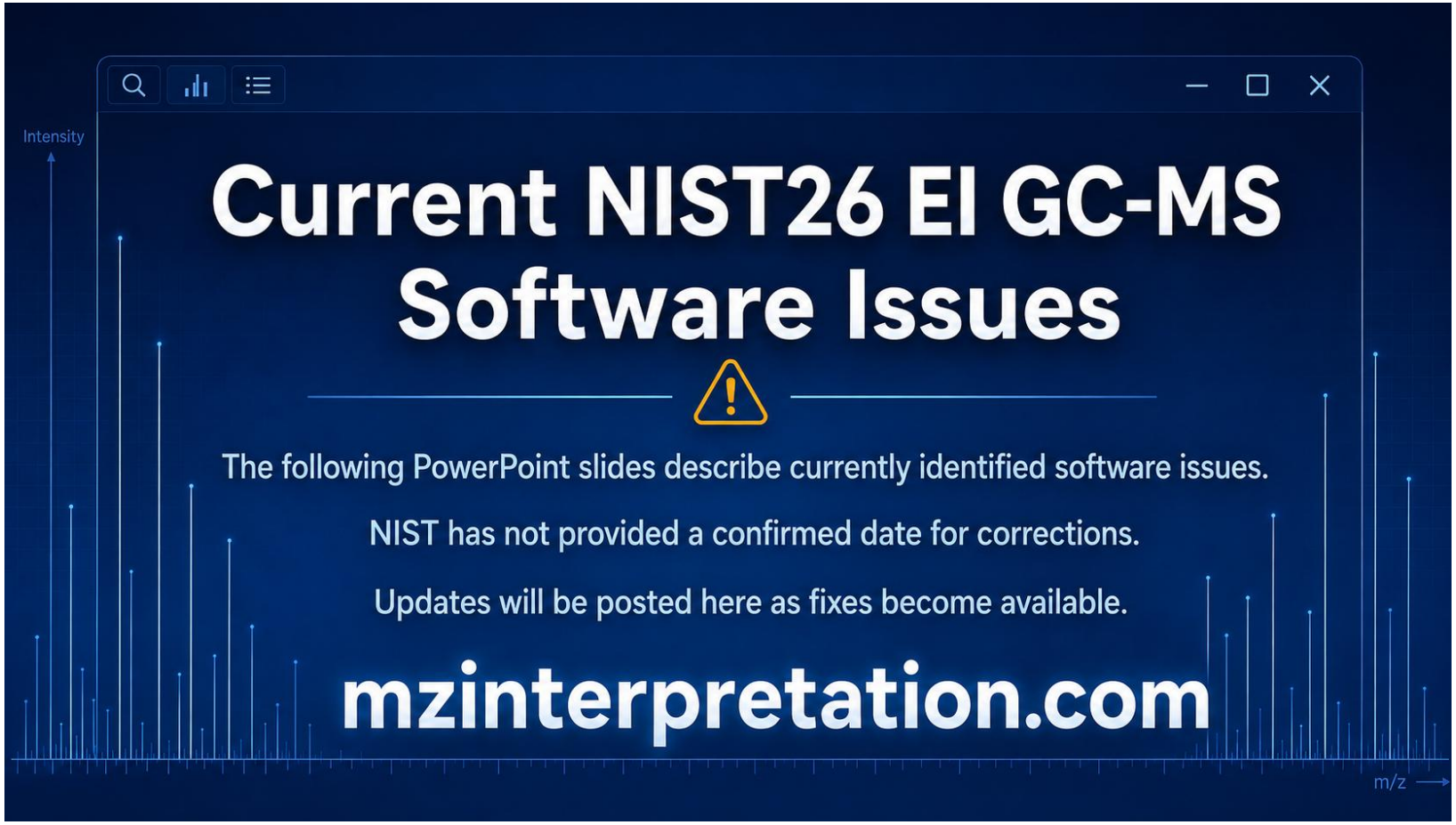
Current NIST26 EI GC-MS Software Issues
Video and Handout

