NIST/EPA/NIH EI-MS Library

2026 Release

35K New NIST Measured/Evaluated Compounds

431K Electron Ionization (EI) Spectra

- 382,180 Compounds, 49,097 Replicate Spectra
- 35 K More Compounds than NIST 23

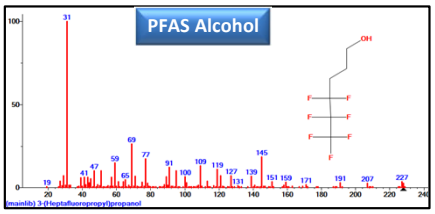
527K Retention Index (RI) Values

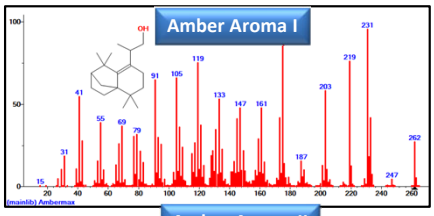
- 216K RI Compounds with EI, >35 K Increase
- AI-RI Estimates for All Compounds

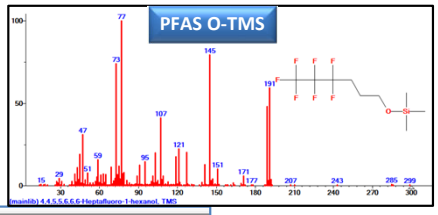
Compounds Selected for Analytical Relevance

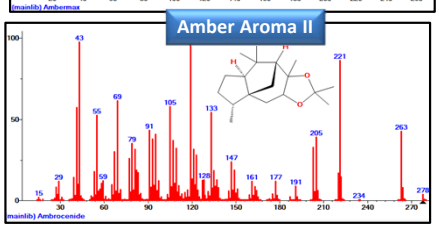
Fully Evaluated with Derivatives, Retention Indices & Class Information

Citation	New	Total
Wikipedia	355	8583
EPA PFAS	275	961
PubChem Lite	8341	55640
CHEMBL	304	3725
TSCA	396	9400
Human Metabolite DB	556	11898
KEGG	181	6925
Protein Data Bank	461	5459









Compound Data

Name: Valeryl fentanyl
Formula: $C_{24}H_{32}N_2O$
MW: 364 Exact Mass: 364.251463 CAS#: 122882-90-0 NIST#: 463844 ID#: 18711
Contributor: NIST Mass Spectrometry Data Center
InChIKey: VCCPXHWAJYWQMR-UHFFFAOYSA-N Non-stereo
Synonyms:
1.Pentanamide, N-phenyl-N-[1-(2-phenylethyl)-4-piperidinyl]-; 2.N-Phenyl-N-[1-(2-p
Other DBs:
-----Wikipedia-----
wikipedia2021_via_cheminfo_SMILES
-----Environmental-----
SUSDATFY22

Collections

Experimental RI median±deviation (#data)
Semi-standard non-polar: 2962±18 (2)
Standard non-polar: 2958±N/A (1)

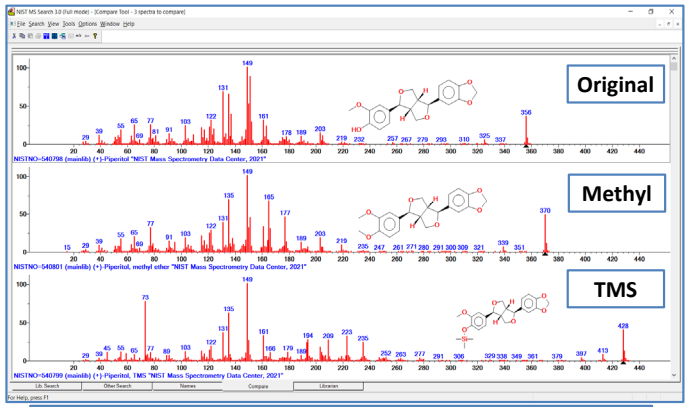
RI Averages

Estimated non-polar retention index (n-alkane scale):
Value: 2938 iu
Confidence interval (Nitrogen-containing): 83(50%) 356(95%) iu

AI-RI Estimates

Retention index
1. Value: 2980.5 iu
Column Type: Capillary
Column Class: Semi-standard non-polar
Active Phase: HP-5MS
Column Length: 30 m

