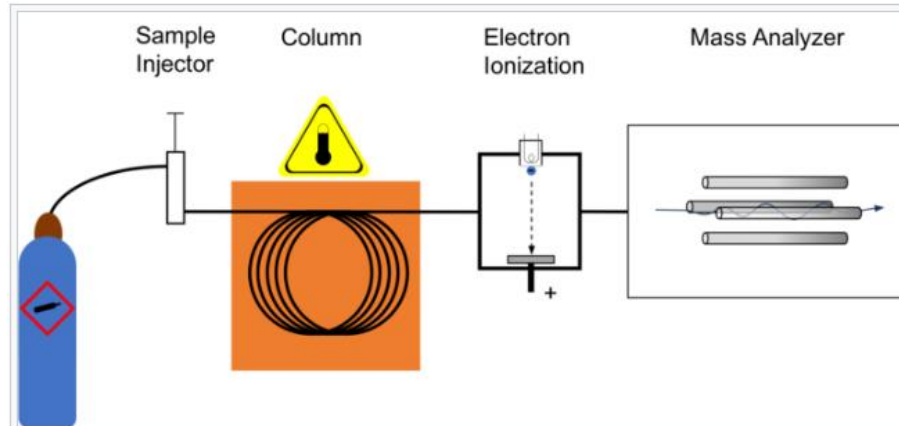


Free NIST GC-MS Software Lab for Universities:

Part 8: Advanced Processing with NIST Software



James Little

August 29, 2023

38 years Eastman Chemical Company

7 years Mass Spec Interpretation Services

<https://littlemsandsailing.wpcomstaging.com/>

[Link to GCMS Schematic Above](#)

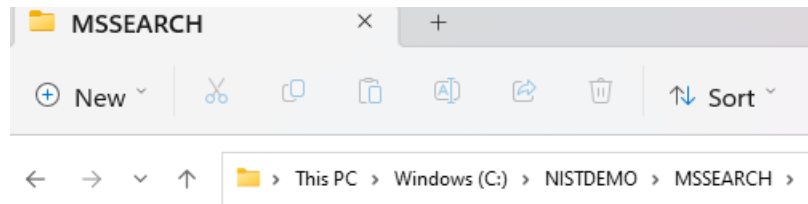
[Link to University Logos](#)

Topics

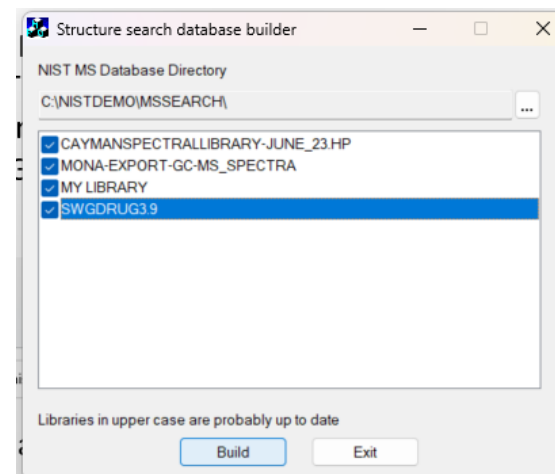
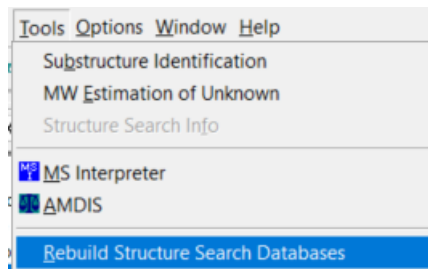
- Use MONA library of over 18,000 EI Spectra and structures within Demo software
- Add SWGDRUG Library, library of drugs and drug related compounds (>3,500 spectra)
- Cayman EI library of >2,000 emerging forensic drug standards
- Buy full version of NIST search, *SHOP around*, prices vary widely!
- Take my advanced Course on NIST search, better for purchased version, but useful for Demo also
- Demo and purchased version processes MSMS data
- MONA database available for MSMS, instructions on my website for NIST software

MONA, SWGDRUG, and Cayman

- MONA, SWGDRUG, and Cayman add ~27,000 additional EI spectra and structures in NIST demo search program
- The Main NIST library delivered with Demo program has ~2,400 spectra
- MONA EI library available on my website in NIST has ~19,000 EI spectra
- The SWGDRUG and Cayman libraries will need to be downloaded by user
- All need to be placed at the following location:



- Make sure that the index files are placed in the proper place as shown in video
- If not, they **will not** search!
- Make sure to update their structure indexes



[Link to MONA EI download on my website](#)

[Link to MONA EI original download site](#)

[Link to SWGDRUG EI library Download Site](#)

[Link to Cayman library download site](#)

Purchase of NIST 2023 MS Search and Library

- Consider buying one copy and putting on your GCMS system at school
- Users will find very valuable in unknown identifications
- **Shop around**, prices will vary more than you can imagine!