J. L. Little



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

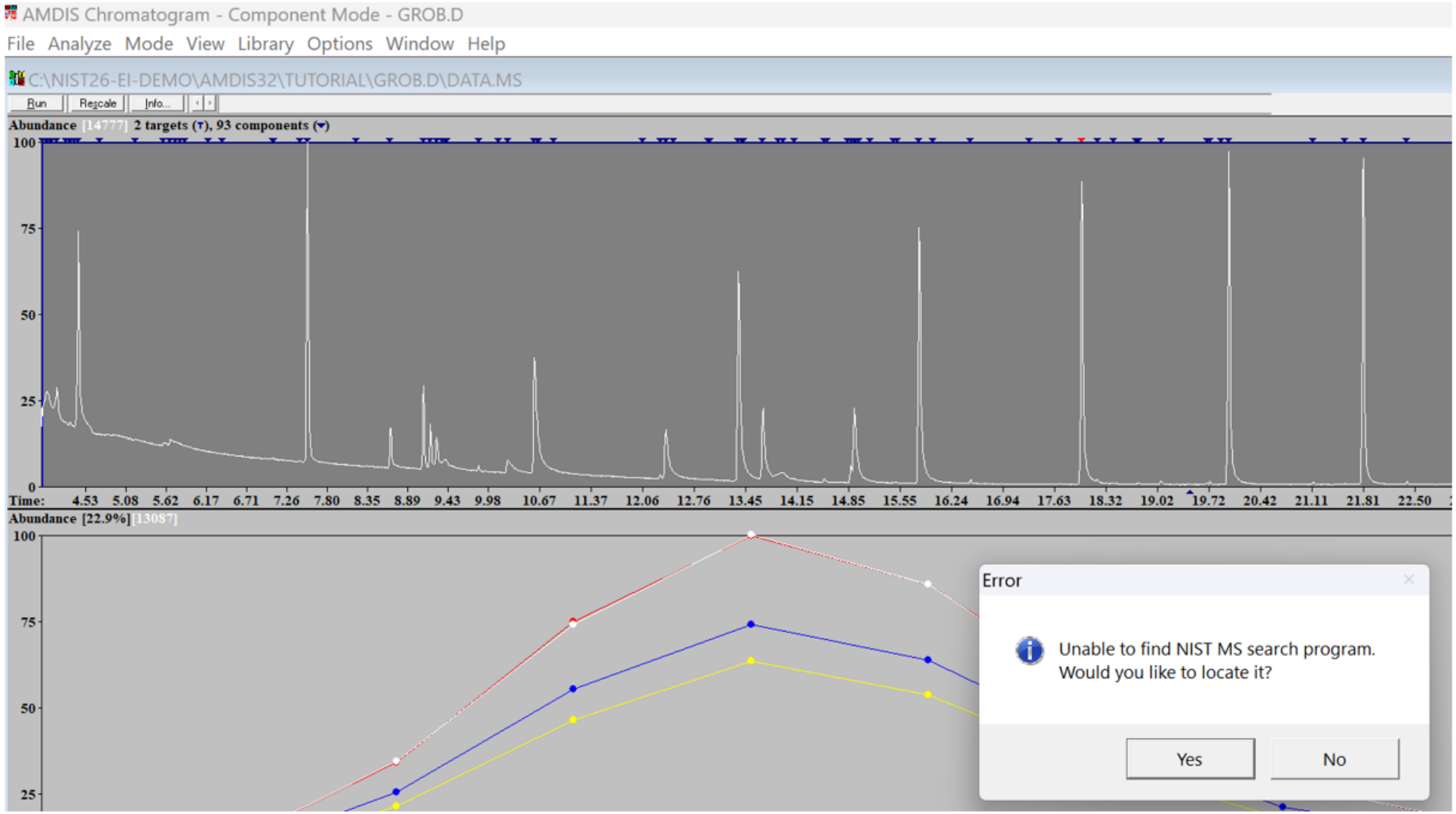
link to course

Index of Software Bugs and Status

Name	Status	Comment	Date	page no.
Cannot Find the NIST Search Executable	Fixed and posted new EI Demo on website	NIST Removed Stand-Alone Amdis	8/29/2026	3-4
Wrong NIST Search Opened by EI DEMO Stand-Alone Amdis	Fixed and posted new EI Demo on website	NIST Removed Stand-Alone Amdis	8/29/2026	5
win.ini concern	when installing demo, can write extra stuff in Win.ini, probably should delete after using, be sure to make backup of win.ini before installing and then restore original, more of problem before NIST removed AMDIS stand-alone from demo	don't know if NIST will address this, only problem if for example, NIST23 or some other older version of software there originally	8/29/2026	6-8
MS Interpreter Concerns	Not really a bug, but can be a problem at times	see solution in handout	8/31/2026	9-15

