

Build a User's HRMS Library and Perform HRMS Library Search from GC Image

Introduction

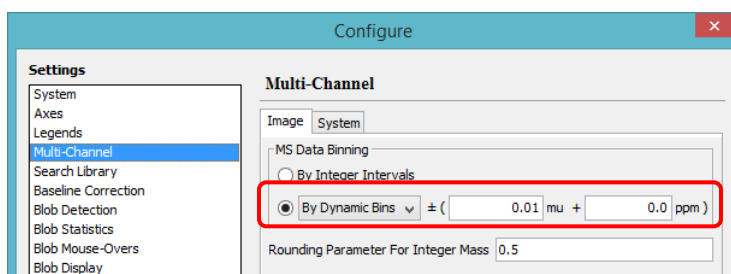
This tutorial application note describes step – by – step how to build a user's HRMS library in NIST MS Search Software 2.2 and perform a HRMS library search using the user's library from GC Image HRMS Software R2.6.

Software

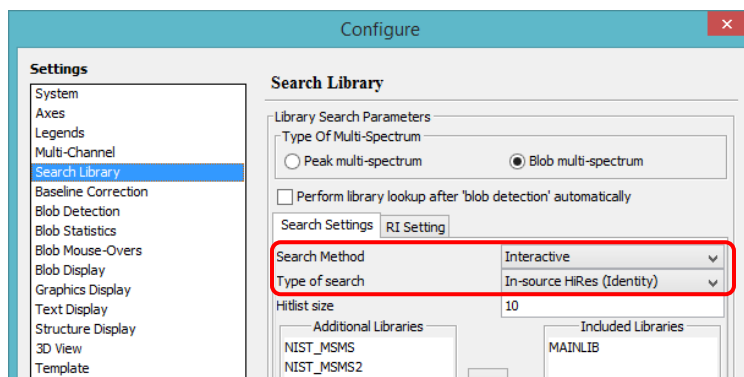
- NIST MS Search Software V2.2 with NIST 14 Library
- GC Image HRMS Software R2.6b4 or later version

Procedure

1. Configure settings in GC Image HRMS Software.
 - 1) Configure – Settings – Multi-Channel – MS Data Binning, e.g., By Dynamic Bins ± 0.01 mu



- 2) Configure – Settings – Search Library – Search Settings,
 - a. Search Method: Interactive
 - b. Type of search: In-source HiRes (Identity)



2. Configure settings in NIST MS Search Software.
 - 1) Options – Spectrum Import Options,

- in the section “Spectra without precursor ion m/z value are”, choose “In-source/EI (accurate m/z)”.
- in the section “In-source/EI accurate ion m/z”, choose the desired number of decimal places.

Spectrum Import Options

EI Spectrum m/z Rounding
 Multiply m/z in imported spectra by and round to the nearest integer
 Example: (CH₂)_n correction is 0.99888
 Optional: Add this term to all m/z before rounding

Tandem Spectrum Accuracy
 Precursor ion m/z: decimal places
 Product ion m/z: decimal places
 In-source/EI accurate ion m/z: decimal places

Adding spectra to Spec List
☒ Prepend (add to the top)
☐ Overwrite (replace)
☐ Ask

Intensity threshold
☐ % of max.
☐ absolute

Spectra without precursor ion m/z value are
☐ EI (nominal m/z)
☒ In-source / EI (accurate m/z)

RI type if unspecified:

☐ Include Synonyms

2) Options – Library Search Options – Search

- In “Spectrum Search Type”, choose “In-source HiRes”.
- In “Presearch”, choose “Off”.

Library Search Options

Search | MS/MS | Libraries | Automation | Limits | Constraints | RI (GC)

