

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

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Mass Spec Interpretation Services

April 25, 2026

mzinterpretation.com

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

Mass Spec (m/z) Interpretation Services Organic Mass Spectrometry



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 (available in June 2026)
- Link for NIST download will be in the resources on my website when available, [see page link](#)
- 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 found in Resources on my website, [see link](#)
- 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

Name	Date modified	Type	Size
nistms-demo2b.exe.HIDpi.bat	5/14/2026 11:1...	Windows Ba...	1 KB
settings_MSMS.INI	5/14/2026 11:1...	Configurati...	15 KB
identifications	5/14/2026 11:3...	File folder	
mona_lcsmms	5/14/2026 11:2...	File folder	
ms_dial_neg_v19	5/14/2026 11:2...	File folder	
ms_dial_pos_v19	5/14/2026 11:2...	File folder	
TestFiles	5/14/2026 11:1...	File folder	
RunMsps	5/14/2026 11:1...	File folder	
MSPepSearch	5/14/2026 11:1...	File folder	
demo-lib	5/14/2026 11:1...	File folder	

3 public libraries

NIST small
demo library

File for Processing and *Suggested* Location

This PC > Local Disk (C:) > NIST26-TANDEM-DEMO > TestFiles

Sort View

Name	Date modified	Type	Size
2026-04-25_QC-Std_Lumos_...	4/30/2026 12:4...	MZML File	84,632...
2026-04-25_QC-Std_Lumos_...	4/25/2026 11:5...	MZML File	109,26...
Checkout_TestMix_AMSMS....	7/2/2025 2:20 ...	MZML File	23,875..
ForTox_TestMix_AMSMS.mz...	8/20/2025 4:00...	MZML File	17,650..
vet_AMSMS-r002.mzML	8/30/2025 9:41...	MZML File	13,847..

First two NIST
demo files

Last 3 files from my
webiste