NIST26 *FREE* Demonstration (Demo) Copy of EI GC-MS Integrated Processing

Video/Handout

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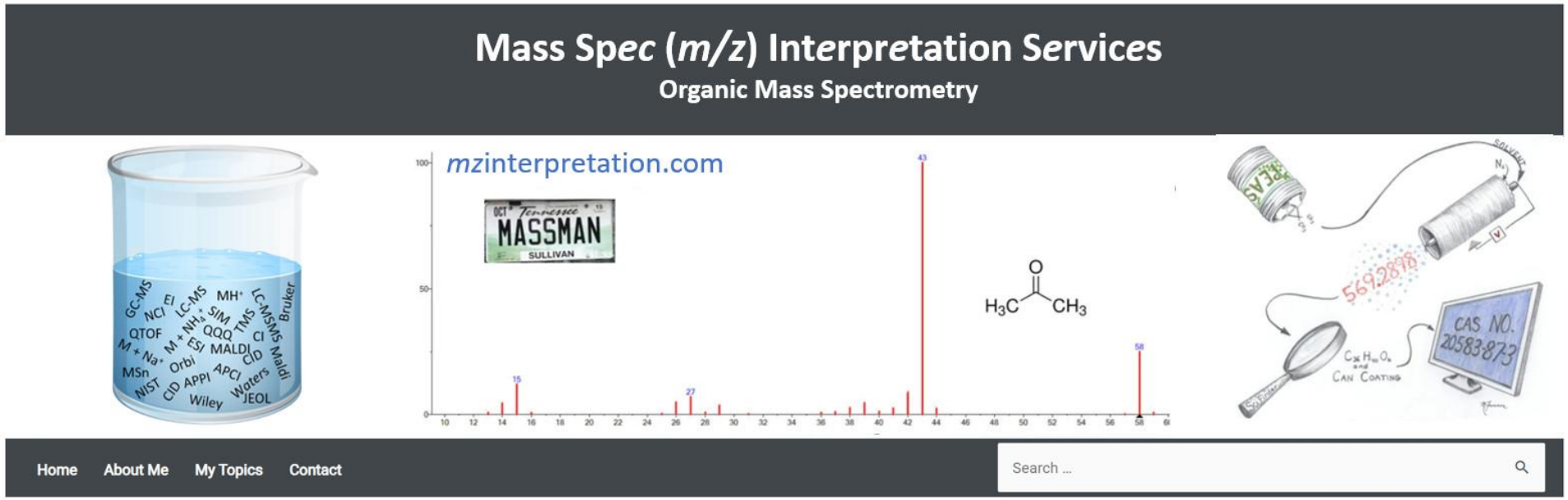
See *Full Course* on NIST26 with new *Integrated* Deconvolution/Library Searching for *EI GC-MS* and *LC-MS/MS*!



Overview

- Fully functional NIST26 EI GC-MS Demo copy
- Demonstrates new integrated AMDIS
- NIST26 Search Chromatogram Tab
- Deconvolution and Library Search together
- AMDIS Stand-Alone ***NOT*** Included
- ***Be aware*** of Win.ini instructions on next page

Topics in Video and Associated Handout:

- Installation of software
- Win.ini concerns
- Location of files
- Content of My Free Libraries
- FREE EI libraries and their relative quality vs. NIST26 libraries
- Demo of 2 test files, nominal and high resolution
- Use of older versions of library with NIST26 Demo Program

Resources:

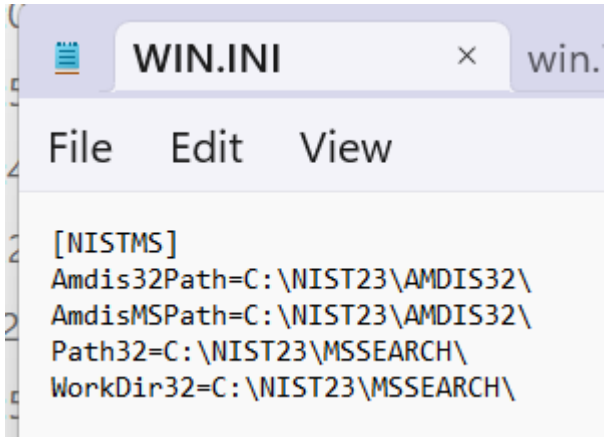
- Fully functional download from NIST, *link to NIST website*
- AMDIS Stand-Alone ***NOT*** Included
- EI GC-MS nominal mass and accurate mass demo files, see location in following slides
- NIST Demo library of 2,373 EI spectra and associated structures
- My additional FREE EI libraries of ~58,000 EI spectra and ~33,000 structures, *link to my website*