Spectrum Search Type
☒ Identity ☐ Similarity
 ☒ in spectrum

Spectrum Search Options
☐ Reverse Search
☐ Penalize rare compounds

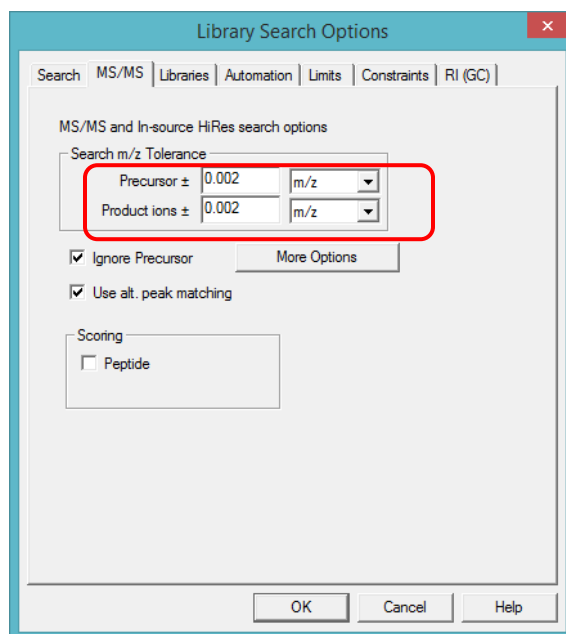
Presearch
☐ Default ☐ Fast ☒ Off
 MW

Other Options
☒ Automation
☐ Auto Report
☐ Apply Limits
☐ Use Constraints

Structure Similarity Search Options
☒ Match Number of Rings ☒ Show Homologues

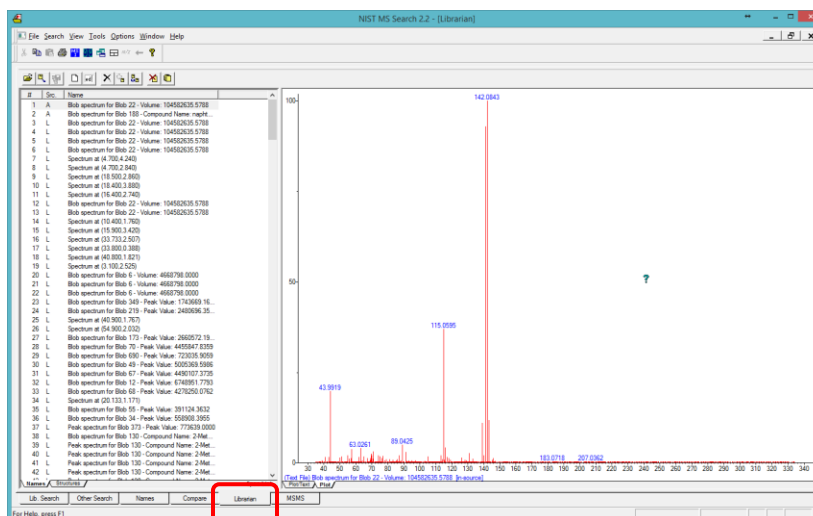
3) Options – Library Search Options – MS/MS

In “Search m/z Tolerance”, input the desired mass accuracy tolerance for search.

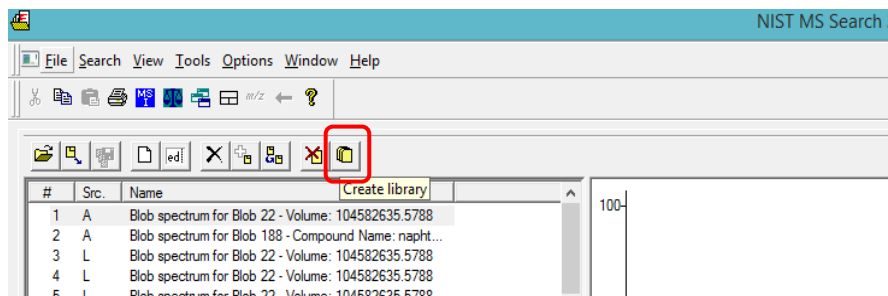


3. Create a user's library in NIST MS Search Software

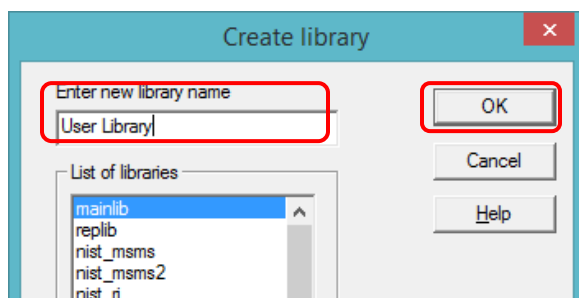
1) In NIST MS Search main page, choose “Librarian” tab.



