

James Little August 29, 2023 38 years Eastman Chemical Company 7 years Mass Spec Interpretation Services <u>https://littlemsandsailing.wpcomstaging.com/</u>

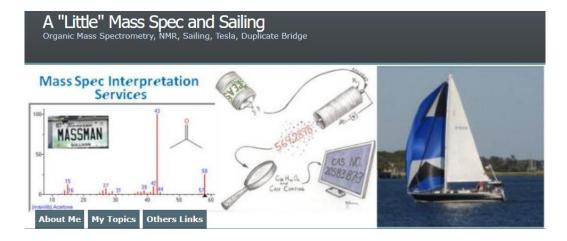
Link to GCMS Schematic Above

Link to University Logos

## Free NIST GC-MS Software Lab for Universities

Part 1: Very Basic Theory of GCMS Analyses

Part 2: Installation of Software Part 3: Library Searches Part 4: Processing GCMS Data with AMDIS Part 5: Understanding EI Fragmentation with MS Interpreter Part 6: Structure Searches with Input from ChemSketch Part 7: Creating a User Library Part 8: Advanced Processing with NIST Software



Link to Training Website

## **Installation of Software**

## NIST Software programs:

- Version 1.7 MS Search
- > AMDIS deconvolution software (data file processing)
- > MS Interpreter (correlation of EI fragment ions to compound substructure)
- > MS Search user Manual
- AMDIS user manual

## **ACD Structural Drawing Software**

# **Installing NIST Software**

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

Link to Downloads

-Scroll down to the following links

Resources

NIST Software Download ACD Free Software MONA EI Library NIST MS Search Manual NIST AMDIS Manual Full Version Training

-Install NIST software by left clicking on NIST Software Download Link

-NIST will download to your Download folder

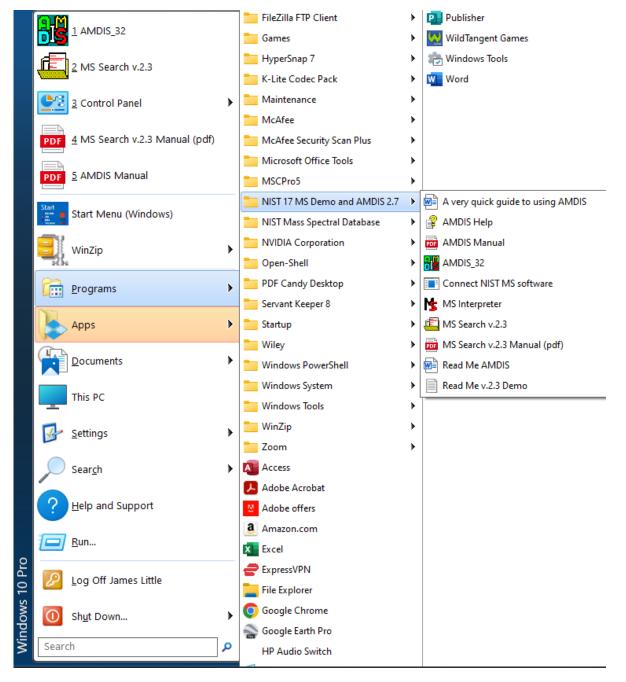
-double left click on the nist17demo.zip file to open zip file

-double left click on the file

-take all the defaults

-should find the files in your program group shown on next page

# Program Group Shown from Start Menu for NIST Demo



## Installing ACD ChemSketch Drawing Program

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

#### Link to Downloads

### -Scroll down to the following links

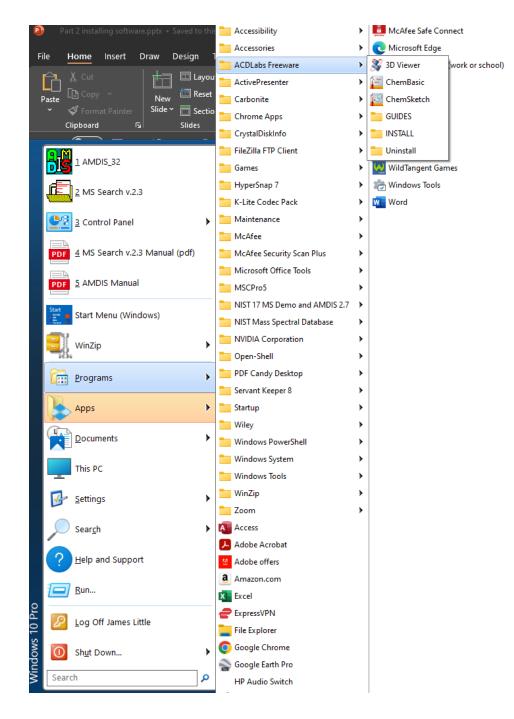
Resources

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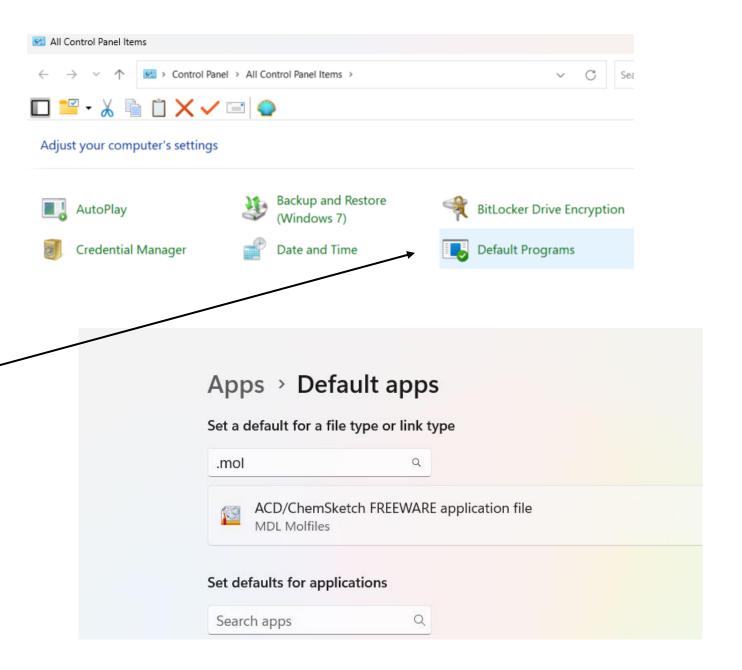
-Install NIST software by left clicking on ACD Free Software link

- -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