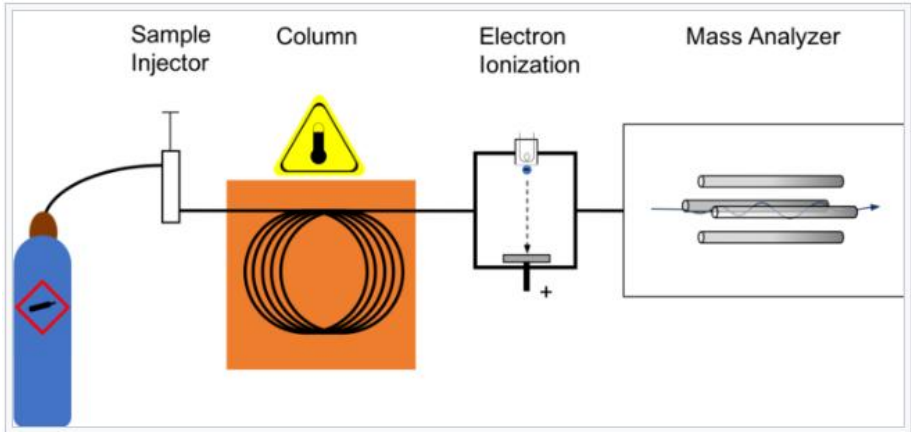
Free NIST GC-MS Software Lab for Universities:

Installation of NIST 26 V4.0 Search Software, Additional NIST EI Reference Libraries, and ACD Drawing Program



James Little

8/29/2026

38 years Eastman Chemical Company

11 years Mass Spec Interpretation Services

https://mzinterpretation.com/

Total University/Introductory Course Link

Link to GCMS Schematic Above

Link to University Logos

Installation of Resources for Course

NIST Software Program:

- Version 4.0 NIST26
- Shown ***only*** in Associated Installation Video
- Latest version no longer includes stand-alone AMDIS
- Only the newly integrated AMDIS, ***much easier*** to use than former

Additional 58,457 EI Reference Spectra with Structures

- User must *manually* download from my web page
- *Link to 58,457 EI spectra and 33,461 Structures*
- *Manually* Copy them to proper directory, NIST26-EI-DEMO/MSSEARCH

