LC/MS Unknown Identifications Using MSMS Libraries
Part VII: Using and Creating Other MSMS Libraries

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- *Retired* Research Fellow, Eastman Chem. Co.*
- *42 years experience unknown identification*
- *Now Consultant, MS Interpretation Services*
- *Specialties[1] EI GC-MS, LC-MS/MS, Chemical Ionization,[2] Accurate Mass, Derivatization,[3,4] MS library management, SciFinder,[5] ChemSpider,[5] Surfactant ID,[6] NMR, GC-IR, organic synthesis, matrix ionization effects,[7] etc.*

Eastman Chemical Company, Main Site, Kingsport, TN
50 Manufacturing Sites Worldwide, ~14,500 Employees

>50 Mass Specs Networked
Worldwide

* https://en.wikipedia.org/wiki/Eastman_Chemical_Company

Table of Contents

Topic **Slide #**

LC/MS Unknown Identifications Using MSMS Libraries

Note: ***Read*** This Before Utilizing Procedures in Handout ***some*** of the ***topics*** in this handout are somewhat ***more challenging***

- ***Buy*** a copy of ***NIST*** MSMS libraries which includes NIST search program
- It is a ***very inexpensive, shop around*** with ***multiple distributors*** for best price!!
- I feel that ***all readily available*** libraries should be used in LCMS and GCMS identifications
- Wiley Libraries (2) and existing user libraries are ***very*** useful, ***you must conve***rt to hybrid format
- I have supplied the MoNA MSMS (~140,000 spectra) and EI Databases (~19,000 spectra) in NIST format, ***download them***[12,13]
- Thus, **give them a try** before creating your own copies
- The ***process*** described in the handout ***is not simple*** and will require a ***time investment*** by the user to create libraries in NIST format for yourself
- These two MoNA databases are ***lower quality*** than those supplied by NIST, but they are ***free*** and will be ***useful***
- User, Wiley, and MoNA libraries are very useful ***complimentary resources*** when used ***with*** the NIST commercial libraries

Part VII: Using and Creating Other MSMS Libraries
My Philosophy

- My philosophy with library searches is to ***use as many libraries*** as possible in the process

- Always remember that library searches are an ***aid to identification*** and all libraries commercial, ‘”crowd-sourced”, or your own personal ones contain errors

- In lower resolution searches, some compounds with different molecular formulae can have very similar spectra

- Accurate mass would resolve the above limitation, but still isomers with the same molecular formulae could have similar spectra

- So ***always be skeptical*** when evaluating results and consider all other sample related history

- After ***“proposing”*** an identity in critical applications, consider trying to ***confirm*** by preparing the component in an enriched mixture by known chemistry, purchasing the material, or evaluating by other analytical techniques

Part VII: Using and Creating Other MSMS Libraries
User Libraries Converted and Approach

Libraries Targeted:

- MoNA,[8,9] a large "crowd-sourced" MSMS library of a variety of classes of compounds (~140,000 spectra) [Free]

- MoNA[8,9], a large "crowd-sourced" EI library of a variety of classes of compounds (~19,000 spectra) [Free]

- Two Wiley Commercial Libraries (~13,000 and ~12,000 spectra) [Purchased]

- Personal user library (~5,000 spectra) with no precursor ion field

Approaches:

- NIST Lib2NIST utility

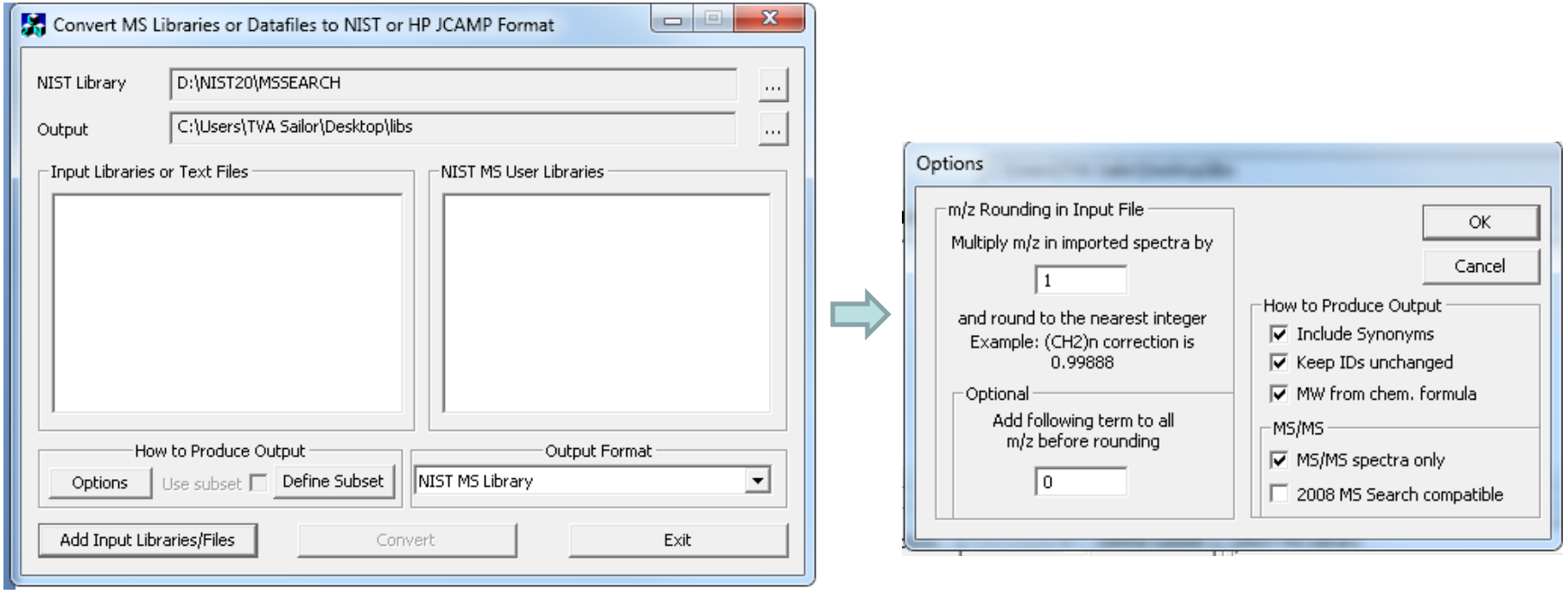
- Version supplied with NIST 2020, Version 1.0.8.8 (beta)

- ***Requires*** a little ***patience*** to complete process

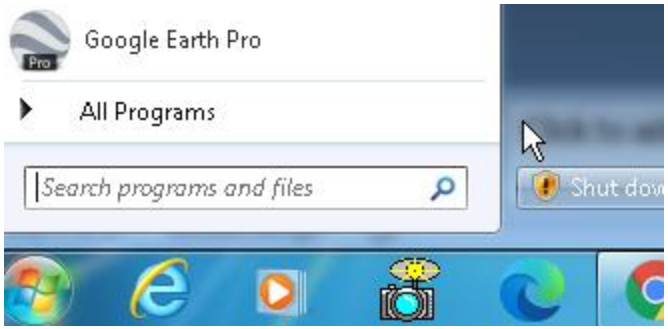
- Placed copy in NIST format[12,13] on the internet for both the MoNA libraries mentioned above

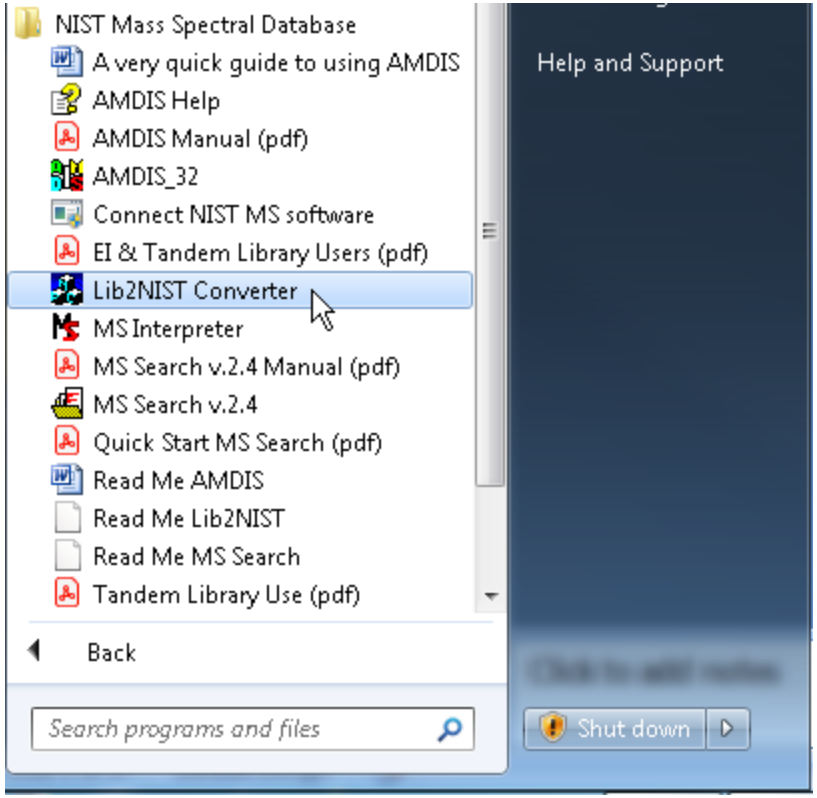
NIST Lib2NIST Utility

- Reasonably easy to use, just put your input in and select output format
- Select ***proper options*** as shown in screen shot on right
- MS/MS selected for MSMS libraries, “de-select” that parameter for EI libraries
- Can be used in many diverse ways, ***see Documentation*** Reference[10]
- Mainly utilized internally by NIST, always changing with new 3 year releases
- I utilized version that came with 2020 NIST library release, Version 1.0.8.8 (beta)