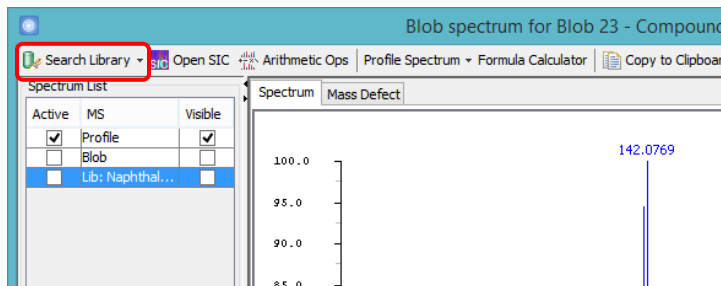
- 2) Click on “Create library” icon.



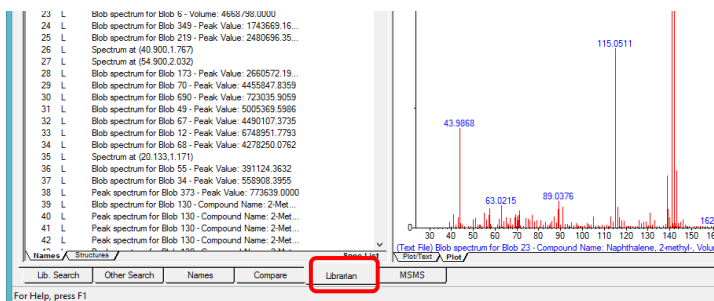
- 3) Enter a new library name, then click “OK”.



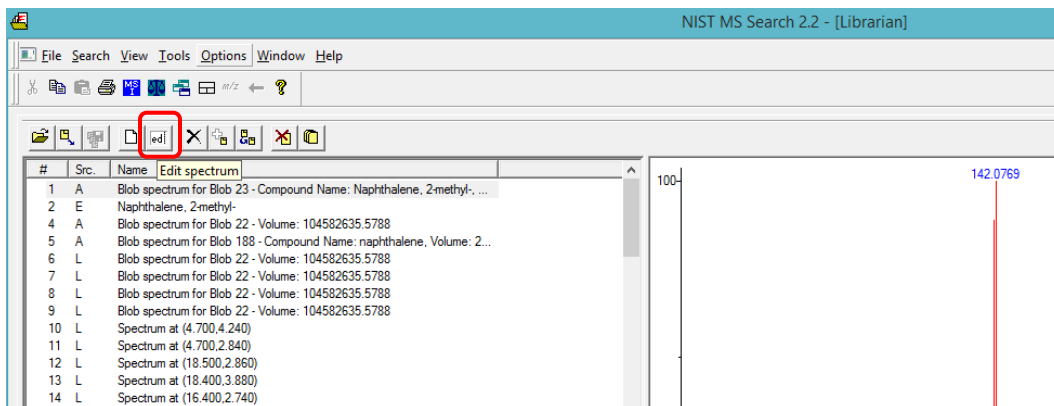
4. Add HRMS spectra into user’s library
 - 1) In GC Image Software, open a mass spectrum.
 - 2) In GC Image MS Viewer, perform a library search. The mass spectrum is sent automatically to the NIST MS Search Software.



3) In NIST MS Search, choose “Librarian” tab.



4) If you want to edit the mass spectrum before adding into a library,
a. Click on the “Edit spectrum” icon.



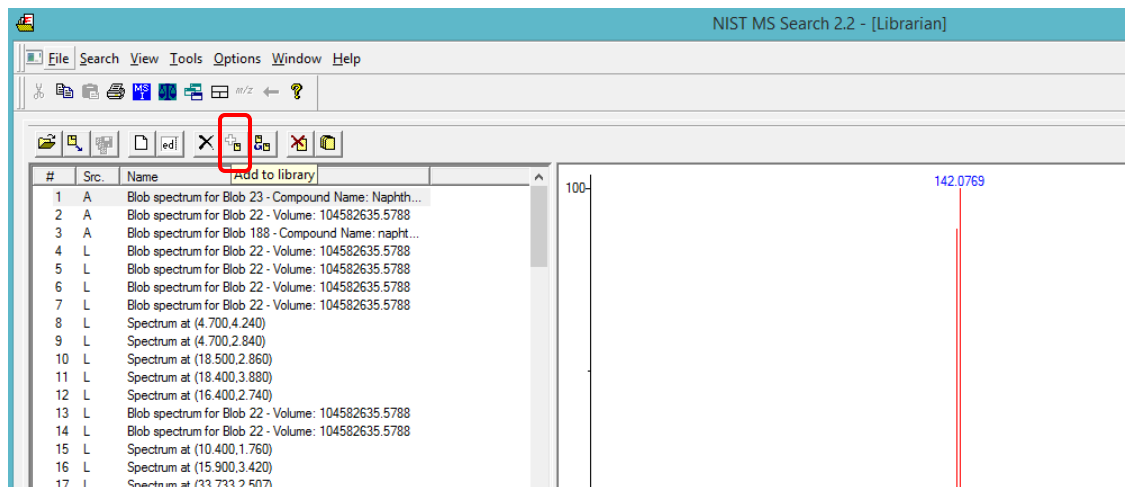
b. After editing, click “Add to Library”.