RI Measured



Piperitol with TMS/Me Derivatives (TFA, Acetyl not shown)

Rich Output

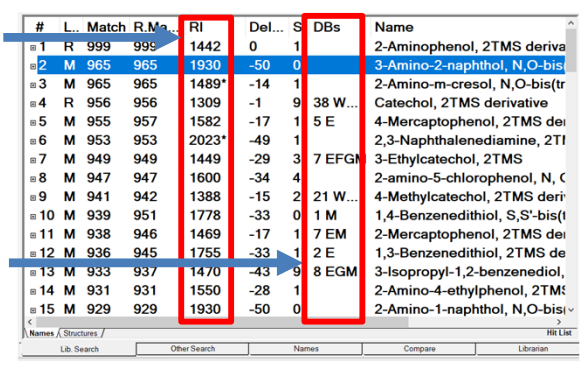
Hit List

Compound/Spectrum Lookup

Retention Index For All Hits (Expt'l or AIRI*)

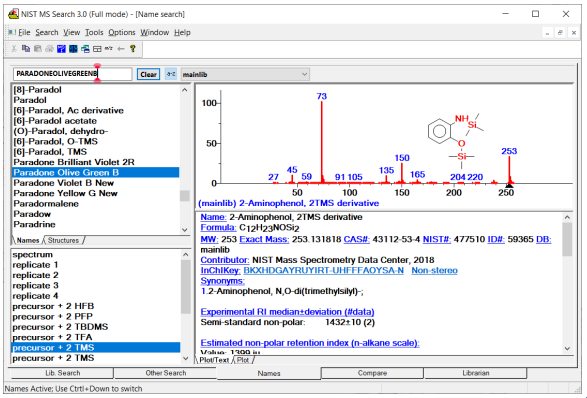
Select Columns
Mass Difference, Reverse Score, Probability, ...

Prior Probability (OtherDBs)



Names

Spectra
Replicates
Derivatives
Stereo



NIST EI Library Software

2026 EI Release

EI MS Analysis Tools

NISTMS

- Full Featured MS Library Search/Display Program
- Multiple Search Methods, Display Modes & Data Types
- 6 Views: Spectrum Search, Feature Search, Compare, Name/Spectrum, Librarian, Chromatogram

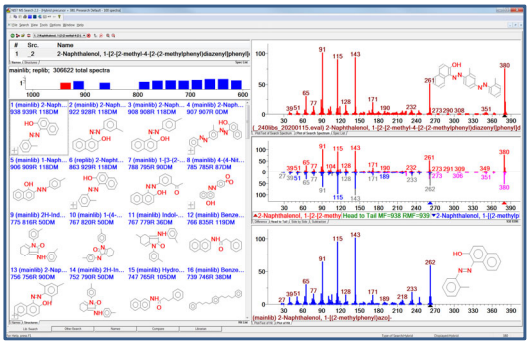
6 Tab Views

1. Query spectrum list
2. Score Histogram
3. Hit List –multiple values
4. Query spectrum
5. Query/Library Compare
6. Library Spectrum

Hybrid Search

- For Compounds Not in Library & for ID Confirmation
- Finds 'Modified' Library IDs and Masses of Modifications With Their Shifted Peaks
- RI and Formula Estimation

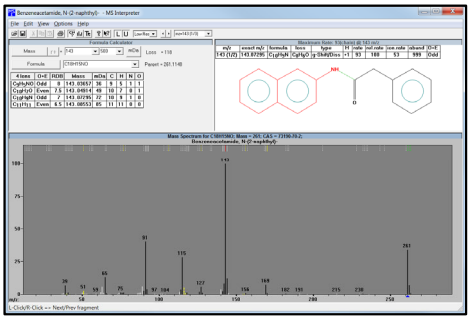
Delta Mass => Chemical Formula



DMass	Replace or Insert
1	H->D, C->C13, NH->O,CH->N
2	CH2->O, C=C->C-C
12	CH2->C=CH2
14	X-Y->X-CH2-Y
16	X-Y->X-O-Y
17	NH->S
18	H->F
28	X-Y->X-CO-Y
30	H->CH3O-H
32	X-Y->X-S-Y
34	H->Cl
50	Phenyl->Naphthyl
76	H->Phenyl
162	H->Glucose