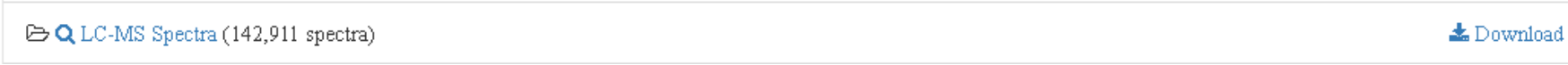


Accessing Lib2NIST Utility





Quality of MoNA and Converting to NIST Format



- Quality of this MoNA[8,9] library, LC-MS Spectra, is reasonable, but much ***lower quality*** than NIST commercial ones
- ***Nevertheless***, Good ***complimentary resource*** for use in conjunction with NIST
- Varies in mass accuracy and presence of Precursor_m/z field utilized in NIST MSMS search
- I placed copy in NIST format on my website,[12,13] place in NIST20/MSSEARCH folder to use
- If you want to do the conversion yourself, I did it in two ways
- The 2nd approach allows one to add lr_ to the front of the name indicating low resolution
- The 1st approach will cause Hybrid MSMS presearch to fail if user precedes the name with lr_

1. From SDF file using Lib2NIST
   a) Download *.sdf format from MoNA site to NIST20/MSEARCH folder
   b) File will be in zip format, unzip to gain access to *.sdf type file for conversion
   c) Use Lib2NIST to convert to NIST format
   d) Make sure final NIST converted copy present in NIST20/MSSEARCH folder

2. From both SDF and MSP file formats using Lib2NIST
   a) Download *.sdf version which contains spectra and structures
   b) Files will be in zip format, unzip to gain access to files for conversion
   c) Convert to NIST file format
   d) Export back to NIST msp ASCII file with folder with structures in Mol file format
   e) Download *.msp file which contains only the spectra
   f) Change the name of the folder with Mol files to match the name of msp file downloaded from MoNA site
   g) Convert the msp with associated Mol files in the folder to NIST Library format
   h) Make sure library is in NIST20/MSSEARCH and folder contains ***no file*** named alias

Low Resolution versus High Resolution MSMS NIST Libraries

- The NIST MSMS search and library software supports low resolution and high resolution libraries
- As you will note, the NIST library contains a ***library lr_msms***
- "**lr**_" preceding a name ***marks*** the library as low resolution
- The user adds this designation after Lib2NIST is utilized ***if*** appropriate
- The information below is noted in the quick start documentation[11]
- I have used "lr_" libraries in hybrid searches simultaneously with high resolution and got results
- MoNA can be used in standard ("hr_") mode *or* low resolution mode ("lr")
- "hr_" is not needed before a library, ***absence*** indicates high resolution

Excerpt *:*[11] *NIST Tandem Quick Start*

lr_msms_nist – contains all low resolution (unit mass accuracy) spectra of 'small molecules'. When searching, the fragment ion tolerance is always set to ±0.5 *m/z* units, regardless of the value set in the MS/MS search tab. The precursor ion tolerance set in the **MS/MS** tab of the **Library Search Options** dialog box is used for all libraries. Use of this library is not recommended for high resolution hybrid searches.

Problems Converting and Searching "User/Crowd-Sourced" Libraries and "Work-Arounds"

- MoNA library required ***two steps*** using both MSP and SDF files to get library to work in Hybrid MSMS in low resolution format

- Typical ***problem*** is the Hybrid MSMS presearch yields ***no results***

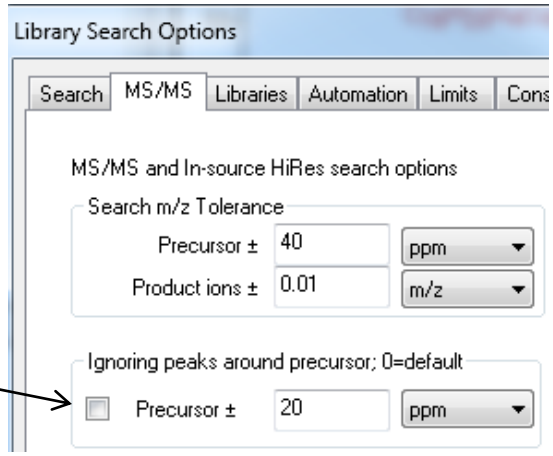
- Results ***can be obtained*** in the other two MSMS search approaches, only hybrid fails

- Results can be obtained if Hybrid MSMS ***presearch is disabled*** in settings, but search ***time greatly increased***

- One can ***search*** in EI Hybrid MS mode, but DeltaMass will be ***shifted +1*** and will be in nominal mass even for high resolution spectra

- Often ***better DotProduct*** results obtained in Hybrid MSMS search ***if*** Precursor box +/- is ***"unchecked"*** in "Library Search Option MS/MS" Tab

Note unchecked!



Composition of the MoNA[8,9] Database Components and Structures for GCMS Derivatives

LC-MS Spectra (142,911 spectra) Download

GC-MS Spectra (18,886 spectra) Download

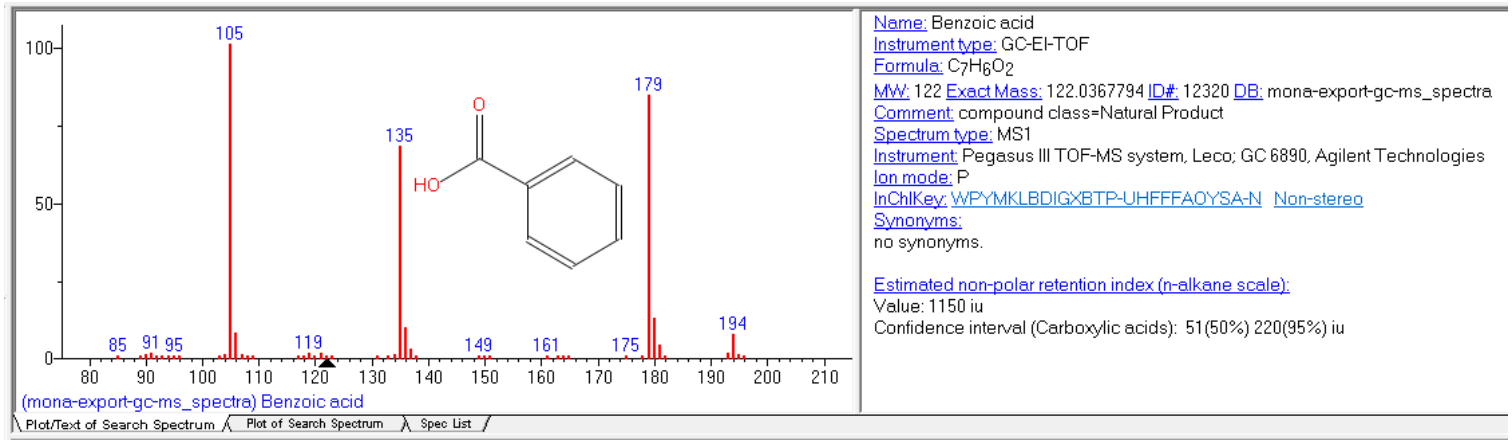
➢Decided to convert ***only the above*** LC-MS and GC-MS MoNA[8,9] spectral libraries, many of the others were either in-silica libraries or were a subset of this library

➢Summarized my observations about the libraries and which were ***subsets*** of the others in this Reference[14]

➢The GC-MS of derivatives show the ***structure of*** the ***underivatized*** structure for the component and ***do not tell*** the user what ***type of derivative*** was formed in the spectral fields for the entries