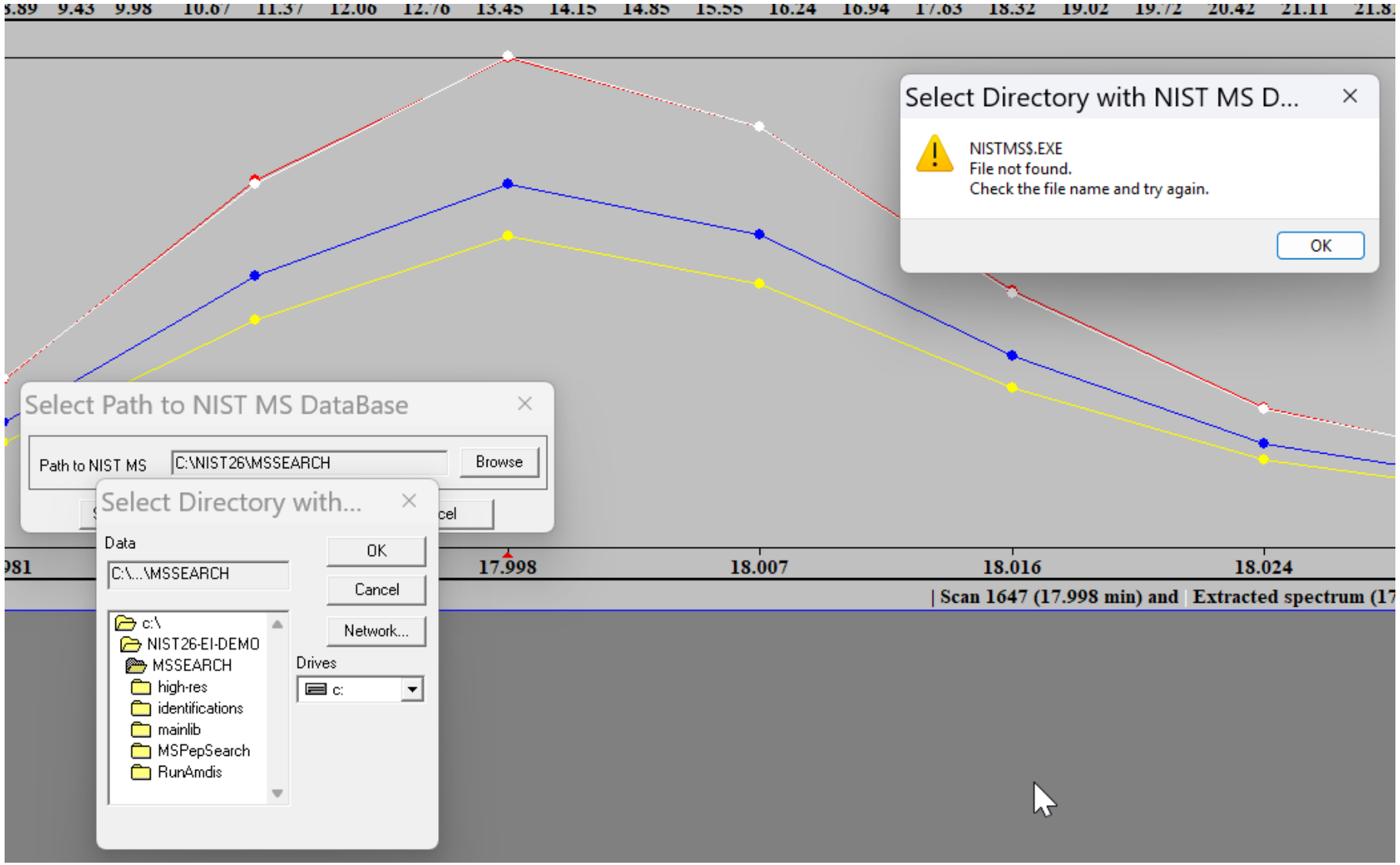
Software Bug: NIST26 EI Demo Stand-Alone AMDIS (Slide 1 of 2)
Cannot Find the MS Search Program

- When stand-alone AMDIS is opened, the AMDIS application cannot fine the Lib Search Program