ACD Structural Drawing Software

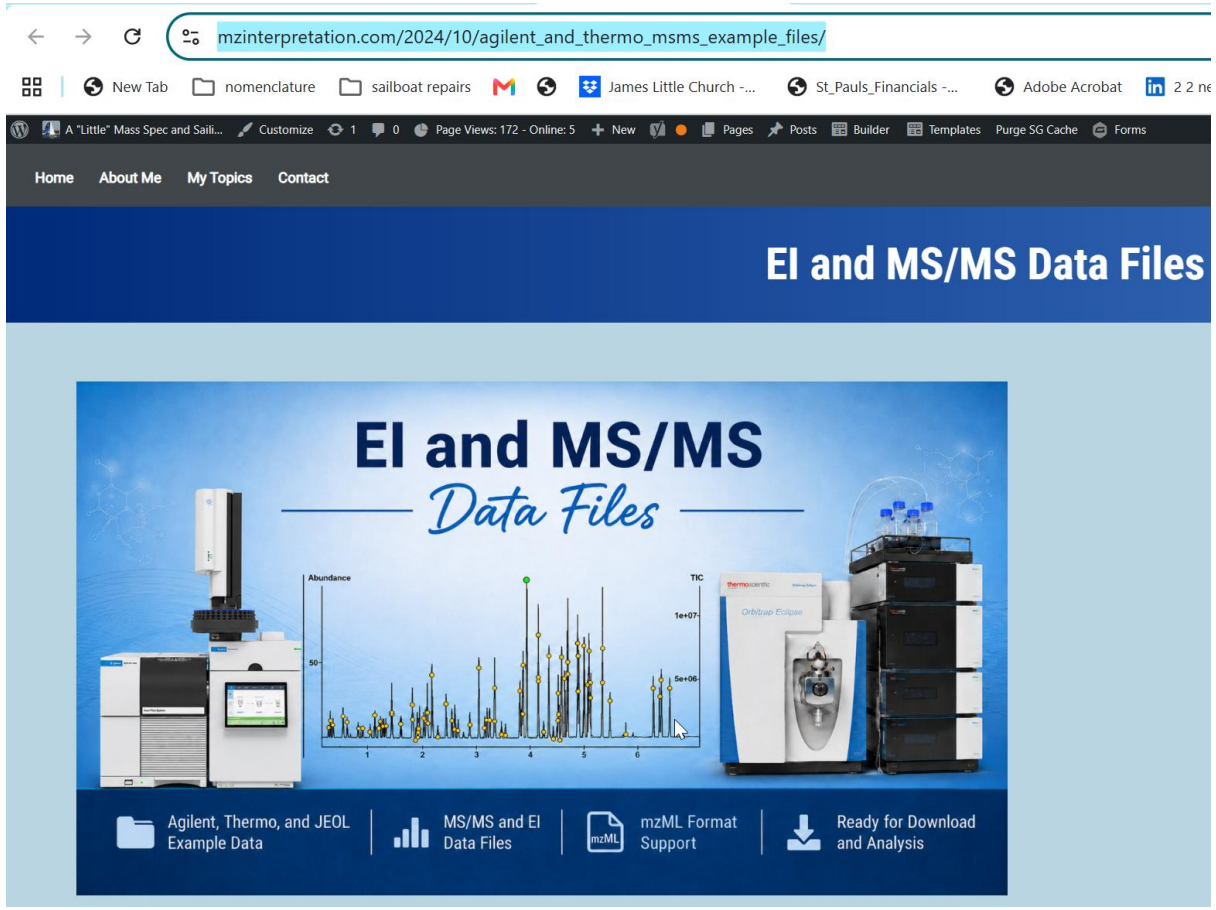
- Steps shown in this handout
- ***Not*** shown in Video

Data Files for Processing

- Often demonstration files included in folder with download of software
- These and MANY more can be found and downloaded at the following ***link***

Demo Files Location

- Can be downloaded to ANY location
- When opening, just browse to that folder
- Some file could be present from download of software
- Varies with the update sometime
- Total list of files at this ***link***