The screenshot shows the 'Spectrum Information' dialog box. The 'Name' field is set to 'Naphthalene, 2-methyl-'. The 'Formula' field is 'C11H10'. The 'Mol. Weight' is 142, and the 'CAS Number' is 91-57-6. The 'Add to Library' button is highlighted with a red box. The 'Peak information' table shows the following data:

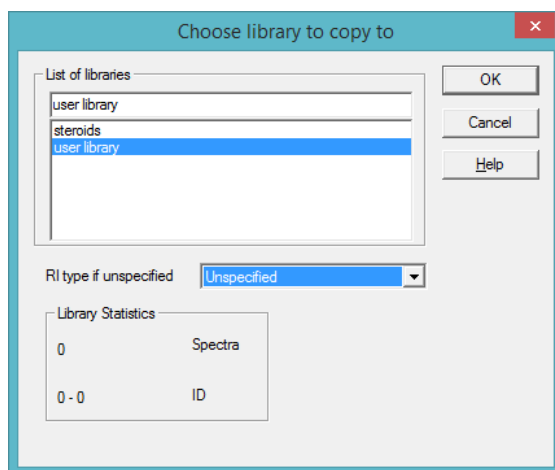
m/z	Abund.	Annotation
39.0145	1.00	
39.0181	7.00	
39.0217	12.00	
39.0253	10.00	
39.0289	5.00	
39.0325	2.00	
39.0361	1.00	
39.0397	1.00	
39.0596	1.00	

The 'Attach Struct' button is also visible, and the chemical structure of Naphthalene, 2-methyl- is shown at the bottom.

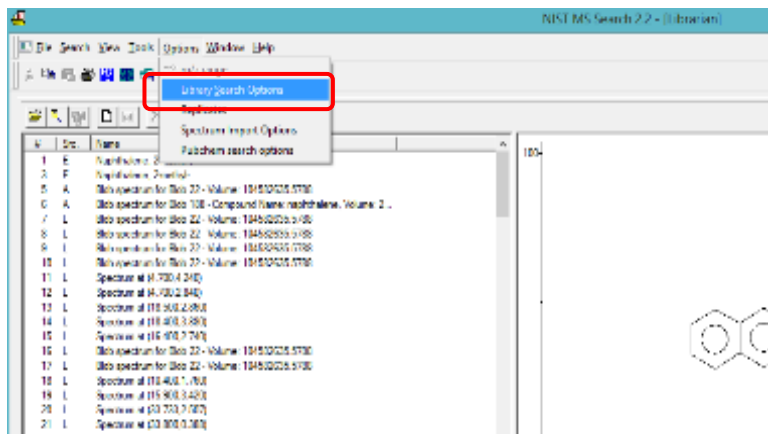
- 5) If you don't want to edit the mass spectrum before adding it to the library, click on "Add to library" icon.



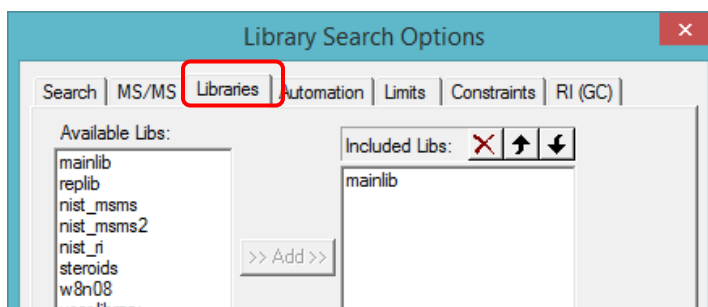
- 6) Choose the library to add the spectrum.