Note: ***Included FREE libraries do not compare to NIST EI libraries in either quantity or quality,***

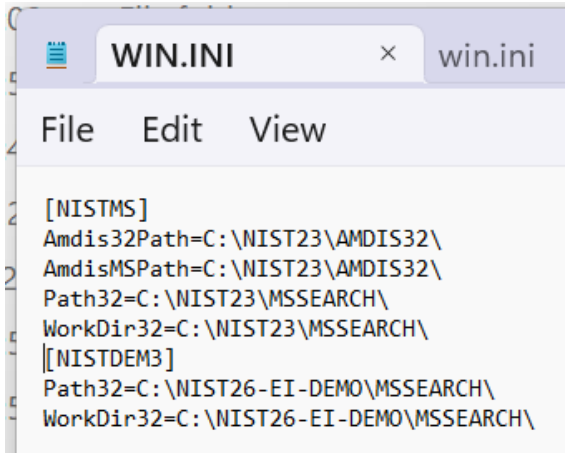
Possible Problems Installing/Uninstalling with Win.ini, especially if previous version of NIST Present (1 of 2)

- ***Make backup copy before installing and make sure use to replace win.ini after uninstalling***
- When downloading the EI demo when previous version of NIST 23, the win.ini is changed
- Can possibly cause issues with the original version, e.g., NIST23, but could be even earlier version
- Thus, be sure to return to original state when *UNINSTALLING* EI demo when evaluation finished
- Originally for NIST23, the win.ini appeared as below as opened in notepad
- Could be different if one uses vendor importing of spectral files for searching to NIST Lib Search
- *REPLACE* with your win_backup.ini file when evaluation finished
- Or edit after finishing when *UNINSTALLING* to remove the EI Demo changes and *MAKE* it the *SAME* as your win_backup.ini file
- Whichever, c:/windows/win.ini is a protected folder
- Requires some administrative privileges
- Might need to take outside that folder and edit
- Then drop it back in C:/windows folder to overwrite it
- ***VERY*** important to make sure file type (extension, .ini) is correct!
- Cannot be save as text, see ***NEXT*** slide