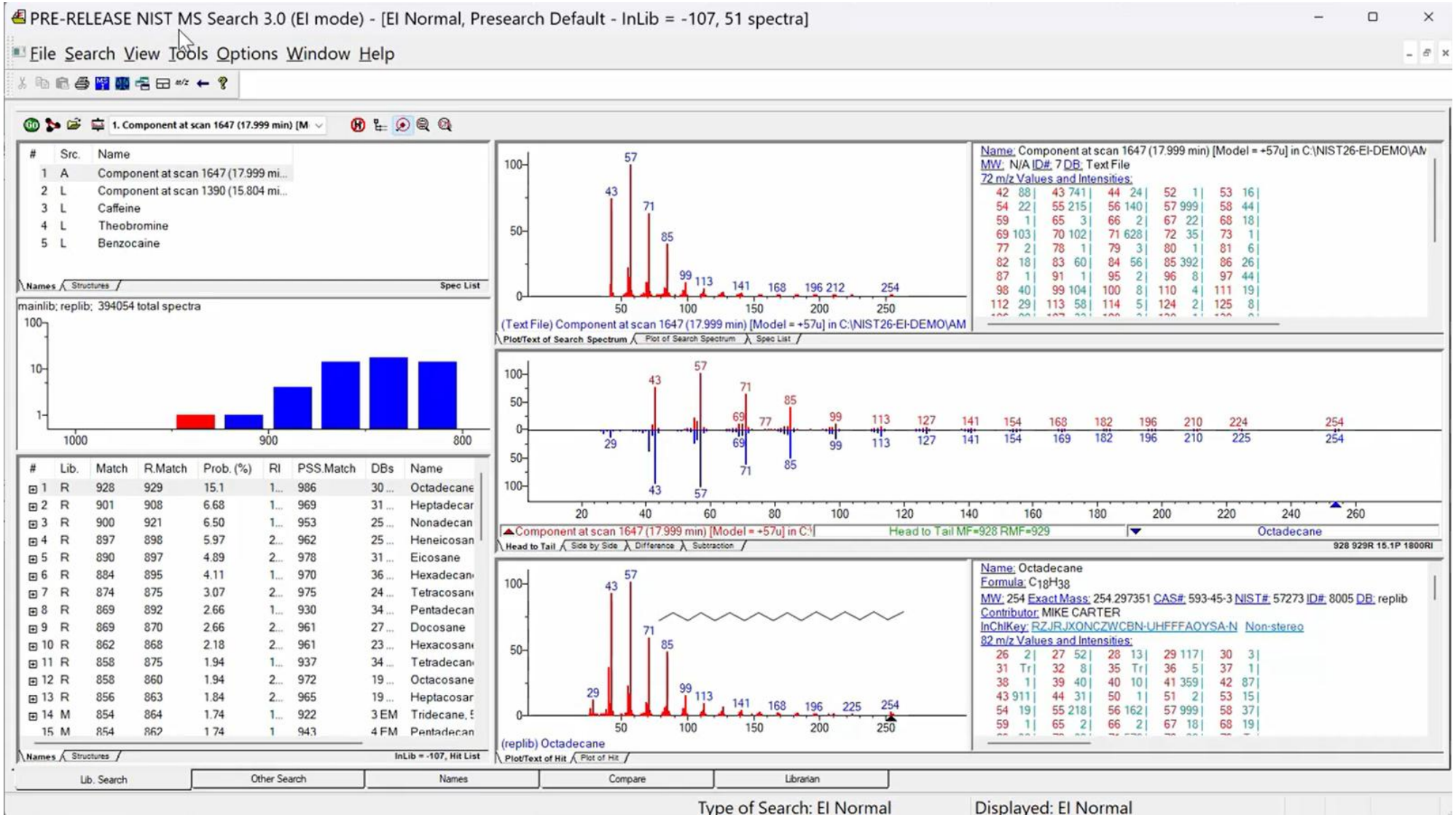
Software Bug: NIST26 EI Demo Stand-Alone AMDIS (Slide 2 of 2)

- When stand-alone AMDIS is opened, the AMDIS application cannot fine the Lib Search Program
- Library has improper executable name, cannot locate it in the NIST26-EI-DEMO folder



Software Bug: NIST EI Demo Problem with Supplied Stand-Alone AMDIS
Wrong NIST Search Opened Stand-Alone AMDIS if e.g. NIST23 present

- If EI Demo software is added to a system with current NIST software containing associated AMDIS
- Previously installed NIST software Lib Search will be opened, NOT the Lib Search included in EI Demo Download