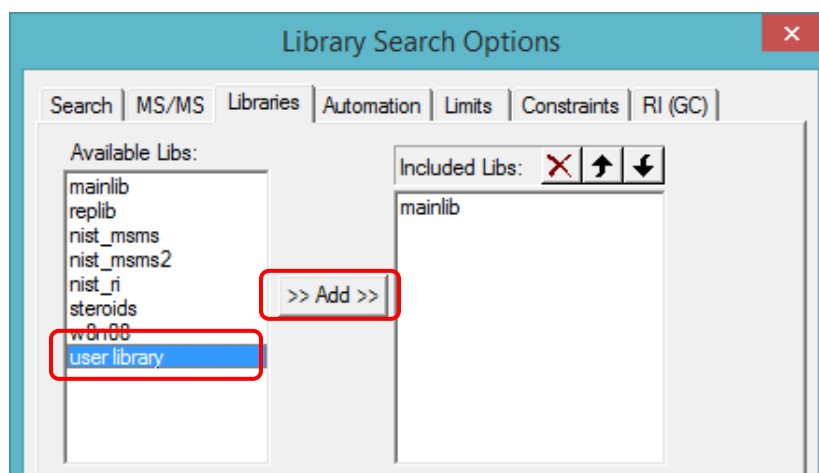
5. Perform HRMS library search from GC Image HRMS Software
 - 1) In the NIST MS Search Software, include the user library in the search library list.
 - a. Choose Options – Library Search Options.



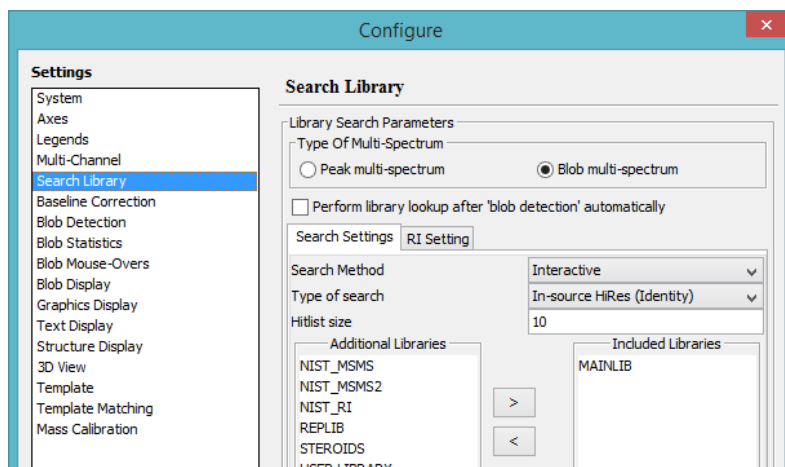
- a. Click on “Libraries” tab



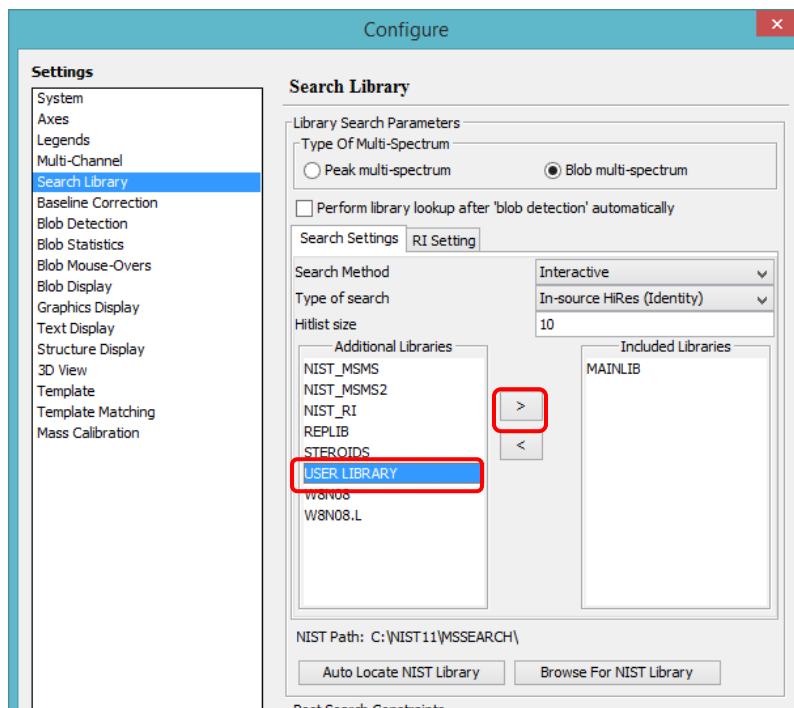
- c. Choose the user library in the left panel, then click “Add” to add the user library to the included libraries list



