

Raw Data Files for EI Low Resolution in the Identifications Folder

Video/Handout

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Mass Spec Interpretation Services

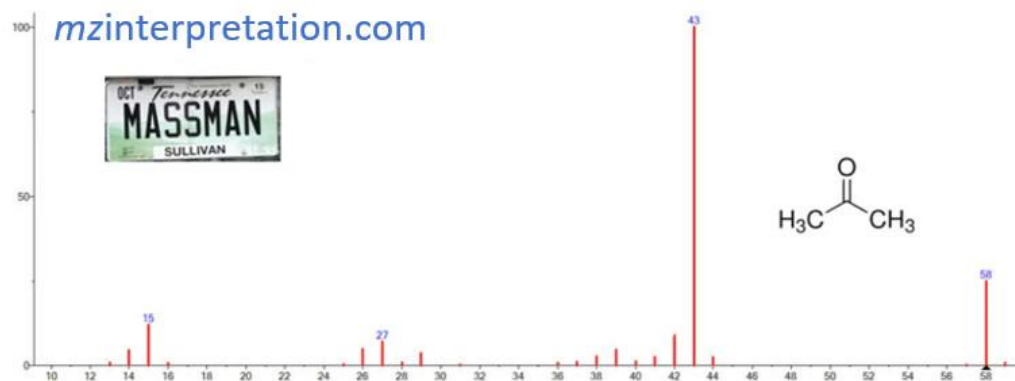
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mzinterpretation.com

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



- Every Analysis Creates a Set of Files Used to Yield the Deconvolution and Library Search Identifications
- Stored in the Identifications Folder in MSSEARCH
- These files shown below for my Grob Analysis in EI, no RI
- I entered these files into ChatGPT with a prompt to see their function
- ChatGPT Report on next few pages
- *Could one use for comparing samples with external user-written application?*
- *Comparing Difference, Good vs. Bad, PCA?*

Open

← → ↕ ↑ This PC > Local Disk (C:) > NIST26 > MSSEARCH > identifications

Organize ▾ New folder

Name	Date modified	Type	Size
GROB.log	4/27/2026 4:29 PM	Text Document	1 KB
GROB.run	4/27/2026 4:29 PM	RUN File	1 KB
GROB.tsv	4/27/2026 4:29 PM	TSV File	32 KB
GROB.ELU	4/27/2026 4:29 PM	ELU File	46 KB
GROB.FIN	4/27/2026 4:29 PM	FIN File	18 KB
GROB.TIC	4/27/2026 4:29 PM	TIC File	2,960 KB

Prompt

i was trying to put some information about raw files NIST creates when doing deconvolution in library search, here is a set for low resolution

Chat GPT Reply

For a **low-resolution GC/MS file**, I would describe the NIST raw/deconvolution support files like this:

NIST creates an “experimental” results folder during chromatogram processing.

This folder contains intermediate files used to document how the chromatogram was processed, how components were found, and how deconvoluted spectra were prepared for library searching.

For **low-resolution EI GC/MS**, the workflow is simpler than accurate-mass EI:

Raw GC/MS data → extracted ion traces → component detection/deconvolution → deconvoluted EI spectra → NIST library search results

The files in the folder are not usually meant as the primary user interface. They are more like a processing audit trail: they preserve chromatographic traces, component groupings, candidate spectra, and diagnostic “check” information used by the NIST program during deconvolution.

Here's a **very brief, clean description** you can drop directly into your page:

- `.TIC` – Total ion chromatogram (raw GC signal vs. time)
- `.ELU` – Detected peaks/components and their elution profiles
- `.FIN` – Final deconvoluted spectra used for library searching
- `.TSV` – Tabulated results (retention times, matches, intensities)
- `.RUN` – Processing parameters and method settings
- `.LOG` – Processing log (timing, number of spectra, search activity)

👉 One-line summary if you want it even tighter:

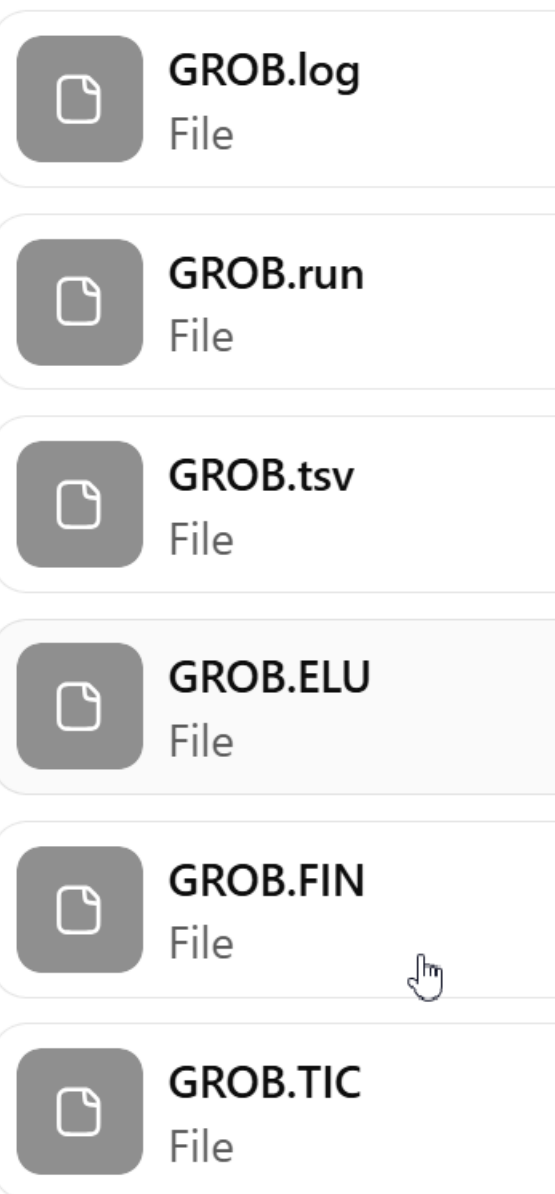
NIST generates TIC (raw data), ELU (peak detection), FIN (deconvoluted spectra), TSV (results), RUN (settings), and LOG (processing record) files during GC/MS deconvolution and library searching.