EI GC-MS Test Files netCDF and Agilent Formats

EI General Files

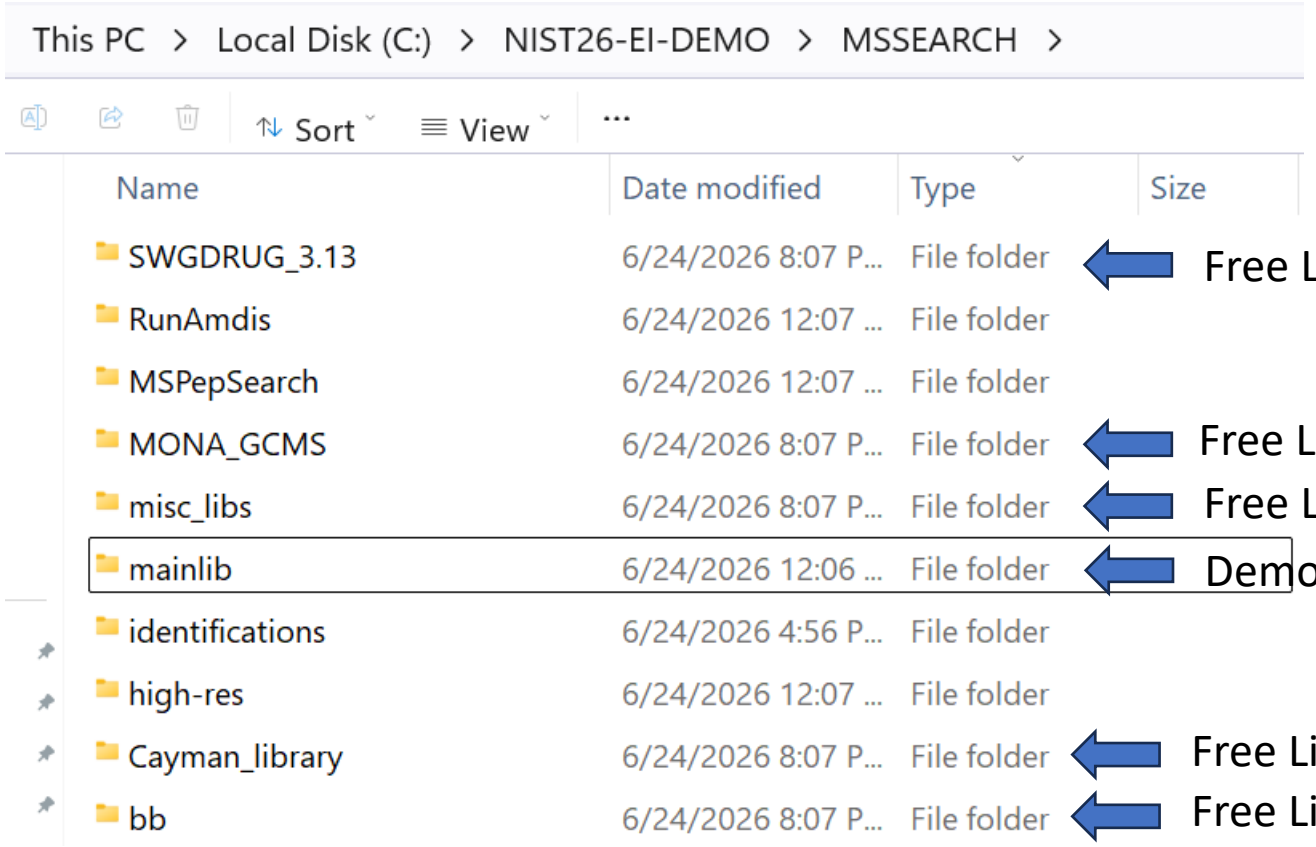
EI Drug Case Files

NIST Tutorial Files

High Resolution Files

Other Misc. Files

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



Free Library from My website