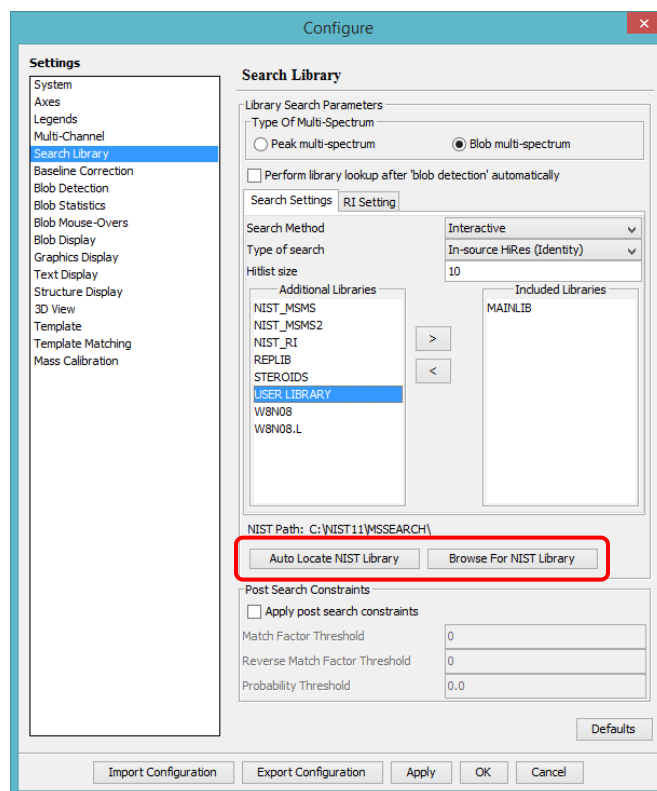
- 2) In GC Image HRMS Software, include the user library in the search library list.
 - a. Choose Configure – Settings – Search Library.



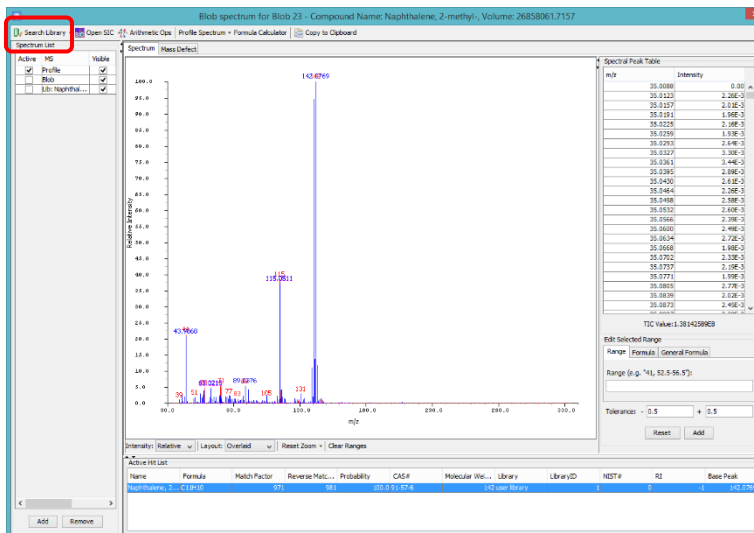
- b. Choose the user library in the left panel, then click ">" to add it to the Included Libraries.



- c. If the user library is not on the Additional Libraries list, click “Auto Locate NIST Library” or “Browse For NIST Library” to locate the user library.



- 3) Perform a HRMS library search from GC Image MS Viewer



- To perform a unit mass library search, Choose Configure – Settings – Search Library in GC Image and set the Search Method to Batch