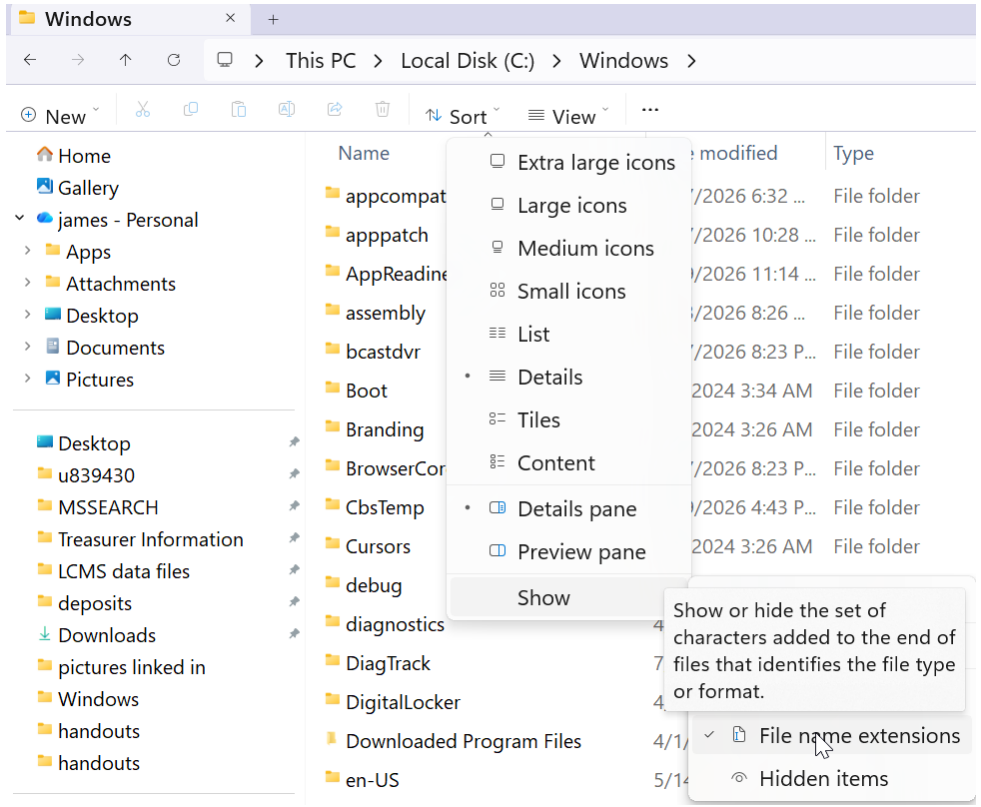


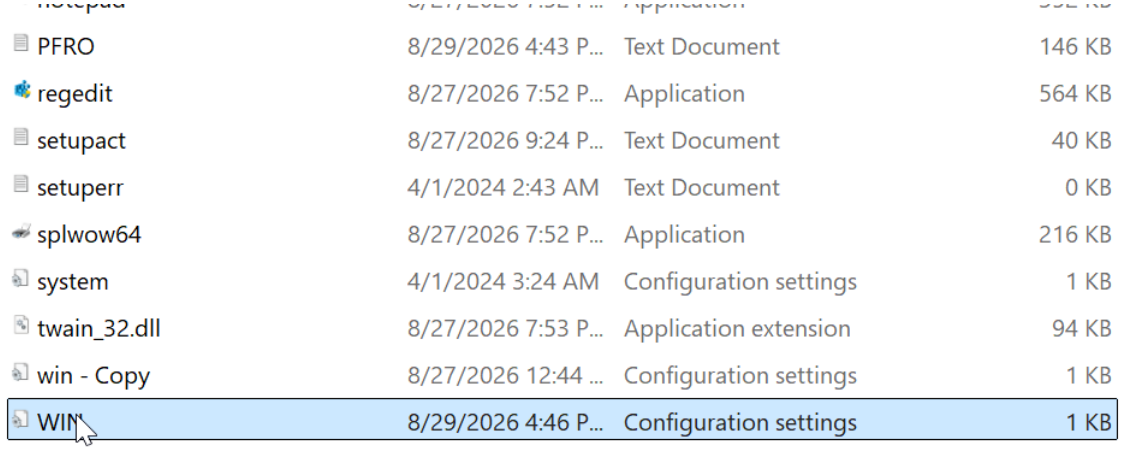
Software Bug: NIST26 EI Demo Stand-Alone AMDIS (Slide 1 of 3)
Possible Problems Installing/Uninstalling with Win.ini, especially if previous version of NIST Present