Before Installation

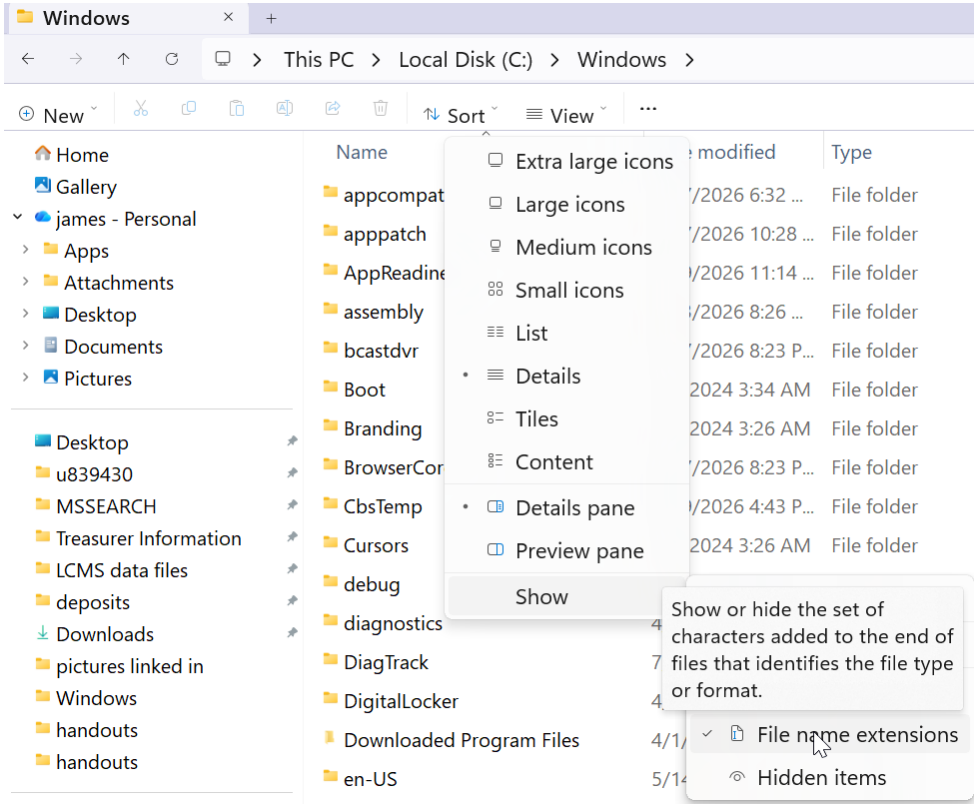


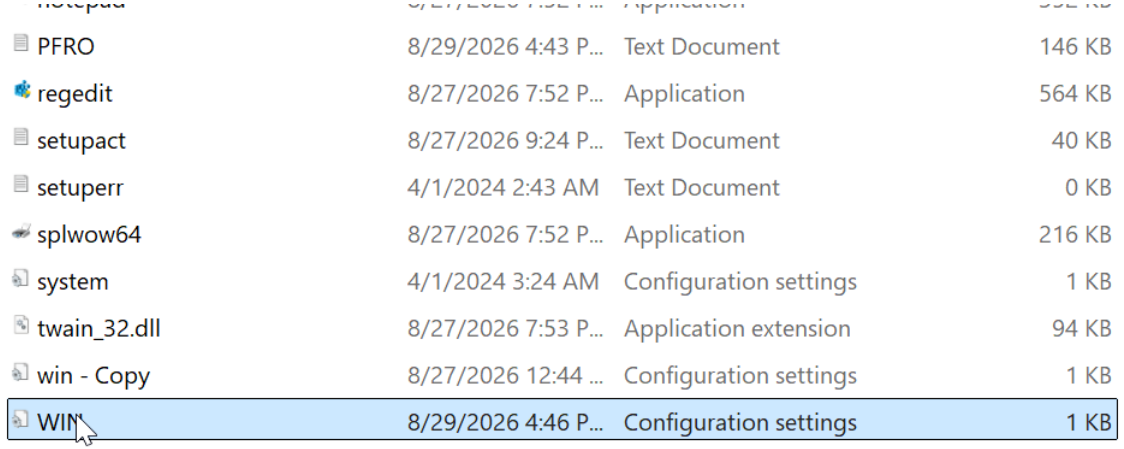
After Installation



Possible Problems Installing/Uninstalling with Win.ini, especially if previous version of NIST Present (2 of 2)