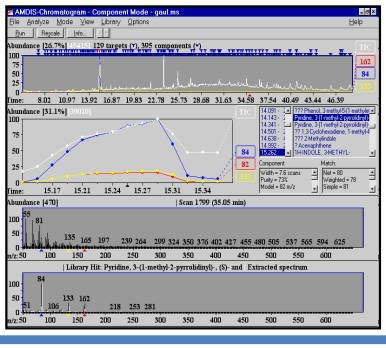
MS Interpreter

- Connect Peaks to Plausible Fragments (in Red)
- Confirm ID
  Compute Fragment Masses
  Connect Peaks to Structures



AMDIS

- 'Purifies' Spectra and Connects to NISTMS



NIST Website *chemdata.nist.gov*

Libraries, Tools, Service

This site provides information and access to NIST mass spectral data products. A variety of data products are available, including EI and tandem MS libraries (small molecule and peptide), a GC retention index collection as well as certain freely available, specialized spectral libraries. Freely available data analysis tools include AMDIS (Automated Mass Spectral Deconvolution and Identification System for GC/MS), the Mass Spectrum Interpreter (connects chemical structures with mass spectra), and the Mass Spectral Digitizer Program. Also available is a fully functional, version of NIST MS Search Program v.2.0f with a small demonstration library.

Recurrent Unidentified Spectral Libraries

There are three NIST user libraries of recurrent unidentified spectra (RUS):

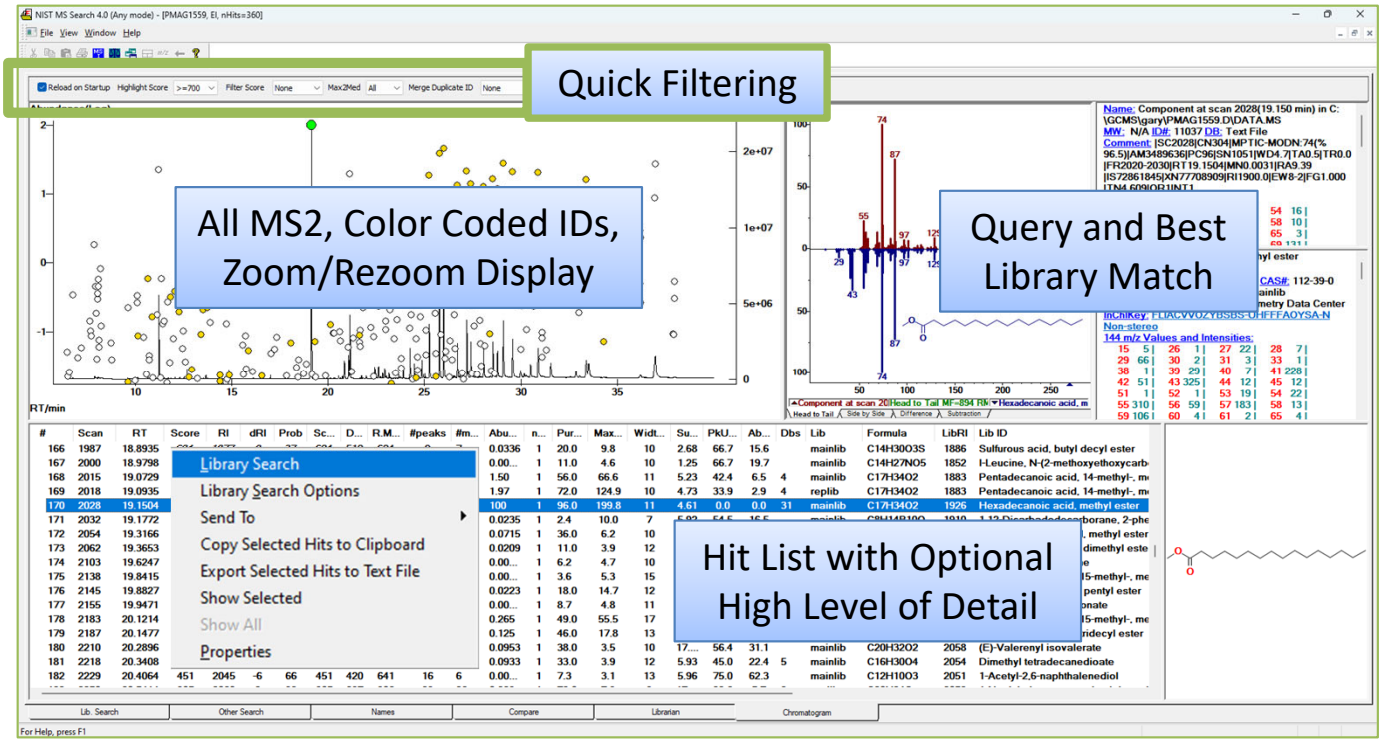
- **Food**: A set of 650+ spectra extracted from a set of dried food material, some of these spectra have tentative identifications. These experiments were done with methoxiamation and TMS derivatization. Data
- **PedUrine**: A set of 200+ spectra from a large set of pediatric urine samples. All of these samples were derivatized with TMS after forming the ethyloxime for the non-acid carbonyl groups; the majority of this
- **EssOil**: A set of 1000+ spectra derived from a large set of essential oils (both commercial and laboratory distilled), solvent extract of various plant materials (leaves, flowers, roots, etc). Most of these data were