- *ALWAYS* make backup of C:\Windows\win.ini *BEFORE* Installation of DemoWhen
- Installing the EI demo when previous version of NIST 23, the win.ini is changed
- Can possibly cause issues
- Thus, be sure to return to original state when uninstalling EI demo when finished
- Originally for NIST23, the win.ini appeared as shown on *Slide 3 of 3.*
- Can then overwrite win.ini with original backup when *UNINSTALLING* EI Demo after evaluation finished
- Or edit after finishing to remove the EI Demo changes
- 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

Software Bug: NIST26 EI Demo Stand-Alone AMDIS (Slide 2 of 3)
Possible Problems Installing/Uninstalling with Win.ini, especially if previous version of NIST Present

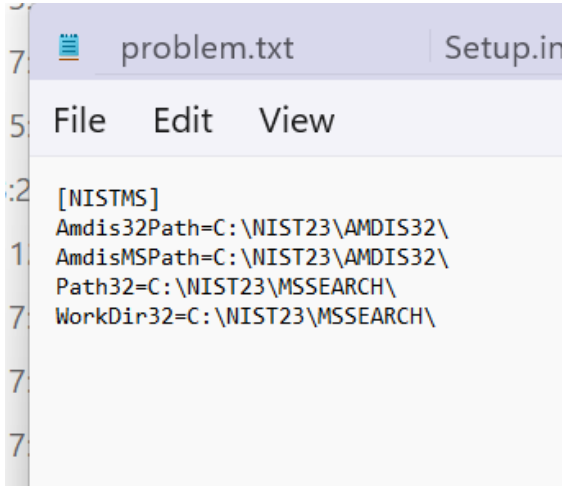
- Make sure after editing, it is still an .ini file extension (Configuration Settings), NOT, .txt, Text Document
- Show file configurations while doing operations!





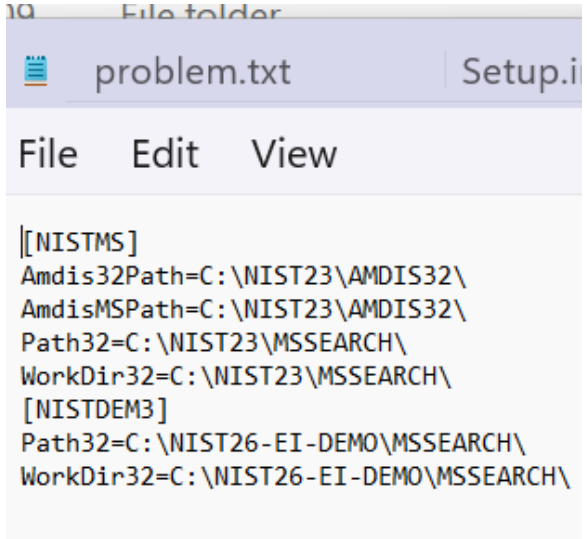
Win.ini Sequence in EI Demo Mode (Slide 3 of 3)
ChemStation Import

NIST23 Installed
EI Only Version



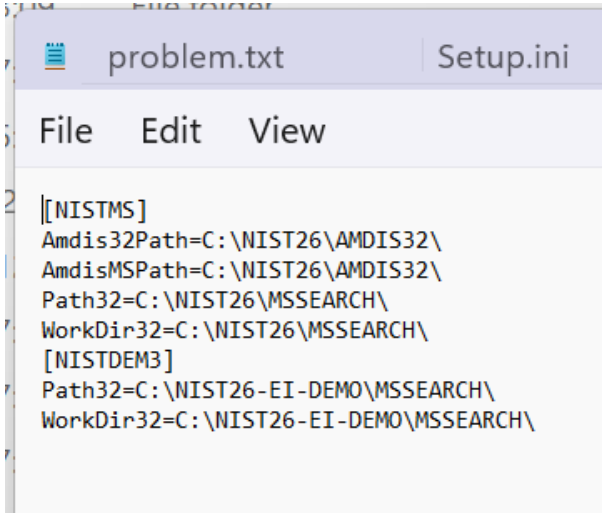
- Chemstation EI Import Works
- Installed ChemStation first
- Then EI Only NIST23

NIST23 EI Only Installed
NIST EI Demo Installed



- AMDIS works as expected to NIST23 search
- ChemStation opens NIST23 not NIST26
- Reasonable result
- Stand-alone chromatogram works
- No demo files since no tutorial folder
- Hi-res demo files present

NIST23 EI Only Un-Installed
NIST26 Demo EI Un-installed
NIST26 Combined EI and MSMS Installed



- Chemstation EI Import Works
- AMDIS works
- *"Residue"* left in win.ini about EI demo
- Does it matter??