➢See TMS derivative of benzoic acid as example below

➢Also the scan range was too high for this type of spectrum



Conversion of Wiley Commercial Libraries with Lib2NIST

➢***Converted*** Wiley Registry of Tandem Mass Spectral Data, MS for ID by Herbert Oberacher (wmsn1) ***using Lib2NIST*** (12,048 spectra)

1) Exported the library in NIST format to MSP with Mol file and SDF formats
2) Converted both back to NIST format which added additional indices needed to perform hybrid search
3) Both worked in Hybrid MSMS format and also worked if converted to lr_wmsn1, low resolution, format
4) Best to ***use this library in high resolution*** mode so ***nothing preceding*** the name

➢ ***Converted*** Maurer/Wissenbach/Weber LC-MS^n Library of Drugs, Poison, and Their Metabolites, 2nd Edition (mwwtox2019_rebuild) (13,027 spectra)

1) Exported the library in NIST format to MSP with Mol file and SDF formats
2) Converted both back to NIST format which added additional indices created to perform hybrid search
3) Both worked in Hybrid MSMS format and also worked if converted to lr_wmsn1, low resolution, format
4) Probably best to ***use this library in "lr",*** low resolution format because all spectra are low resolution

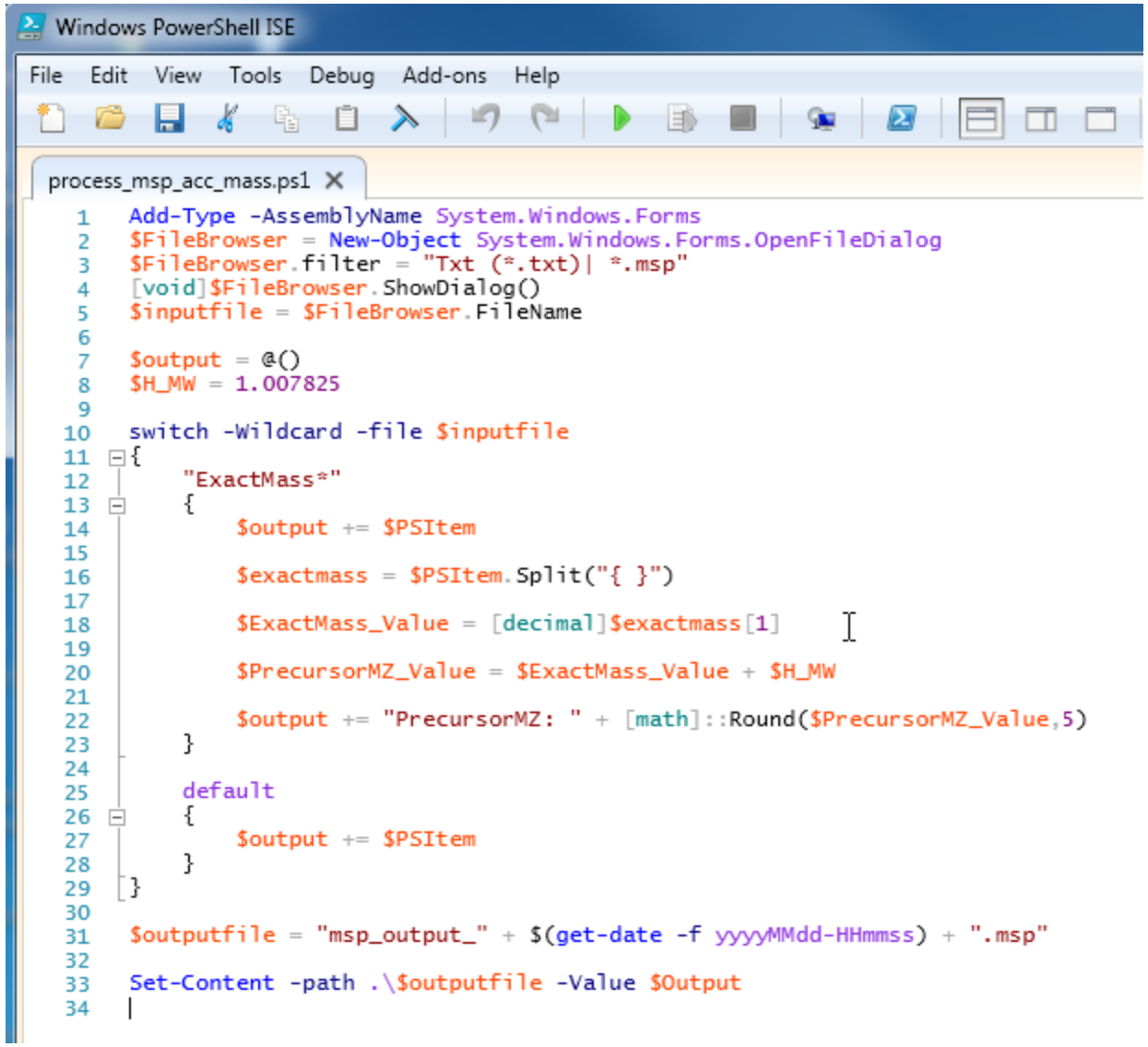
Conversion of Personal User Libraries with No Precursor_m/z Field

- Our ***Eastman library*** was all in low resolution mode and had ***no*** Precursor_m/z field
- Majority were “in-source” spectra with M+H, M+NH4, M-H or M+Acetate/formate precursor ions
- Some were QQQ MSMS
- M+NH4 and M+H yield ***essentially same*** MSMS spectra, so all added as M+H
- ***PowerShell*** “program” (script)[15] written ***to add Precursor_m/z*** field in conjunction with Lib2NIST
- Final libraries in positive and negative mode in “lr_” mode created for use with hybrid MSMS search

Approach:

1) ***Somewhat tedious process***, but libraries ***perform well*** and used in conjunction with NIST, Wiley, and MoNA for searches
2) Export libraries in Lib2NIST in MSP format
3) Import back with “MW from chem formula” option in Lib2NIST to add MW and accurate MW fields to all entries in NIST library file
4) Export once again to MSP format
5) Run PowerShell script[15] to create and insert Precursor_m/z to MSP file
6) Create the final library in NIST format with Lib2NIST
7) ***Precede*** the ***name*** with ***“lr_”*** and install in NIST20/MSSEARCH folder

PowerShell Example Script for Adding Precursor_m/z Field to User Library



Creating/Adding User Library within NIST Search Program

- ***Eastman Chemical Co.*** has added over **>50,000 entries** to our Corporate EI and MSMS libraries over the last 42 years

- ***Critical asset***[16] in R&D, manufacturing, and pollution control

- ***Automatically***[17] Distributed Nightly to large network users/instruments

- ***Performed*** by ***Batch Files***[17] with command line access to ***Lib2NIST***

- Very ***cost effective*** approach and ***reliable***

- **Current work** shows approach to enter **accurate mass** spectra ***with precursor*** ions

- ***Basic steps*** in current approach for accurate mass with precursor ions

- ***Very initial work***[18] was in-source nominal mass spectra with ***no precursor ions***

Types of Components Added to Library

Anything a user would find useful, thus ***much more*** "diverse" than purchased commercial EI and MS/MS databases

Thus, ***users must realize*** Eastman database is an ***aid to identification*** and should be used accordingly.

- ***Most entries*** high quality with ***high confidence*** and exact structure

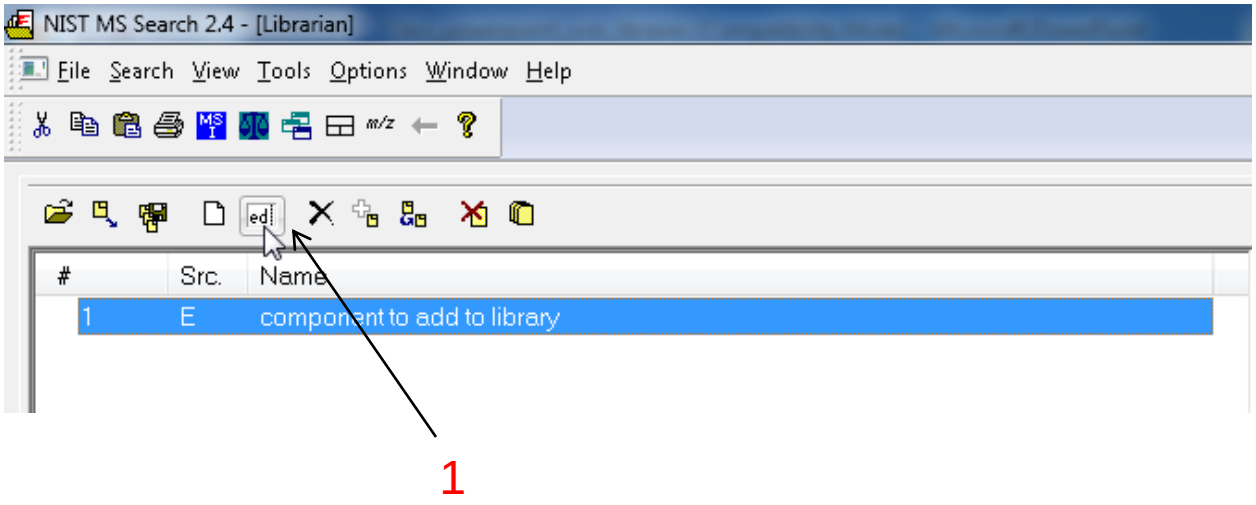
- Some entries will have "?" or "??" in front of name to show best educated guess

