Copy Get\_Lib.bat to your DeskTop, Double Left Click on the My Computer Icon and then double left click on the Schedule Task Icon or JIT Scheduler (<http://www.gibinsoft.com/shareware/jit/>). I like the JIT (Version 4 is free) better than Windows Scheduler since no password or password updating is associated with the tasks.



If you don't have this program, call the computer support group. It was not with the original Windows 95 install, but was added with Internet Explorer 4.0. If the Schedule Task Program is running, you will see a Small Icon on the bottom right side of your task bar at the bottom of your screen with a clock in its lower right corner:



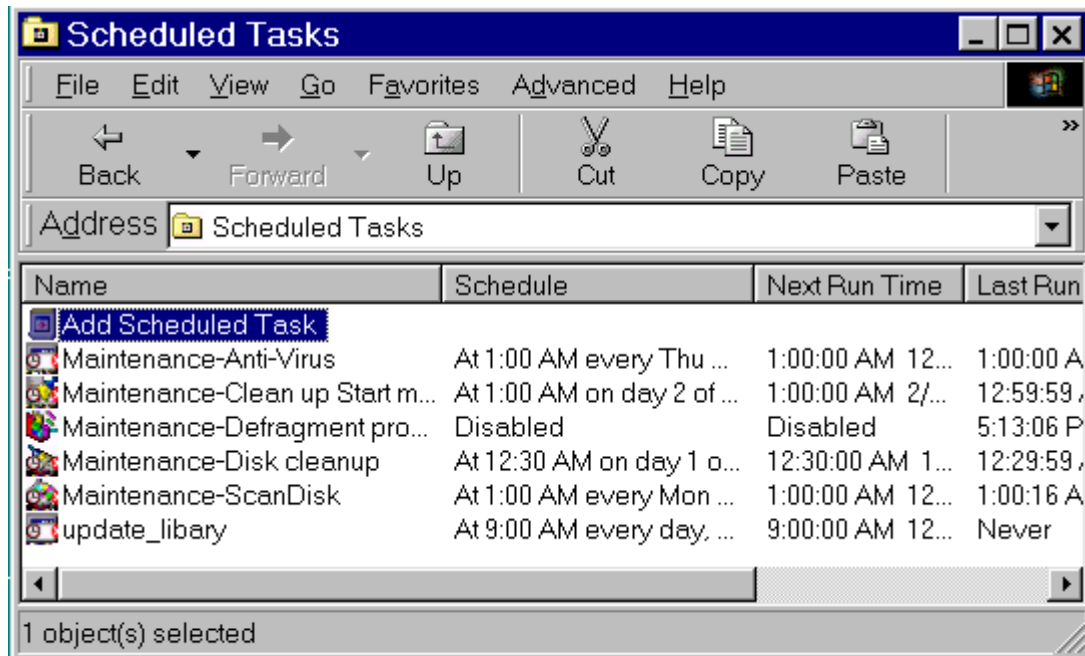
If it isn't running, go to Advance item on your Scheduled Tasks menu and select "Start Using Task Scheduler" option.



Then after started running, click the Add Scheduled Task entry under the name column. This will carry you through a Wizard to setup your program. Browse until you find the Get\_Lib.bat file which you placed on your desktop. Your Desktop is actually one level above C: and My Computer when browsing. Set it up to run the program once daily. 8:00 AM would be a good time, just make sure your computer is connected to the network at the specified time. After you finish, you menu should have get\_lib.dat added to the Scheduled Tasks Window.

***You have to change the password for your scheduled task when you change your logon password.***

Just go to Scheduled task program, double left click on your task, and select set Password option. Also you can view the log for Task scheduler by clicking the "Advanced" option on the Scheduler Task bar. Might want to also select the "Notify me of missed Tasks" option in the "Advanced" option.



**Scheduled Tasks**

File Edit View Go Favorites Advanced Help

Back Forward Up Cut Copy Paste

Address Scheduled Tasks

Name	Schedule	Next Run Time	Last Run
<a href="#">Add Scheduled Task</a>			
Maintenance-Anti-Virus	At 1:00 AM every Thu ...	1:00:00 AM 12...	1:00:00 A
Maintenance-Clean up Start m...	At 1:00 AM on day 2 of ...	1:00:00 AM 2/...	12:59:59 ,
Maintenance-Defragment pro...	Disabled	Disabled	5:13:06 P
Maintenance-Disk cleanup	At 12:30 AM on day 1 o...	12:30:00 AM 1...	12:29:59 ,
Maintenance-ScanDisk	At 1:00 AM every Mon ...	1:00:00 AM 12...	1:00:16 A
update_libary	At 9:00 AM every day, ...	9:00:00 AM 12...	Never

1 object(s) selected