NIST26 *FREE* Demonstration (Demo) Copy of MS/MS Integrated Processing

Video/Handout

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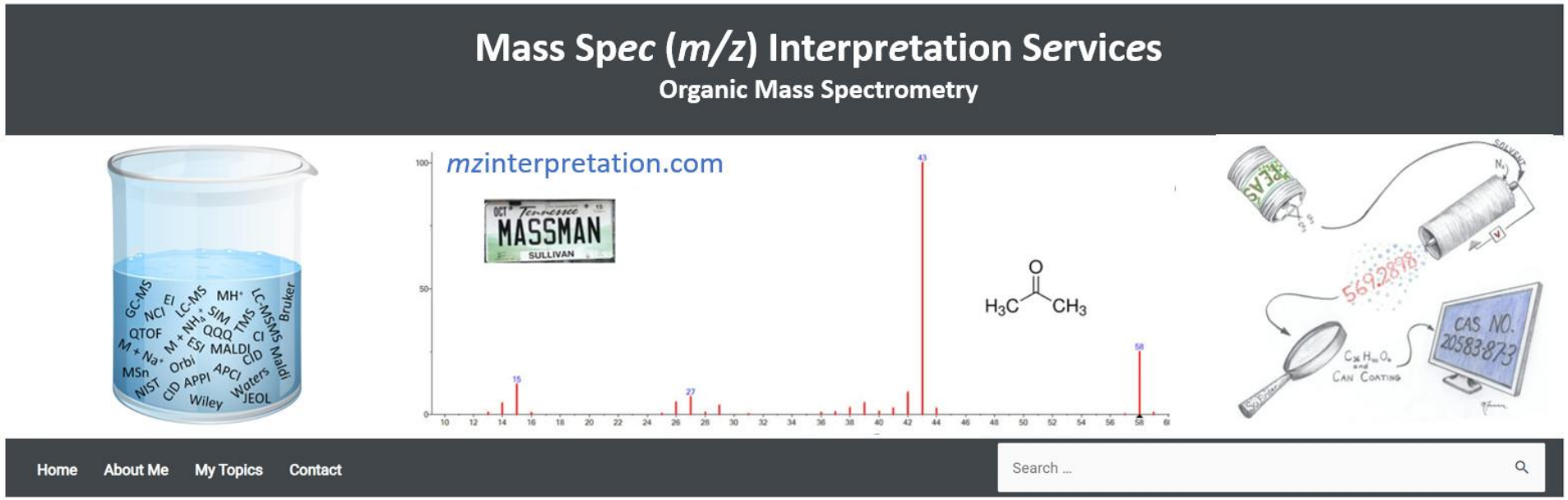
See *Full Course* on NIST26 with new *Integrated* Deconvolution/Library Searching for *EI GC-MS* and *LC-MS/MS*!



Overview

- Fully functional Demo copy to demonstrate powerful new deconvolution/library searching software
- Integrated in library search in NIST26
- Handout for details of installation
- Software demonstrated in associated video

Resources:

- Fully functional download from NIST, *link to NIST website*
- Demo library from NIST of 26 compounds and 830 associated MS/MS spectra
- Test files (2) of sample in positive and negative mode containing NIST26 demo compounds
- 3 Files from *mzinterpretation.com* of common commercially available compounds in mzML format
- 3 Public libraries from *mzinterpretation.com* in NIST format, *see link*
- Public libraries contain >520K MS/MS spectra and >150K structures from MoNA and MS-Dial
- Basic Theory of LC-MS, *see link*

Note: 3 Public libraries don't compare to NIST MSMS spectra in either quantity or quality, but do contain compounds not found in NIST26 Library, ***suggest searching all of them***