- Many components added with reference to common names for commercial plasticizers, lubricants, surfactants, antioxidants, UV stabilizers, polyesters, *etc.*

- Many entries added with reference to plant and R&D processes with unknown structure, but do include accurate mass and confirmation of MW by CI

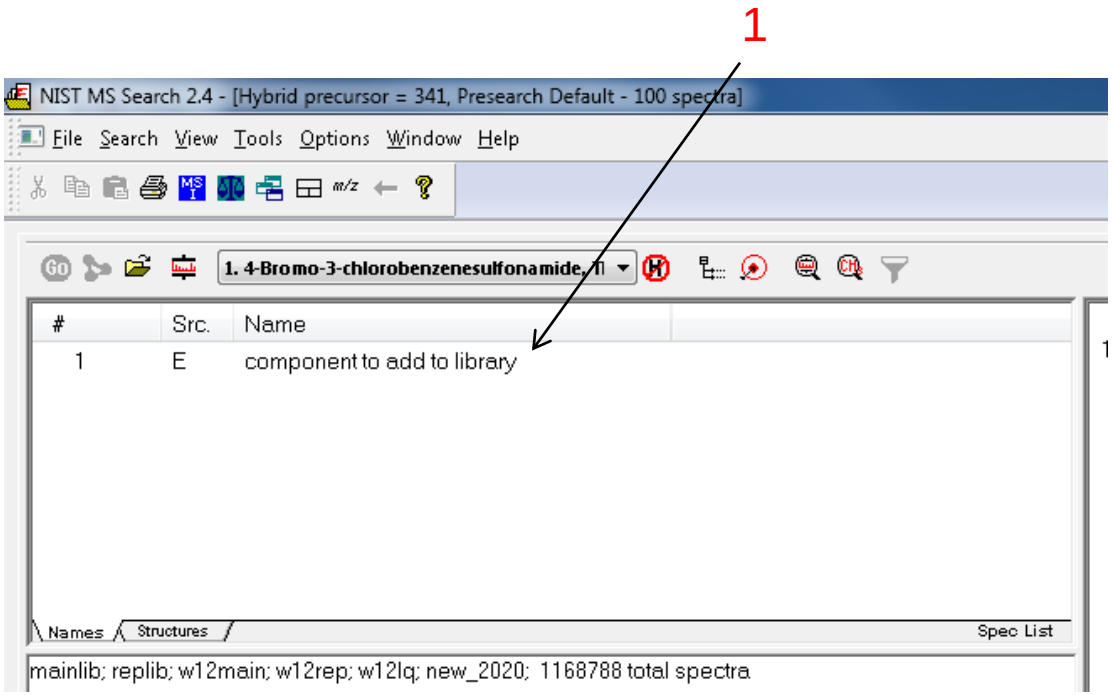
Creating a User Library Spectrum: Opening Edit Spectrum

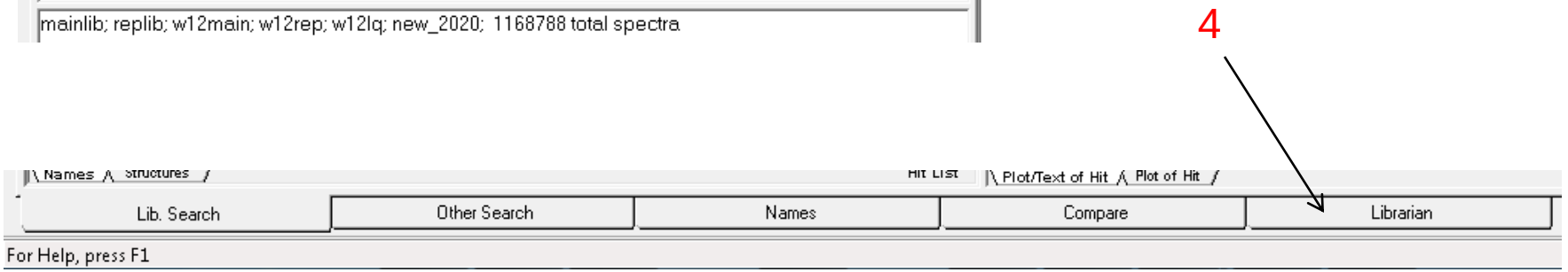
1) **LMB** “ed” (edit spectrum) button on toolbar



Creating a User Library Spectrum

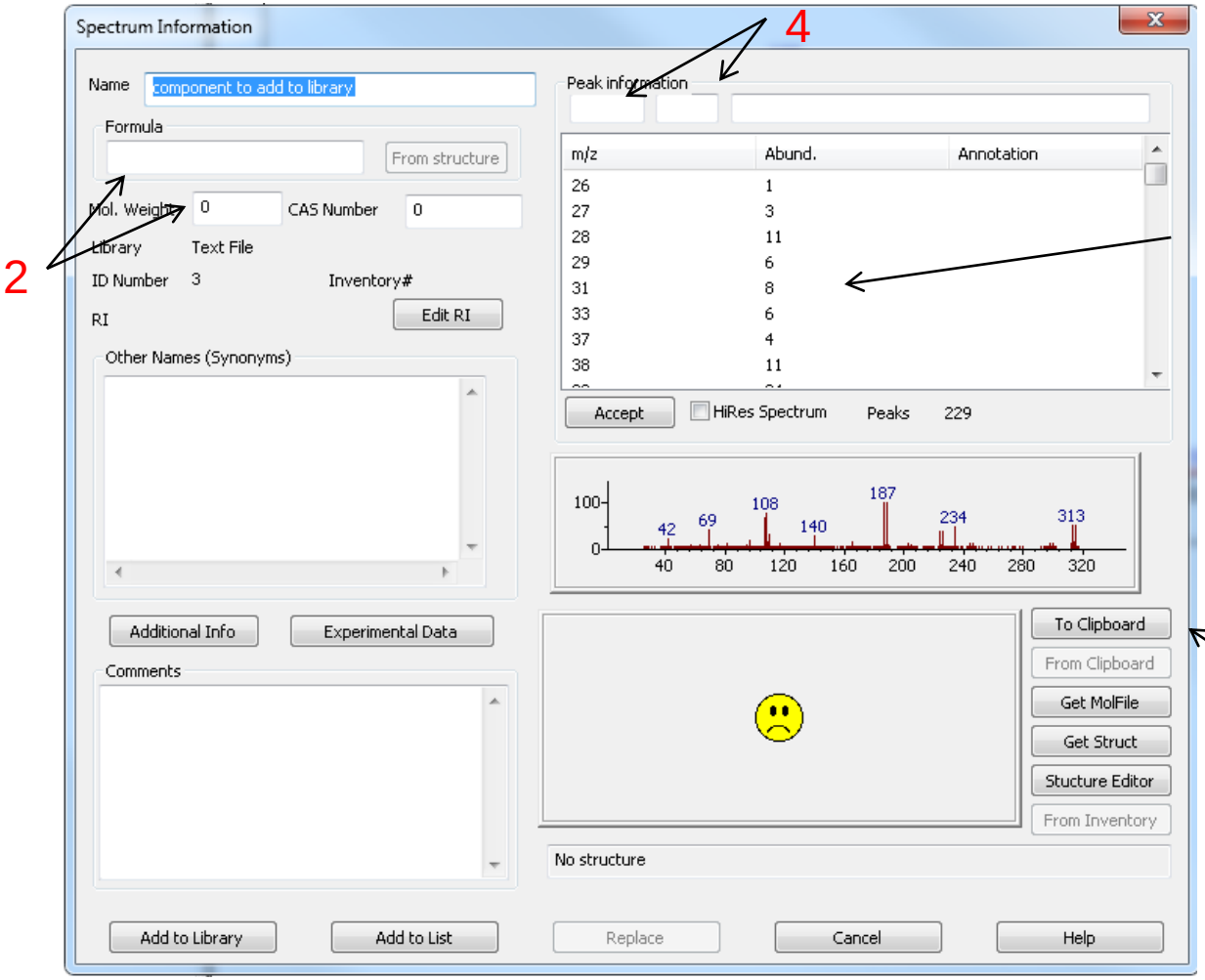
1) Import the spectrum from data processing application from manufacturer
2) Spectrum will be in the Spec List Window
3) Draw the structure in drawing program and copy into windows clipboard
4) **LMB** Librarian Tab