Software Bug: MS Interpreter (Slide 1 of 7)

- Probably not really a bug
- Sometimes you might be having trouble with the program, and it will not open
- Possibly an earlier version might be present on the system, and you want to change to a newer version?
- Some instructions from different sources on the next few pages
- You need to be the *TRUE Administrator of your PC*
- Might require help from a IT corporate or university administrator to access Admin Rights on your computer
- Discussion of OLE and MS Interpreter by ChatGPT on next slide

Software Bug: MS Interpreter (Slide 2 of 7)

➢ Chat GPT Explanation

MS Interpreter uses **OLE registration because NIST MS Search treats it as an external software component that must be located, started and controlled programmatically**.
When you select **Send To → MS Interpreter** or press **F9**, NIST MS Search needs to:

- Locate the installed MSPCALC.EXE.
- Start the correct copy of MS Interpreter.
- Transfer the selected mass spectrum.
- Transfer the chemical structure, when available.
- Instruct MS Interpreter to display and analyze the information.

OLE registration places MS Interpreter's COM/OLE identity and executable location in the Windows Registry. NIST MS Search can then request MS Interpreter through Windows without knowing its folder directly.

Administrator access is required

Registering, unregistering or repairing MS Interpreter normally requires **Windows administrator privileges** because the necessary information is written to protected areas of the Windows Registry.
Therefore, to correct an OLE-registration problem, you generally must either:

- Sign in using an account with administrator rights; or
- Right-click MSINTREG.BAT, MSINTUNR.BAT or MSPCALC.EXE and select **Run as administrator**.

Within MS Interpreter, the corresponding commands are:
Options → OLE Registration → RegServer
and, when removing an obsolete registration:
Options → OLE Registration → UnregServer
Simply running these commands from a standard user account may appear to work but fail to update the protected registry information. In a company-controlled environment, such as Eastman, the user may need the IT department or a system administrator to perform the repair.
Moving, renaming or replacing MSPCALC.EXE may leave Windows pointing to an old program location. The old registration should then be removed and the correct copy registered again with administrator privileges.
Most other NIST programs do not require OLE registration because they communicate through command-line instructions, temporary files, shared folders or direct program calls rather than acting as registered Windows automation servers.
Although NIST calls it **OLE registration**, its primary purpose here is Windows **COM automation and program discovery**, not embedding an object in a document. NIST's instructions specifically require running the registration utilities or MSPCALC.EXE **as Administrator**. NIST MS Interpreter documentation

Program arrangement	Communication method
NIST MS Search → MS Interpreter	Registered OLE/COM connection
Vendor software → NIST MS Search	Files, macros, command lines or nistms$.exe
Other NIST utilities	Direct execution or file exchange

Software Bug: MS Interpreter (Slide 3 of 7)

- Instructions from NIST
- Need to be *TRUE administrator* for the system to perform operations for MS Interpreter

- Download the archive with MS Interpreter Registration program MSINTREG.ZIP
- and unpack the msintreg.exe file to the folder with the NIST MS Interpreter software (MSPCALC.EXE, Frag32.dll, Qual.dll, etc.).

- Purpose:

- The program MSINTREG.EXE is supposed to completely replace instructions on registering NIST MS Interpreter in case all MS Interpreter files are in a single folder on user's PC.

- How to use instructions:

- (1) The purpose of Windows 32-bit console application msintreg.exe is to connect NIST MS Interpreter to NIST MS Search. It is designed to work under Win XP, 7, 8, 8.1, 10, 11.
- (2) Shutdown NIST MS Search if it is running.
- (3) Copy file msintreg.exe to the folder containing MS Interpreter files.
- The minimal set of MS Interpreter files is: MSPCALC.EXE, Frag32.dll, Qual.dll.
- (4) Run msintreg.exe in that folder.
- Normally, Windows would request Administrative credentials to run msintreg.exe.
- (5) In case of an error, a system-modal dialog entitled MSIntReg is displayed. In this case:
- Before clicking OK, take a look at the console output to find out what caused the error.
- To resolve the problem, you may need to close MS Search, remove read-only attribute, update MS Interpreter files and/or reboot Windows and repeat (4).
- (6) To restore MSPCALC.INI removed by MSIntReg, shutdown MS Search and MS Interpreter, then copy MSPCALC.INI.BAK to MSPCALC.INI.