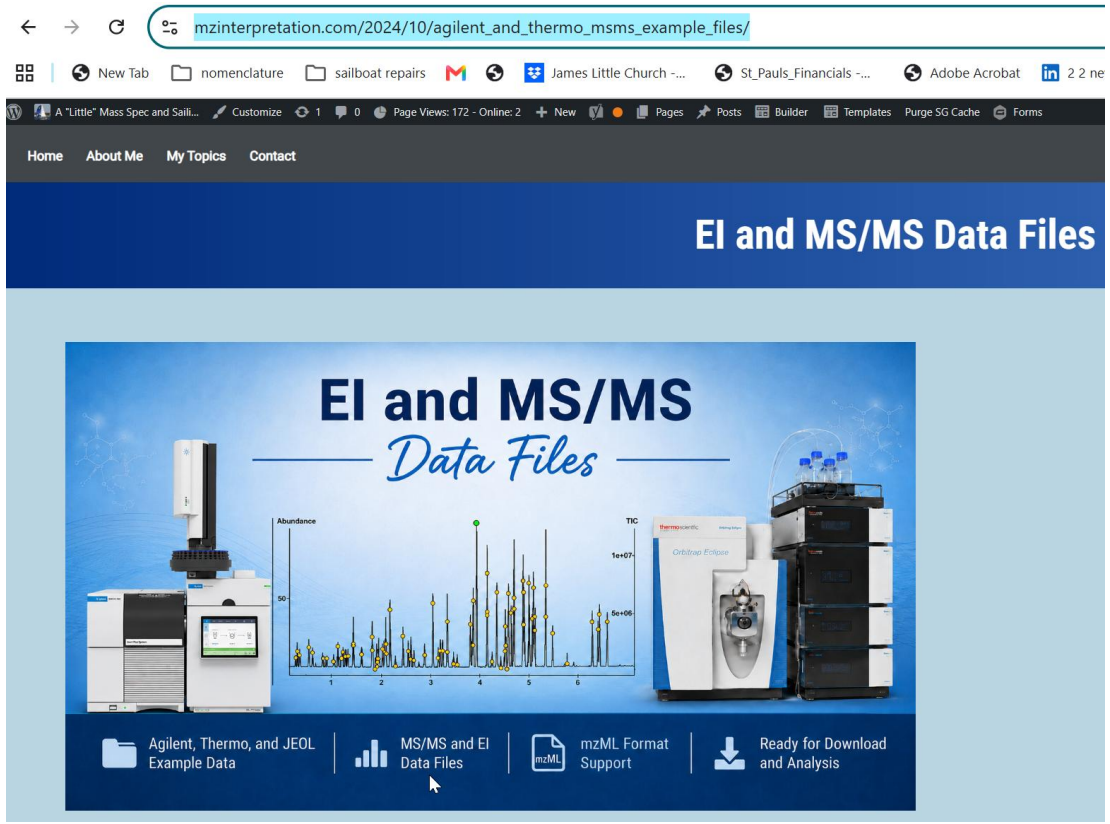
- Make sure after editing, it is still an .ini file extension (Configuration Settings), NOT, .txt, Text Document
- Show file configurations while doing operations!





Demo Files Location for Nominal Mass
Users' Files Kept in *Any* Location

- All EI Files found on my website at following *Link*
- Some can be found as resources on NIST installed software program
- Files can be downloaded to any folder
- User could then browse to that folder from NIST program
- Both nominal (low-resolution) and high-resolution examples

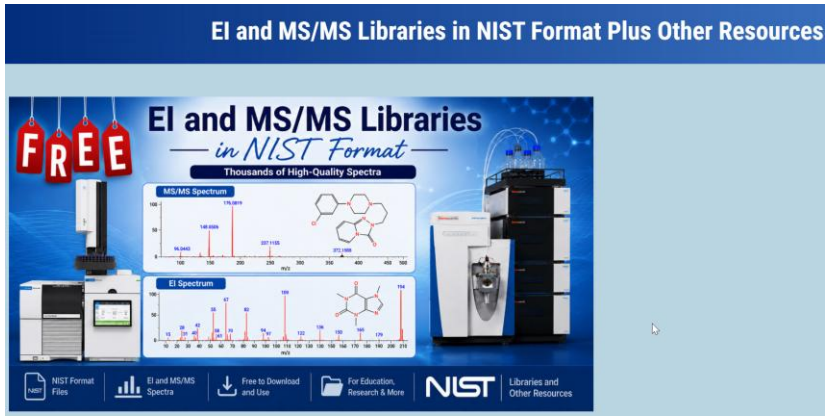


EI GC-MS Test Files netCDF and Agilent Formats

EI General Files
EI Drug Case Files
NIST Tutorial Files
High Resolution Files
Other Misc. Files

Library Files *Must be Kept* in NIST-EI-DEMO/MSSEARCH Folder

- Libraries are found at the following ***link***
- Must be downloaded in specific location to be accessed by NIST Program



This PC > Local Disk (C:) > NIST26-EI-DEMO > MSSEARCH >

Sort View ...