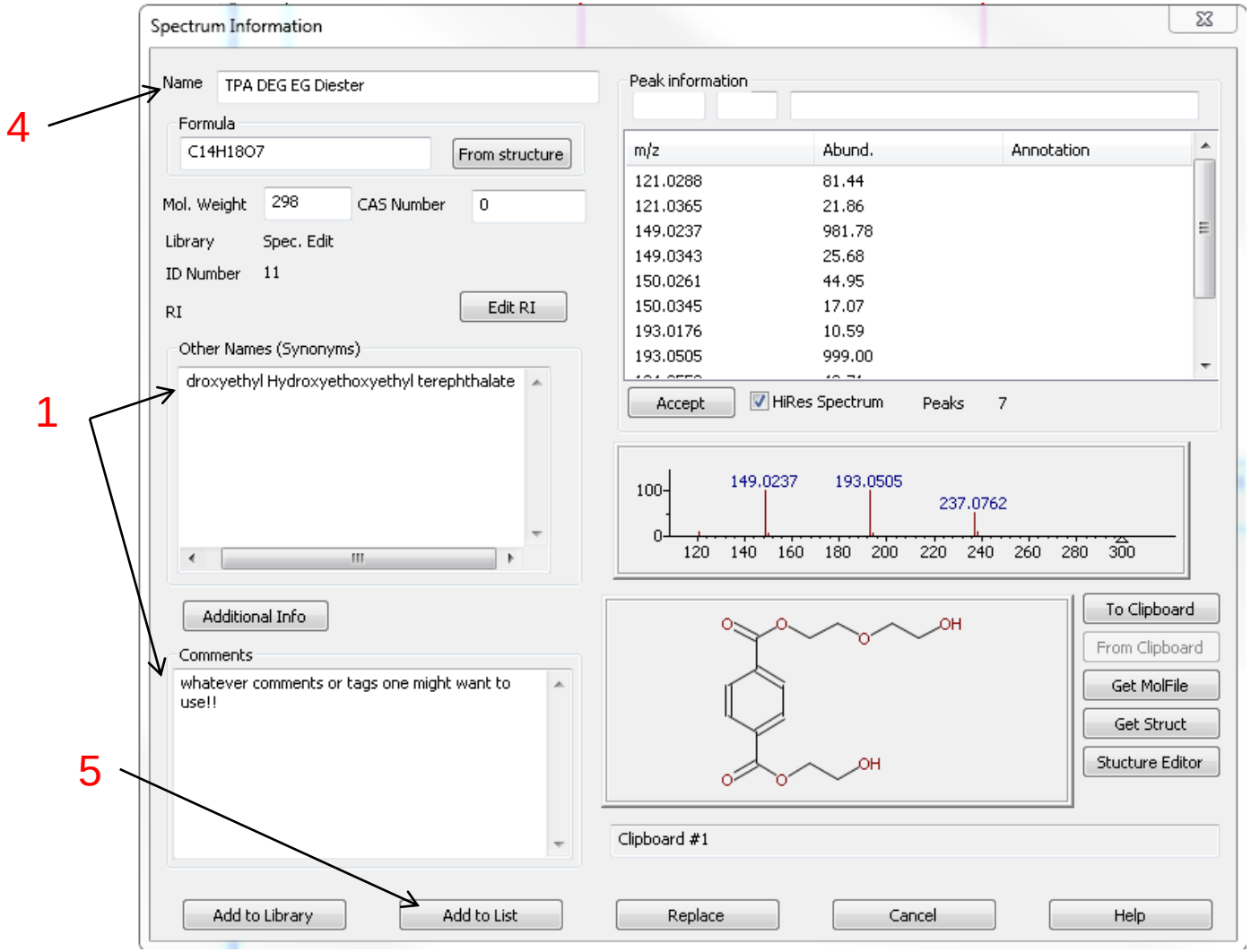
Creating a User Library Spectrum: Spectrum Information Window

1) ***LMB "***To Clipboard" to paste structure from windows clipboard into window
2) Mol. Weight and Formula will be automatically calculated
3) To delete peaks, **LMB** to select peaks and then must push ***Delete*** key on keyboard to delete, ***no*** button within NIST program!
4) To add peaks, type in peak information, *m/z* and Abund., and accept; annotation not needed



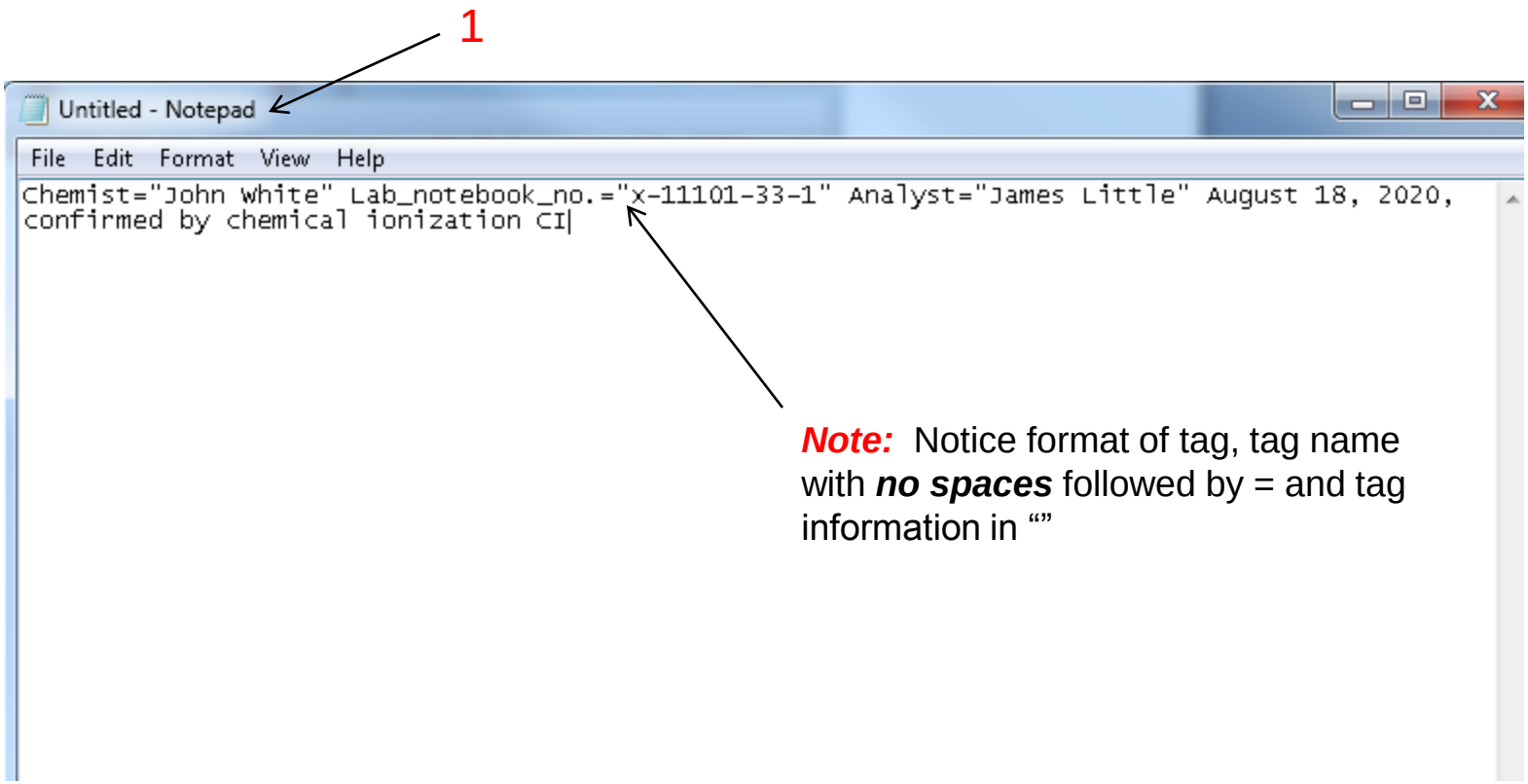
Creating a User Library: Adding Comments and Synonyms