Very Approximate Estimates from ChatGPT, Grok, and Other Sources

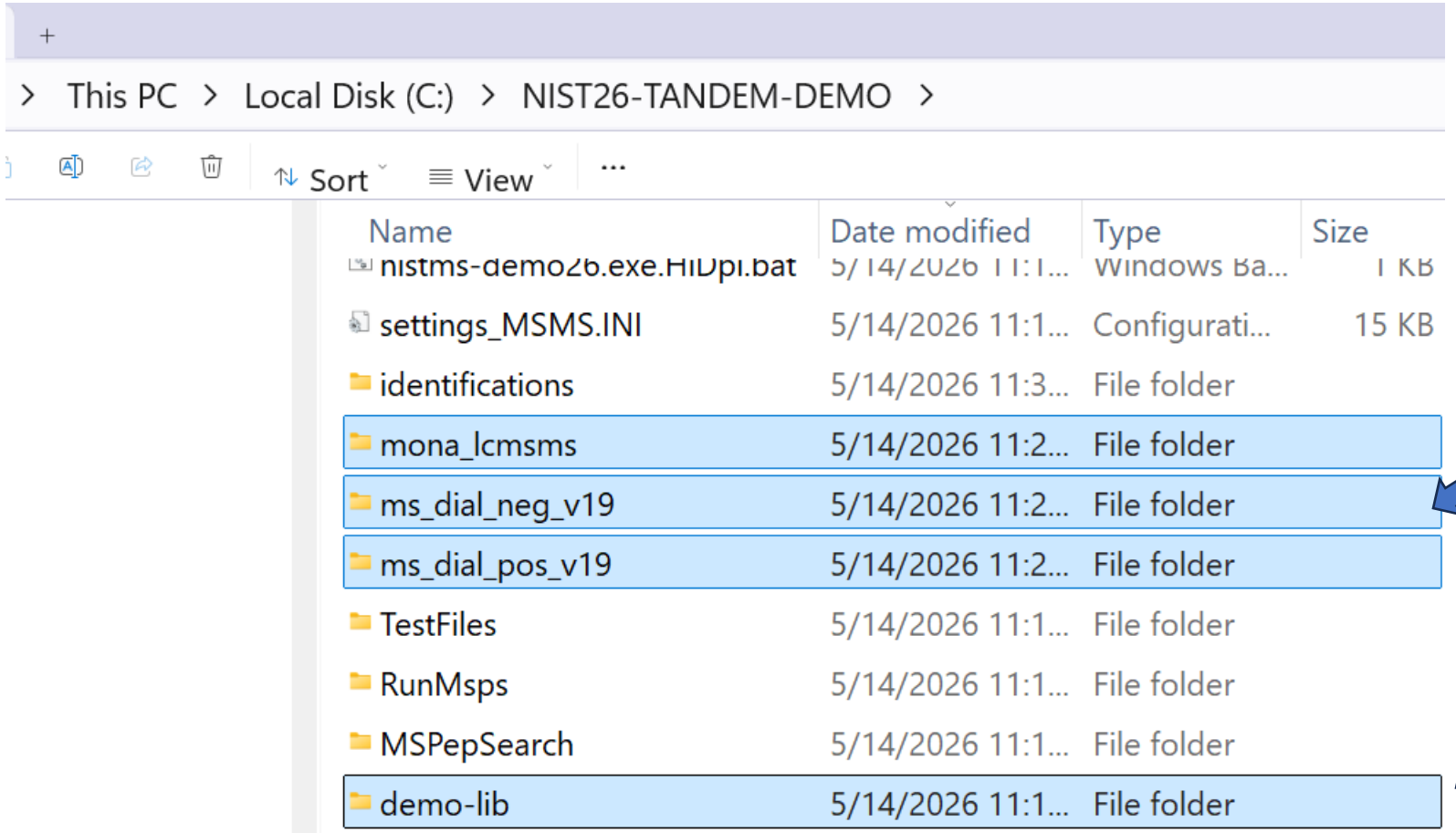
Library	Approx. Unique Compounds	Approx. MS/MS Spectra	Structures Available in NIST	Comments
National Institute of Standards and Technology NIST 2026 Tandem MS/MS	68,635	~3.2 million	68,635	Fully curated and structure-linked
MassBank of North America MoNA LC-MS/MS	~30,000–50,000	~150,000+	~50,000 (when imported with accompanying SDF)	Adds many compounds not present in NIST
MS-DIAL V19 MSP Libraries	~30,000–100,000*	~365,000	0 (unless external structures are supplied)	Spectral-only MSP entries by default