Name	Date modified	Type	Size	
SWGDRUG_3.13	6/24/2026 8:07 P...	File folder		← Free Library from My website
RunAmdis	6/24/2026 12:07 ...	File folder		
MSPepSearch	6/24/2026 12:07 ...	File folder		
MONA_GCMS	6/24/2026 8:07 P...	File folder		← Free Library from My website
misc_libs	6/24/2026 8:07 P...	File folder		← Free Library from My website
mainlib	6/24/2026 12:06 ...	File folder		← Demo Library supplied by NIST
identifications	6/24/2026 4:56 P...	File folder		
high-res	6/24/2026 12:07 ...	File folder		
Cayman_library	6/24/2026 8:07 P...	File folder		← Free Library from My website
bb	6/24/2026 8:07 P...	File folder		← Free Library from My website

Caution in Use of My FREE EI Libraries

- Always be skeptical of results, especially with my lower quality FREE EI libraries
- However, there can be errors in any EI library including commercial ones
- Library results yield a *proposed structure*
- An *aid to identification*
- User must carefully interpret the final results
- Consider sample origin, other related species in sample, organic chemistry, etc.

Library Name	No. EI Spectra	No. of Structures	Quality	Comment
mainlib	2,373	2,373	Very good	Library from NIST supplied with Demo
SWGDrug_3.13	3,598	3,593	good	Library downloaded from internet, drug related
Cayman	2,262	506	good	Library downloaded from internet, drug related
Misc_lib	20,049	10,547	Unknown/ Good	From internet and Kodak library; 10,501 are Kodak ~95% good quality, remaining unknown, wide variety of compound types
MONA	18,914	18,815	good	Crowd sourced, wide variety of compound types
BB	13,634	0	good	Six peak index from ASTM and Eastman Chem. Co., wide variety of compound types, useful for low MW compounds and when no full spectrum available
Total	**60,830-2,373 =58,457**	**35,834-2373 =33,461**		**Values NOT including NIST MainLib**