1) Add **Comments** and **Other Names (Synonyms)** to Spectrum Information window
2) User can create Tags that will be displayed on a separate line for the library entry (described later)
3) Format for tag such as notebook number would be lab_notebook_no= "x-11101-33-1“
4) Generate name with drawing program and paste into field or enter your own
5) After complete, select “Add to List”



Creating a User Library: Using Windows Notepad and Tags

1) ***Tip:*** If adding the same comment many times to different spectra, **create in Windows Notepad** and paste into Spectrum Information Window using **Ctrl V** on keyboard
2) My Tags below are chemist, lab_notebook_no., and Analyst
3) When ultimately displayed, they will show up as ***separate line items*** and are removed from the Comments display

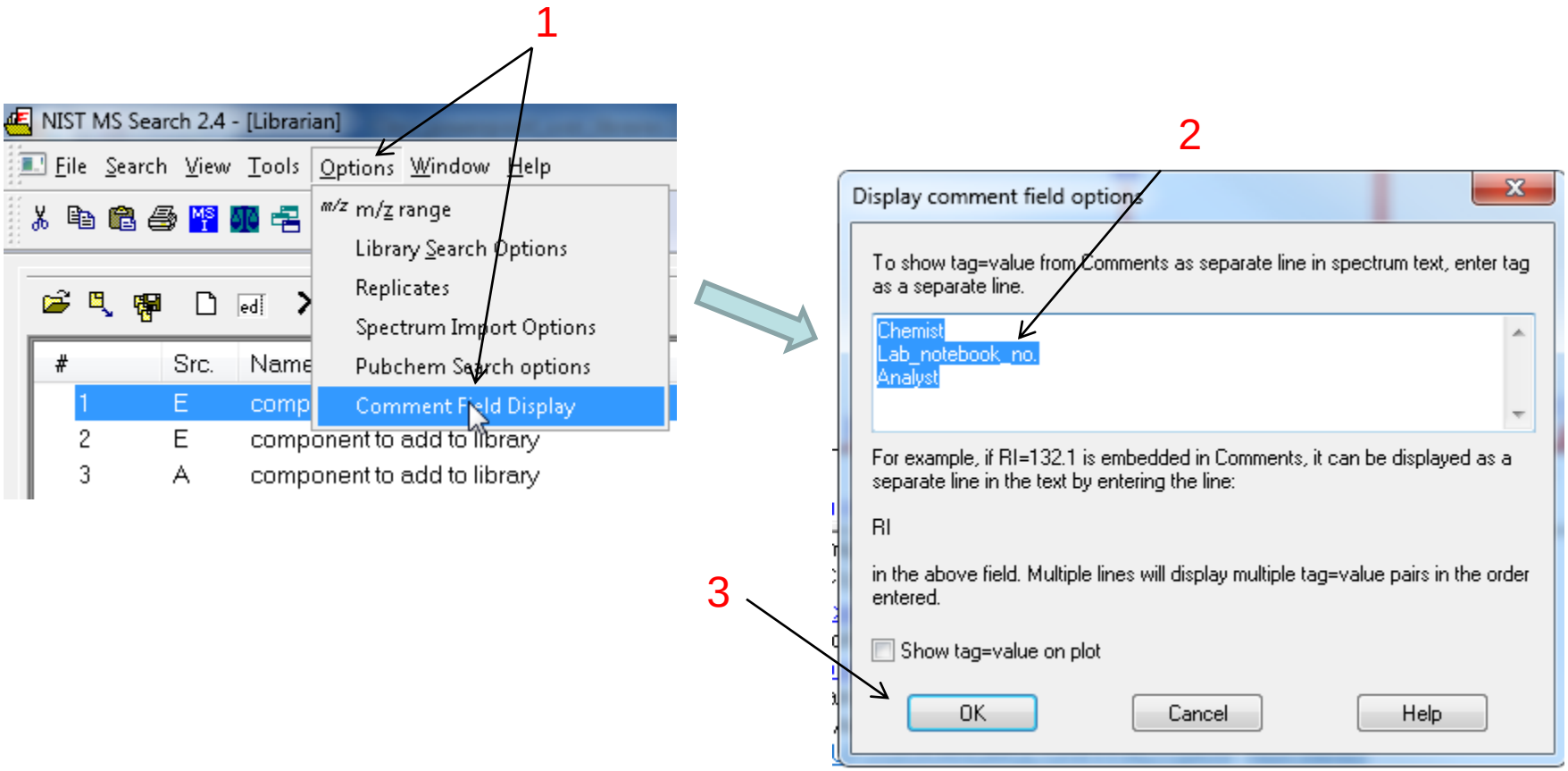


Creating a User Library: Comment Field Display with User Tags

1) ***LMB*** on Options, Comment Field Display

2) Add the ***user defined Tags*** Chemist, Lab_notebook_no., and Analyst to ***Display comment field options*** window

3) **LMB OK** to accept values



Creating a User Library: Comment Field Display Showing User Tags

1) User library comments ***without*** Tags
2) User library comments ***with*** Tags
3) The InChIKey and Estimated retention index automatically added by NIST program

1

Name: component to add to library
Formula: $C_{10}H_8BrF_4NO$
MW: 313 Exact Mass: 312.972538 ID#: 6 DB: Spec. Edit
Comment: Chemist="John White" Lab_notebook_no.="x-11101-33-1" Analyst="James Little" August 18, 2020, confirmed by chemical ionization CI
InChIKey: IUFOQIOKANQMQL-UHFFFAOYSA-N Non-stereo
Synonyms:
1.PM 2201 derivative
2.TFA derivative of PM 2201
3.Morrison's Amine, TFA derivative

Estimated non-polar retention index (n-alkane scale):
Value: 1422 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu

2

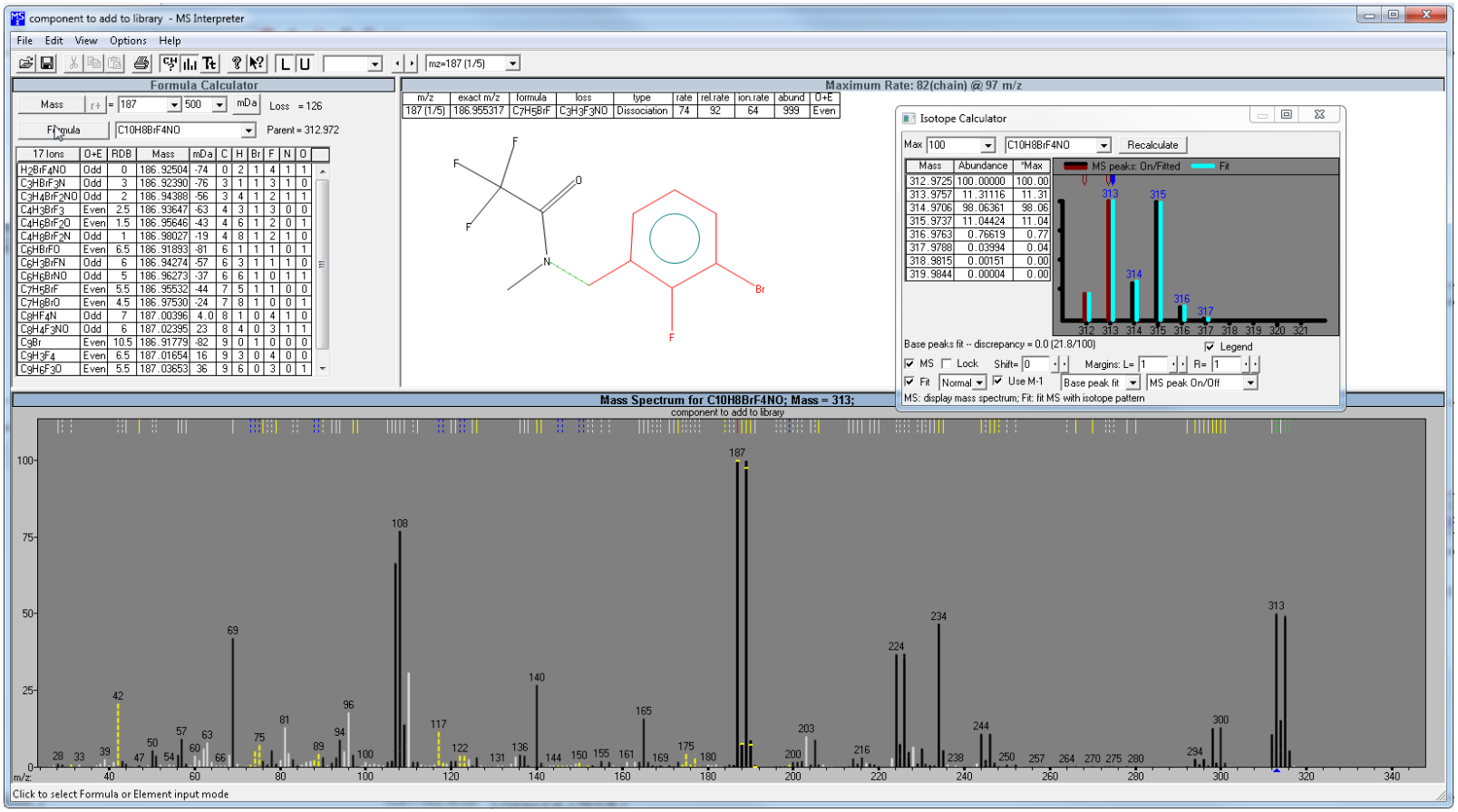
Name: component to add to library
Formula: $C_{10}H_8BrF_4NO$
MW: 313 Exact Mass: 312.972538 ID#: 6 DB: Spec. Edit
Chemist: John White
Lab_notebook_no.: x-11101-33-1
Analyst: James Little
Comment: August 18, 2020, confirmed by chemical ionization CI
InChIKey: IUFOQIOKANQMQL-UHFFFAOYSA-N Non-stereo
Synonyms:
1.PM 2201 derivative
2.TFA derivative of PM 2201
3.Morrison's Amine, TFA derivative