*The number of unique compounds represented in the MS-DIAL MSP collection varies widely depending on which libraries are included and how duplicates are removed

Installation of Software

- Download NIST Demo software from NIST website
- *Link to NIST Website*
- NIST Test files located in NIST demo search folder
- NIST Demo lib located in NIST demo search folder
- Public libraries found on my website, see link
- Test files of common compounds in mzML format on my website, *see link*
- Place additional test files in NIST Test Files Folder
- Place 3 Public libraries in Demo folder

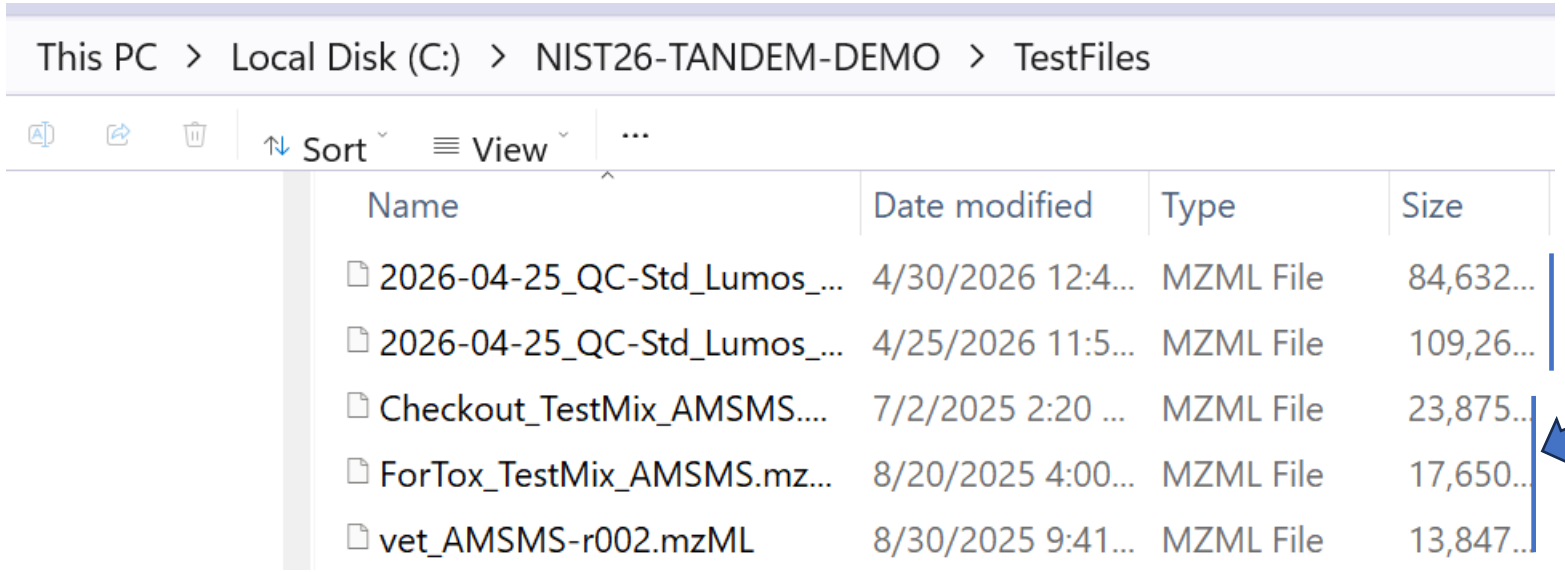
Libraries for Searching and ***Required*** File Locations



3 public libraries

NIST small demo library

File for Processing and *Suggested* Location



First two NIST demo files

Last 3 files from my webiste