A concise webpage wording:

During chromatogram processing, NIST creates an experimental results folder containing intermediate files used for deconvolution and library searching. For low-resolution EI GC/MS data, these files document the extracted ion information, detected chromatographic components, deconvoluted spectra, and diagnostic checks used to generate the final library-search results. Most users will work from the final NIST chromatogram and library-search windows, but these raw output files can be useful for understanding how the software separated overlapping components and generated searchable spectra.

If you upload the actual set, I can label each file type one by one.

Great — this is exactly the kind of real dataset that makes your webpage much stronger. I'll map what you uploaded into a **clean, interpretable structure for low-resolution EI GC/MS (NIST/AMDIS-style processing)**.



Prompt: could One compare two samples using these files to tell differences

Chat GPT Response

Yes — **especially using the .TSV file.**

You could compare two samples by matching components by:
retention time + library ID + major ions / spectrum

Then compare:

- compounds present in one sample but not the other
- peak areas or intensities
- relative abundance changes
- new or missing deconvoluted components
- match-score changes

The best files for comparison would be:

- **.TSV** = easiest for sample-to-sample comparison
- **.FIN** = useful if you want to compare deconvoluted spectra directly
- **.ELU** = useful for checking peak shape/elution behavior
- **.TIC** = broad overview only, not ideal for compound-level comparison

A good webpage sentence:

These output files can also support sample-to-sample comparisons. The tabulated results file is the most practical starting point, allowing components to be compared by retention time, library identification, and peak response. More detailed comparisons can be made using the deconvoluted spectra and elution profiles.

What Your File Set Represents (Low-Resolution EI GC/MS)

You've essentially captured the **full internal processing stack** for a chromatogram run:

1. Processing / Audit Log

- `GROB.log` →  GROB

This is the **execution record of the library search + deconvolution**

Key details from your file:

🗨️ Ask ChatGPT

- 91 spectra processed
- ~178,757 library comparisons
- ~24 peaks per spectrum
- Deconvolution step executed at the end

👉 Interpretation for your webpage:

This file documents the computational workload and confirms that deconvolution and library searching were successfully completed.





Core Data Files (What the Software Actually Uses)

2. Chromatographic Data

- GROB.TIC
→ Total Ion Chromatogram (TIC)

👉 This is your **primary GC trace** — what users visually see in the chromatogram window.

” Ask ChatGPT

3. Elution / Component Detection

- GROB.ELU
→ Elution profile / detected peaks

👉 Contains:

- Peak start/stop times
- Apex locations
- Possibly grouped ion traces



👉 This is where **components are defined before deconvolution**

4. Deconvoluted Results

- **GROB . FIN**

→ Final deconvoluted spectra

👉 This is the **most important file conceptually**:

- One spectrum per resolved component
- Cleaned up from overlapping peaks
- Ready for library searching

5. Tabular Summary

- **GROB . tsv**

→ Tab-delimited summary

👉 Typically includes:

- Retention times
- Match factors
- Compound IDs
- Peak intensities

👉 Think of this as **exportable results for reporting**

6. Run Configuration / Control

- GROB . run

→ Processing parameters

👉 Likely stores:

- Deconvolution settings
- Peak detection thresholds
- Library search options

👉 This is key for **reproducibility**

How It All Fits Together (Low-Res EI Workflow)

Here's a clean version you can use directly:

During low-resolution EI GC/MS processing, NIST generates a series of intermediate files that document each stage of chromatogram analysis. The TIC file represents the raw chromatographic signal, while elution files define detected components based on ion behavior across time. Deconvolution produces a final set of resolved spectra (FIN files), each representing a single chemical component extracted from overlapping peaks. These spectra are then used for library searching. Supporting files, including logs and run parameters, provide a complete audit trail of the processing steps and ensure reproducibility.

Key Insight (Worth Highlighting on Your Site)

This dataset shows something important:

 **Only 91 spectra were searched**

(from your log)

That means:

- The system **did NOT search every scan**
- It searched only **deconvoluted component spectra**

 This is a powerful teaching point:

NIST/AMDIS reduces thousands of scans into a small number of chemically meaningful spectra before library searching.