Estimated non-polar retention index (n-alkane scale):
Value: 1422 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu

Possible Quality Checks Before Adding Spectra to User Library

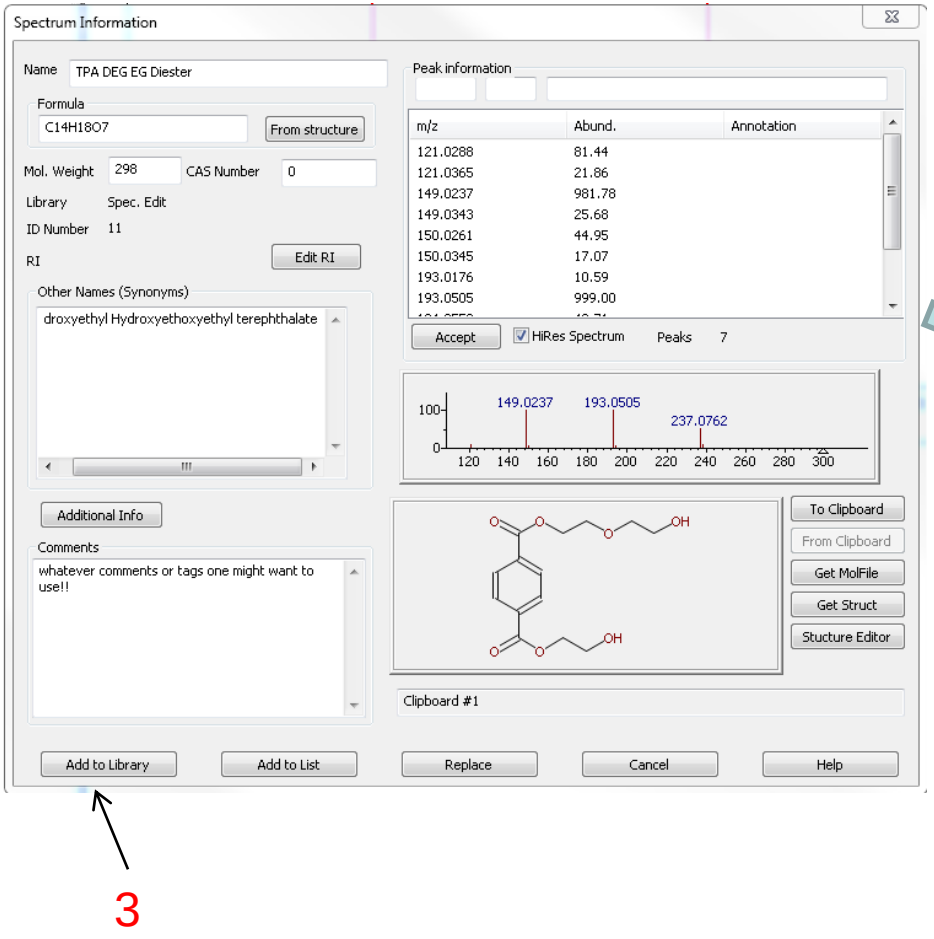
I ***always*** as a minimum do options 2 and 5

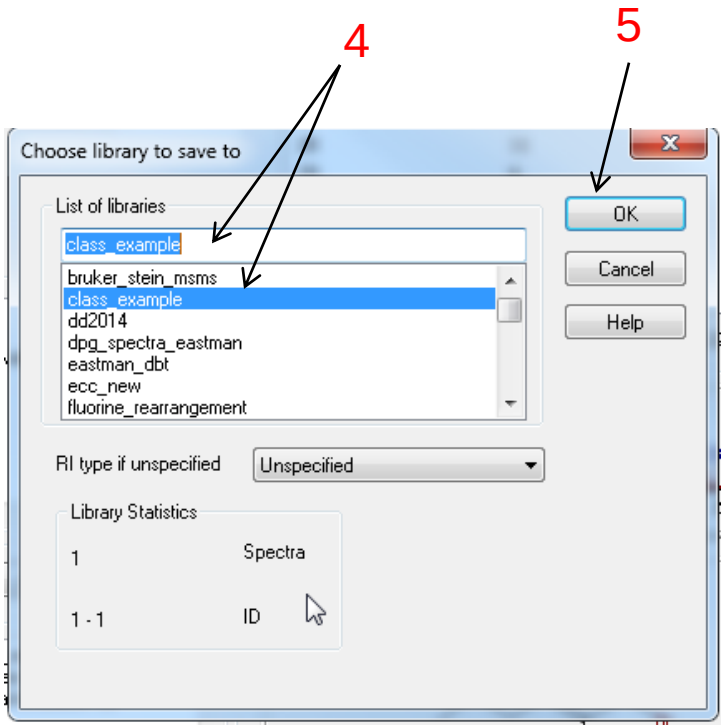
1) User entry added to SpecList
2) Check to see if exact spectrum present using InChIKey exact structure search
3) Similarity structure search to find model compounds
4) ***MSMS*** searches to see if consistent with current library entries
5) Send to MS interpreter, see if major peaks "***in the black***," thus explained



Addition of Spectrum to User Library or Creating New Library

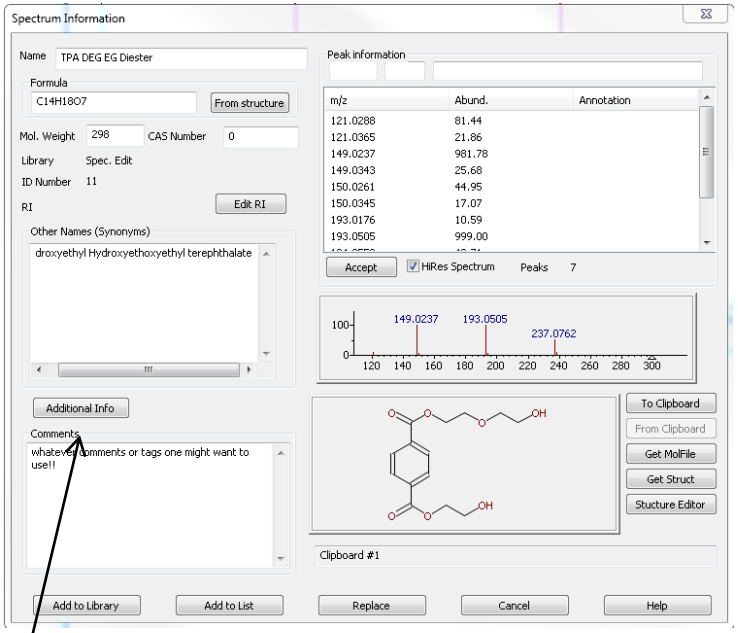
1) **LMB** to select entry to be added
2) **LMB** “ed” button in Librarian Tab to display Spectrum Information window
3) **LMB** “**Add to Library**”
4) Then add to a current user library, ***or*** if creating ***new*** library, type in its name
5) **LMB OK**