Free Library from My website

Free Library from My website

Demo Library supplied by NIST

Free Library from My website

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

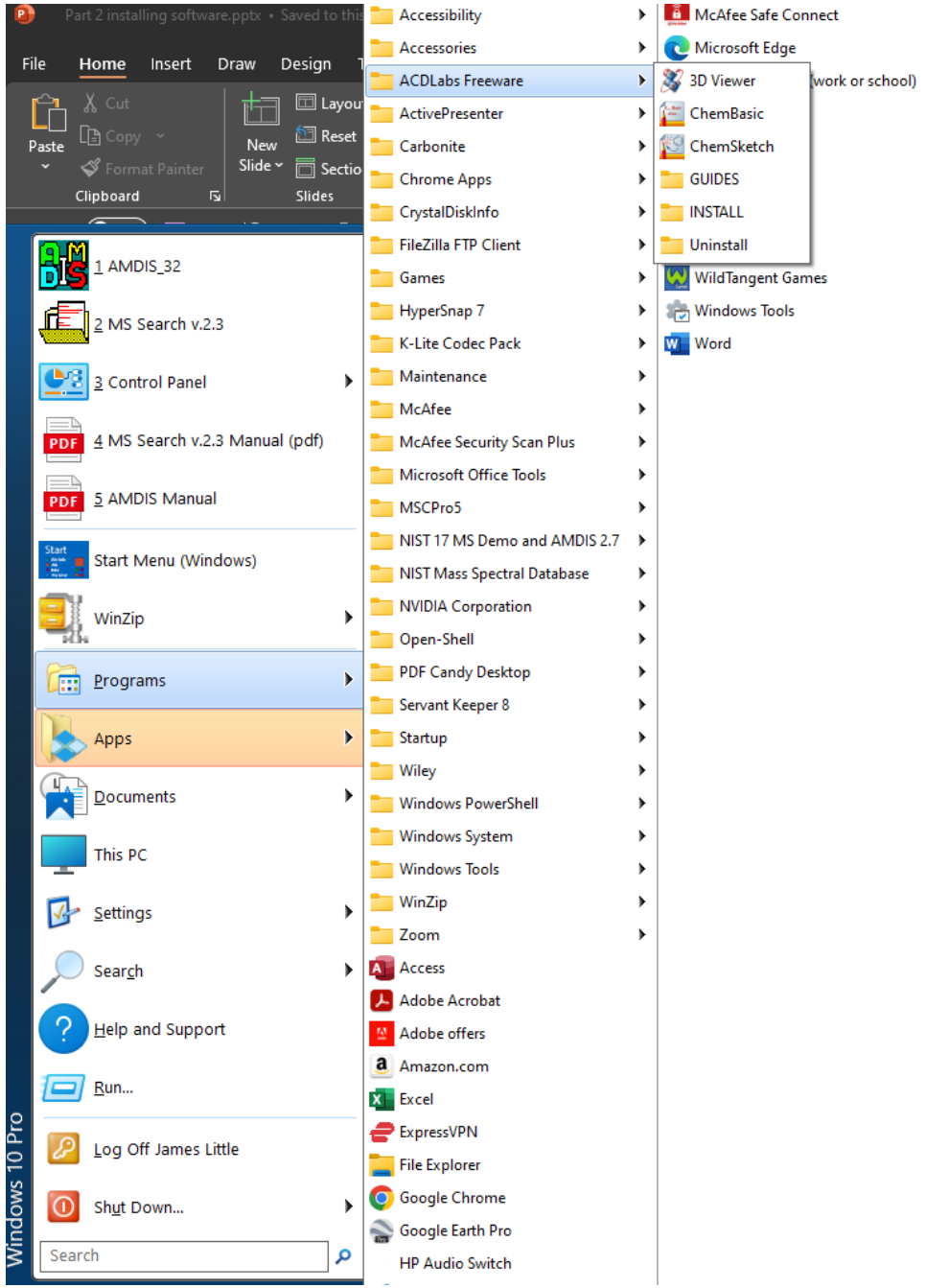
Installing ACD ChemSketch Drawing Program