- Details:

- A successful run of msintreg.exe may look like this
- ==begin==
- MSIntReg.exe: Connect MS Interpreter to NIST MS Search (ver. 1.0.2 build Thu Aug 1 11:51:28 2024)
- Searching for the minimal set of MS Interpreter components
- Searching for MSPCALC.EXE... - success
- Searching for Frag32.dll... - success
- Searching for Qual.dll... - success
- Searching for running NIST MS Search
- Running NIST MS Search not found.
- Trying to kill running NIST MS Interpreter process/task "mspcalc.exe"
- SUCCESS: The process "Mspcalc.exe" with PID 57572 has been terminated.
- INFO: Found NIST MS Interpreter file MSPCALC.INI
- Deleted file MSPCALC.INI.BAK
- Renamed MSPCALC.INI to MSPCALC.INI.BAK
- Unregistering NIST MS Interpreter... - success
- Registering NIST MS Interpreter... - success
- ==end==
-

Software Bug: MS Interpreter (Slide 4 of 7)

- MS Interpreter from NIST Website Approach
- https://chemdata.nist.gov/dokuwiki/doku.php?id=chemdata:interpreter

Introduction

New Version – March 2023 (v. 3.4.5). Updated mechanisms and their rates for all fragmentation types (EI, Tandem positive and negative mode). This program connects mass spectral peaks to their probable chemical structure origin and can be quickly invoked from the NISTMS program with the F9 key or right mouse button followed by send to MS Interpreter. It also enables the display of isotopic envelopes, chemical formula calculations and other related calculations and user interface control.

Here is the link to download MS Interpreter:

Download MS Interpreter Ver.3.4.5 (2023 Release)

Version 3.4.* replaces all earlier versions under 32-bit and 64-bit Windows.

MS Interpreter was described in a poster in the meeting of the International Mass Spectrometry Society, Edinburgh, UK, 2003, “An Automated Method for Verifying Structure-Spectral Consistency Based on Ion Thermochemistry”

MS Interpreter ASMS presentations (PDF) are also available: ASMS 2017 ASMS 2018, ASMS 2019

No documentation is available except built-in help system. Select Help/What's New from MS Interpreter menu to get a list of newly added features, or open file MSPCALC.chm

Software Bug: MS Interpreter (Slide 5 of 7)

Installation

How to install MS Interpreter ver. 3.4

The following instructions assume that you do not have a earlier version of MS Interpreter installed on your PC.

1. Extract files from this package to a directory on your computer.
2. Run MSINTREG.BAT as Administrator. This will register the new MS Interpreter. This process lasts 1-3 sec., no new application window will be open. Or you can run newly extracted file MSPCALC.EXE as Administrator; select from its menu Options/OLE Registration/RegServer.
3. Optionally create a shortcut to MSPACALC.EXE and name it “MS Interpreter”.

How to replace an earlier version of the MS Interpreter

How to verify that MS Interpreter is properly installed

1. Run NIST MS Search (your current version).
2. Open a mass spectrum in any of the MS Search windows
3. Right-click the window and select “Send To”, “MS Interpreter” from the floating menu.

The MS Interpreter window should pop up and display the selected spectrum and (if present) the chemical structure. The Help/About box should display “MS Interpreter Version 3.4” or later.

Software Bug: MS Interpreter (Slide 6 of 7)

How to Reattach MS Interpreter to the NIST MS search program

Download the archive with MS Interpreter Registration program:

Download MS Interpreter Registration program archive

1. Unpack the ***msintreg.exe*** file to the folder with the NIST MS Interpreter software (mspcalc.exe, frag32.dll, Qual.dll).
2. Close the NIST MS Search program
3. Run this program (msintreg.exe)
4. Restart the NIST MS Search program.

More detailed instruction is in the Readme.txt file included in the msintreg.zip archive.

➢ Software Bug: MS Interpreter (Slide 7 of 7)

- Sometimes I have had success
- UnRegServer, then RegServer
- You need to be the *TRUE Administrator of your PC*
- Might require help from a IT corporate or university administrator to access Admin Rights on your computer
- MS Interpreter can be opened from program group
- MS Interpreter program is really named Mspcalc