My Opinion on Order of Quality

MAINLIB >>> BB* > SWGDrug or Cayman > Misc_lib > MONA

Higher Quality *Lower Quality*

*Lower relative match due to only 6 largest peaks

After Initial Evaluation, Consider Purchasing Updated or New NIST26 EI Library

NIST/EPA/NIH EI-MS Library

2026 Release

35K New NIST Measured/Evaluated Compounds

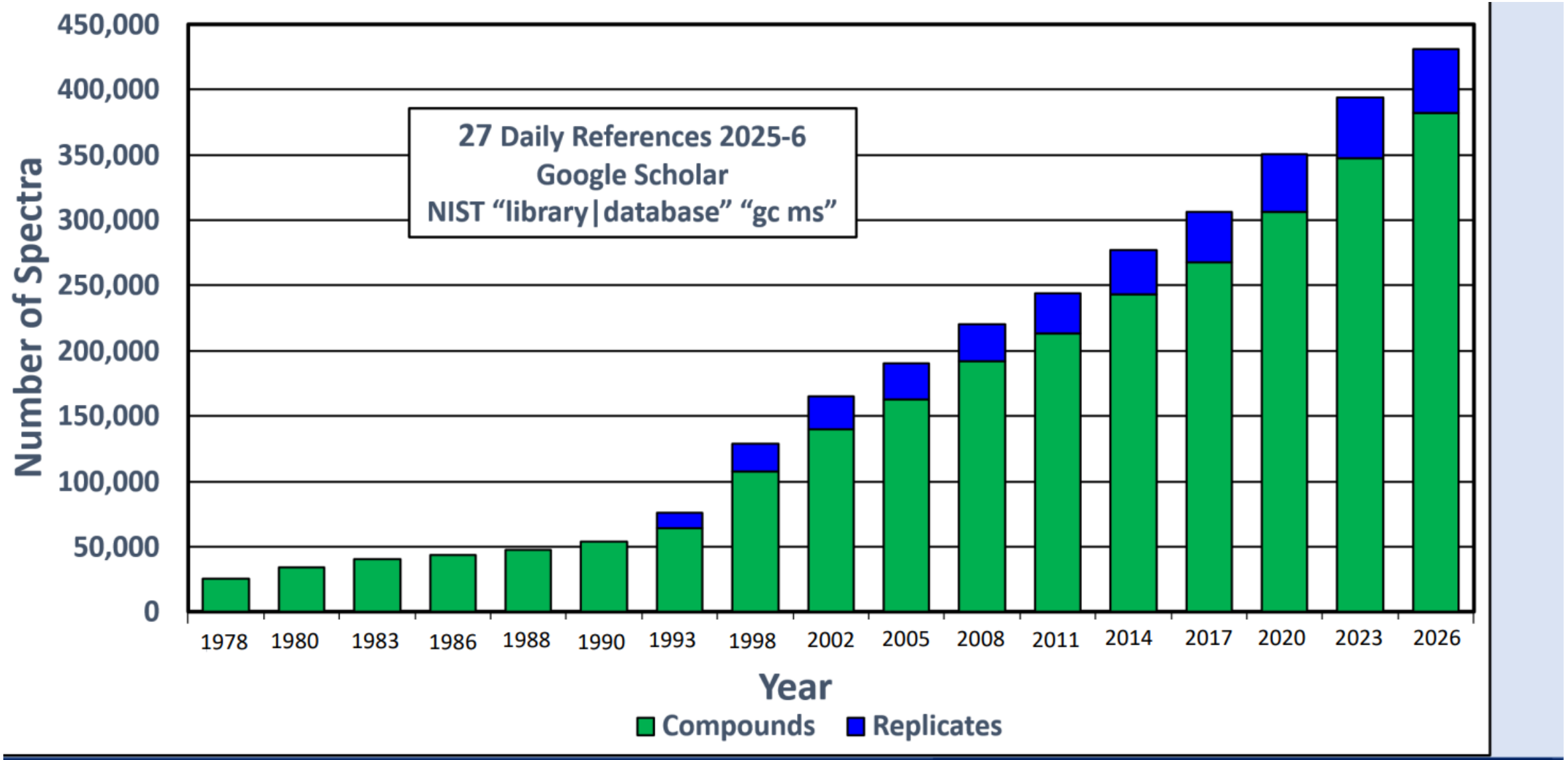
431K Electron Ionization (EI) Spectra

- 382,180 Compounds, 49,097 Replicate Spectra
- 35 K More Compounds than NIST 23

527K Retention Index (RI) Values

- 216K RI Compounds with EI, >35 K Increase
- AI-RI Estimates for All Compounds

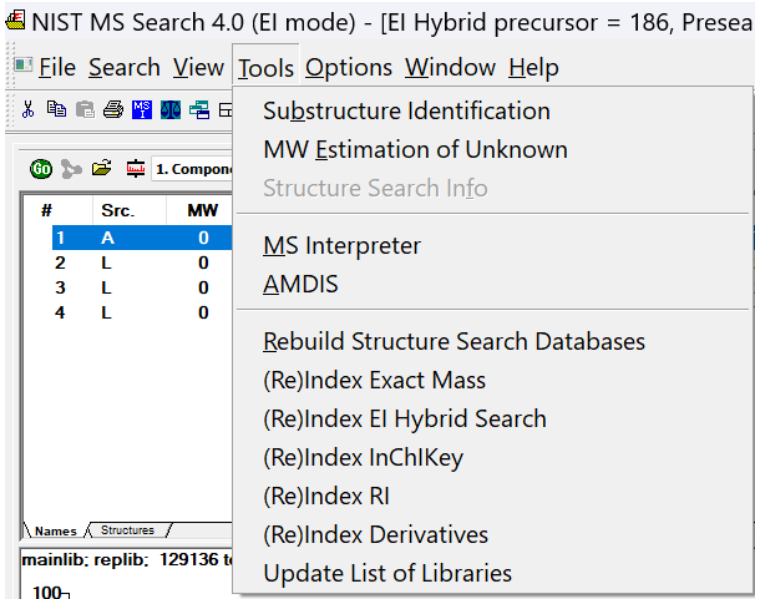
Growth Over Time of NIST EI Library



Wide Variety of New Compounds from Diverse Databases

Use of Older Versions of NIST Libraries

- Tested with NIST98 EI library of 129,136 spectra
- Remove mainlib (NIST demo library) from NIST26-EI-DEMO/MSSearch Folder
- If libraries named WinMain and WinRep in older versions
- Rename mainlib and replib
- Place library files in NIST-EI-DEMO/MSSEARCH Folder
- Run Tools and Update both mainlib and replib with (Re)Index EI Hybrid Search
- Run Tools and Update both mainlib and replib with (Re)Index InChiKey
- (Re)index makes hybrid search work, but only delta mass column shown
- ***Other newer hybrid search functions such as dForm and pctRelForm not populated***



Found in Lib Search Tab