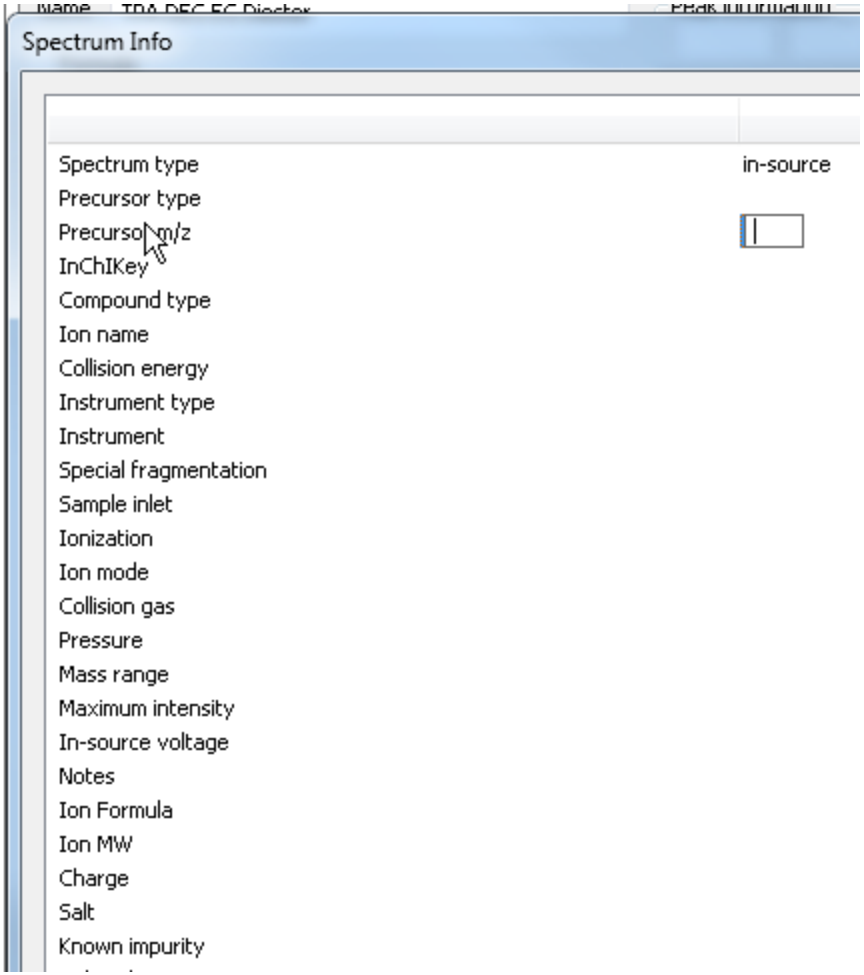


What If My Library Imported Spectrum Contained *No Precursor_m/z* Field?

- Can add your spectrum imported from the manufacturer's processing program
- Open "Additional Info"
- ***LMB click*** on the field such as Precursor m/z ***twice***, then field will turn from blue to white and value can be entered
- The ***field*** will ***show*** up ***after*** either the entry is added to the list or actual library



"Additional Info" button



What If I Need to Add Several *Different F*ields *for a Set* of Spectra?

- Very inefficient if one wants to add several different fields to a spectrum separately
- These fields would be ***useful*** for taking advantage of ***"Filtering"*** the list ***after*** the MSMS search
- One can use note pad which contains a list to be ***pasted*** into the ***synonym field (***use control C, control V)
- These will be added to the spectrum and ***will appear after*** the spectrum is added to the list or a library
- Add each one on a separate line using a carriage return when creating in Notepad

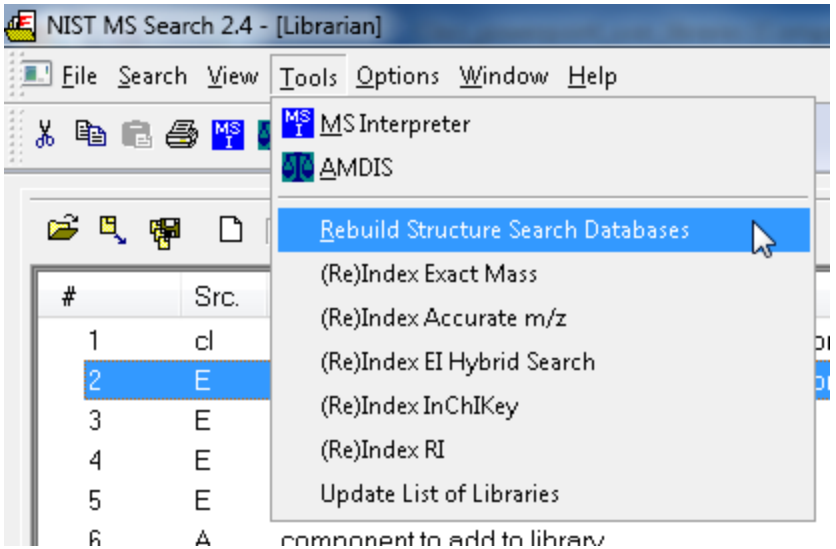
Syn.tag	MSP file tag	MS Search display
$:00	Spectrum_type	Spectrum type
$:01	Compound_type	Compound type
$:02	Ion_name	Ion name
$:03	Precursor_type	Precursor type
$:04	PrecursorMZ	Precursor m/z
$:05	Collision_energy	Collision energy
$:06	Instrument_type	Instrument type
$:07	Instrument	Instrument
$:08	Special_fragmentation	Special fragmentation
$:09	Sample_inlet	Sample inlet
$:10	Ionization	Ionization
$:11	Ion_mode	Ion mode
$:12	Collision_gas	Collision gas
$:13	Pressure	Pressure
$:14	Mass_range	Mass range
$:15	Maximum_intensity	Maximum intensity
$:16	Cone_voltage	Cone voltage
$:17	AUX	AUX
$:18	Link	Link <= never displayed
$:19	Ion_Formula	Ion Formula
$:20	Ion_MW	Ion MW
$:21	Charge	Charge
$:22	Salt	Salt
$:23	Known_impurity	Known impurity
$:24	Related_CAS#	Related CAS#
$:25	Salt/mix_CAS#	Salt/Mix CAS#
$:26	Peptide_sequence	Peptide sequence
$:27	Peptide_mods	Peptide mods

e.g. For ion mode, put $:20P, the field number is 20 and the value is P for positive, take a look at some of the fields in typical hr_msms library entry

After Additions or Creating a New User Library
(Re)Index Indices for Structure, Hybrid Search, InChIKey for User Libraries

- This is ***critical step*** to create index files needed for proper searching after adding an entry to a library
- ***Only*** the “simple” library identity searches will work ***without*** this step for MSMS spectra
- Typically update the “Rebuild Structure Search Databases” and possibly I”nChiKey”for MSMS spectra
- MSMS spectra cannot be (Re)Indexed for MSMS Hybrid mode internally, only EI Hybrid
- This requires ***either*** a batch file command as part of Automatic Nightly Distribution Process or a ***manual approach*** using a two step ***export/import using Lib2NIST***
- “Update of List of Libraries” makes a newly created library appear in NIST program ***without*** first having to close program

Note: EI only inside NIST program, MSMS external batch file approach as part of nightly distribution process



Automatic Network Distribution of Eastman User Libraries

Software Essentials and Approach

No Expensive Hardware, Software, or Licenses!

- DOS files written by user[5] such as Get Lib, Send Lib, etc.
- DOS files interact with Lib2NIST utility supplied by NIST
- Process managed by inexpensive Windows scheduling program
- Individual User libraries ***automatically*** merged, distributed and archived ***daily***
- Additions and any new entries available to all users worldwide

Users

Get Lib

1) Users send files for help
2) MS Expert sends results in PDF files, adds new entries to library

Standard Corporate Network and Servers

1) Get Lib
2) Send Lib

1) Merges user libraries
2) Sends merged library to server
3) Sends archive copy to server

Standard Computer automatically merges and archives corporate Library using DOS batch files

MS expert

Excerpt of Typical DOS Script[5]

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

Live Demo on YouTube
LC/MS Unknown Identifications Using MSMS Libraries
Part VII: Using and Creating Other MSMS Libraries

Webinar References (*Internet Links*)

1. *James Little Mass Spectral Resource Website*
2. *Chemical Ionization for MW Determination*
3. *Trimethylsilyl Derivatives for GC-MS*
4. *Methyl Ester Derivatives for GC-MS*
5. *SciFinder/ChemSpider and Accurate Mass LC-MS Data for Unknown ID's*
6. *Surfactant Identification*
7. *Lipid Matrix Ionization Effects in LC-MS*
8. *MassBank of North America Overview*
9. *MassBank of North America Downloads*
10. *Lib2NIST Documentation*
11. *Tandem NIST Search Quick Start Guide*
12. *MoNA MSMS Library in Hybrid NIST Format*
13. *MoNA EI Library in NIST Format*
14. *Components in MoNA Libraries*
15. *PowerShell Script for Adding Precursor_m/z Field to User Library*
16. *Corporate Database Critical Eastman Chemical Co. Asset*
17. *Nightly Automatic Update of User's Library on Corporate Network*
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