NIST/EPA/NIH EI-MS Library, 2023 release

394,054 electron ionization (EI) spectra

- 347,100 compounds, 46,954 replicate spectra
- 40,231 more compounds than NIST 20

491,790 retention index (RI) values

- 180,610 RI compounds – 40 K increase
- 153,472 compounds with both RI & MS

[Link to List of Vendors](#)

Advanced Training for NIST Search on My Website

- Very useful for more detailed training in use of Demo version
- Great resource if you buy full copy of NIST search and associated EI reference libraries!
- Start with Part 0 if using Demo version, Part I if purchased 2023 version
- Take a close look at NIST Hybrid Search, Part IV
- Two test spectra of Theobromine and Xanthine that are not found with standard search!
- Delta mass values from hybrid search easily point to their identified
- Change from Identity to Similarity/hybrid search in Library Search options window, then Go
- Note the delta mass value of 14 for Theobromine indicating difference in methylene group
- Note the delta mass value of 16 for Xanthine showing difference of hydroxy group

The webinars demonstrate both Versions 3.0 (2023) and V2.4 of the NIST search. If you are using V3.0, start with Part 0. If you are using V2.4, start with Part I.

Videos:

Part 0: Changes in EI NIST23 Program (V3.0)

Part I: Spectral Searches with NIST MS Search

Part II: Structure Searches with MS Search and Using MS Interpreter

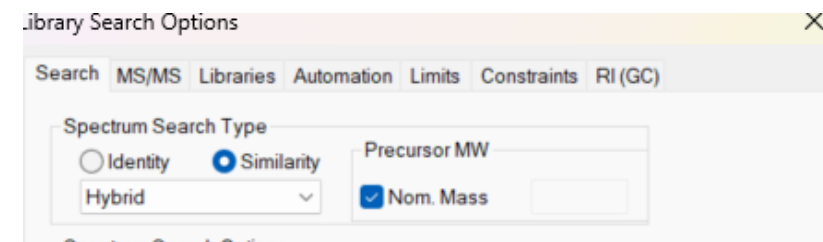
Part III: AMDIS (NIST) for Processing EI Mass Spectral Data Files

Part IV: Advanced NIST Hybrid Search of EI and MS/MS Spectra

Part V: Creating and Sharing User EI and MS/MS Libraries

Part VI: Creating and Using Retention Indices in NIST Software

| | | |
|---|---|-------------|
| 4 | L | Theobromine |
| 5 | L | Xanthine |



[Link to Advanced Training NIST Search Website](#)

➤ MSMS (Tandem) NIST Library Searches

- The demo version of the software will do MSMS searches to identify unknowns analyzed by LC-MS
- Not demo libraries sent with the Demo version
- AMDIS cannot not process LC-MSMS data files
- Most manufacturers can export to NIST MS Search program
- MONA free MSMS library available on my website
- MSMS advanced training for V2.4 available on my website
- NIST 2023 comes with both EI and MSMS libraries plus version 3 of the NIST search

NIST Tandem Mass Spectral Library, 2023 release

- 51,501 compounds
- 60% increase over the 2020 release
- 399,267 precursor ions
- 2.4 million spectra

Fragmentation methods

- 49,590 HRAM (high res accurate mass) compounds
- 51,292 QTOF, HCD, IT-HRAM, QqQ compounds
- 49,561 ion trap compounds (low res., up to MS⁴)
- 561 APCI HRAM “extractables and leachables”

Precursor ion types

- 44,191 protonated
- 19,620 deprotonated
- 14,318 water/ammonia loss
- 44,547 other in-source generated

[Link to Advanced MSMS training on my website](#)

[Link to MONA MSMS library on my website](#)