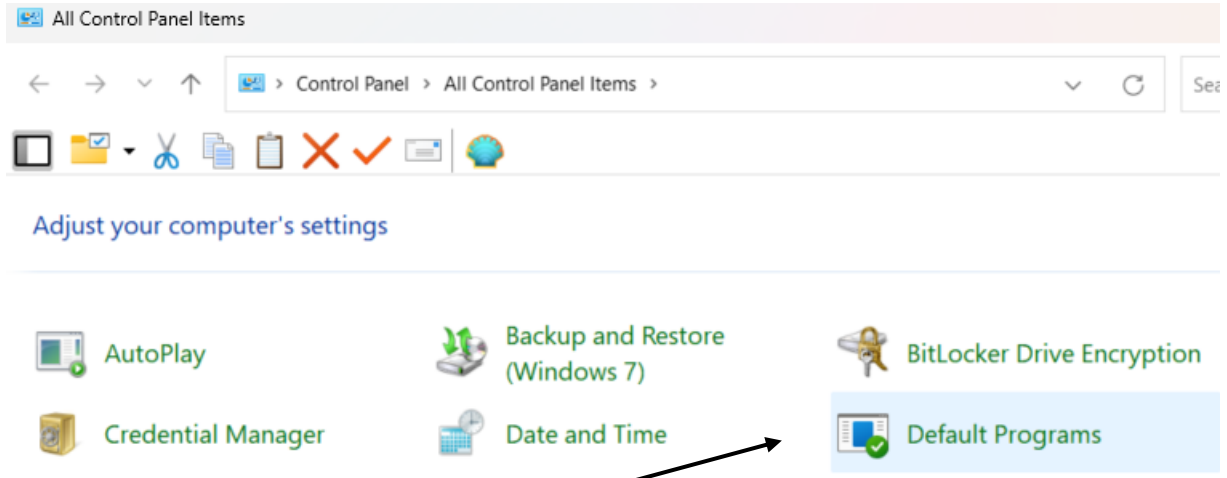
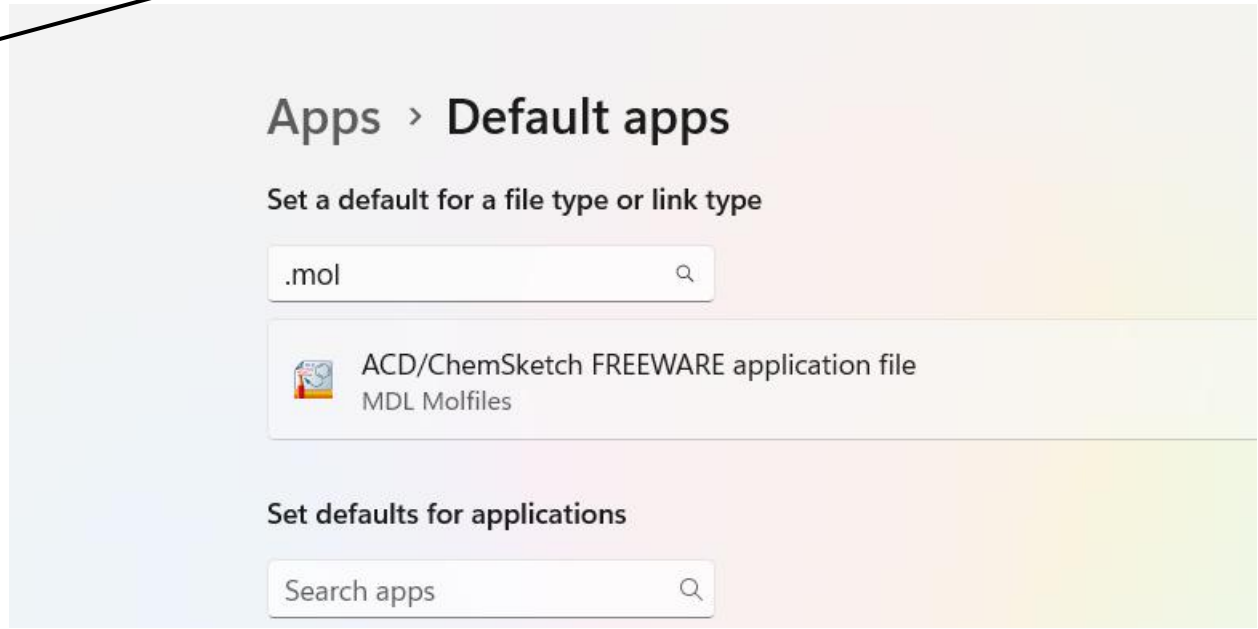
-Go to Resources on my web page at the following link

Link to Downloads

-Install ACD software by left clicking on ACD Free Software link
-ACD will download to your Download folder
-double left click on the ACDLabs202310_ChemSketch_FInstall.zip
-double left click on the file displayed
-take all the defaults
-should find the files in your program group shown on next page

Program Group Shown from Start Menu for ACD ChemSketch Free Program



Checking to Confirm that ChemSketch is Default Program for .mol file

-.mol file is the type of file used in clipboard to send files between ACD ChemSketch and NIST Programs
-Type control panel in Start menu at bottom of windows screen
-select Default Programs option
-make sure .mol uses ChemSketch
-see display to left