Freely Available Data and Software

Tools

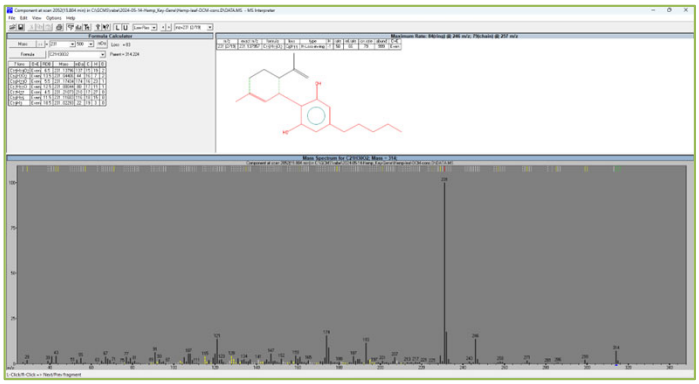
- Mass Spectrum Interpreter – Major New Release – February 2019 (v. 3.4). Information and downloads for version 3.4 of this program which connects mass spectral peaks to their probable chemical structure origin (EI and MS/MS, both nominal and accurate mass).
- NIST MS Software and Data - updates, demo, documentation, MSPepSearch, Lib2NIST, RUS libraries and support programs.
- AMDIS – computer program that extracts spectra for individual components in a GC/MS data file (Instructions for using AMDIS with MS Search – 11-25-2019)
- Mass Spectrum Digitizer Program – a tutorial on how to use the program (includes program download) that allows the digitization of graphical spectra
- The NIST Glyco Mass Calculator - a tool to aid in the analysis of glycoforms
- DIMEDR - A Novel Algorithm for Agglomerating Incongruent LC-MS Metabolomics Datasets.
- MS_Piano (New, 2021) - A new software tool for annotating peaks in collision induced dissociation (CID) tandem mass spectra of peptides and N-glycopeptides.

NEW Full GC/MS Chromatogram Analysis by NIST EI Library

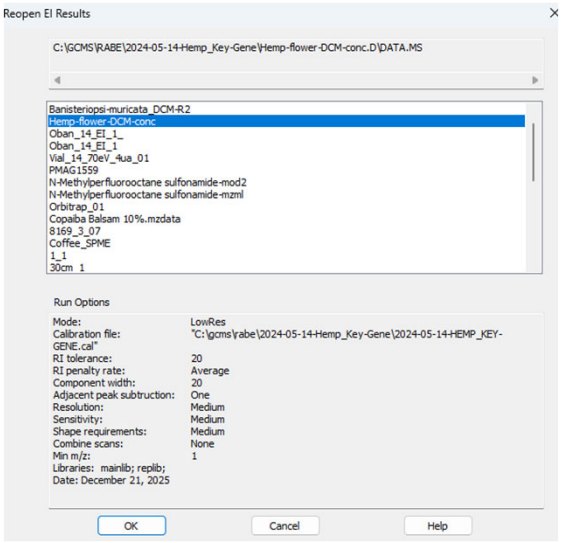


AMDIS Deconvolution
Low and High Resolution
Multiple Data Formats
Use External Libraries

Hybrid and Other Searching
Multiple Sorting & Filtering
Export to Spreadsheet
Many Display Options

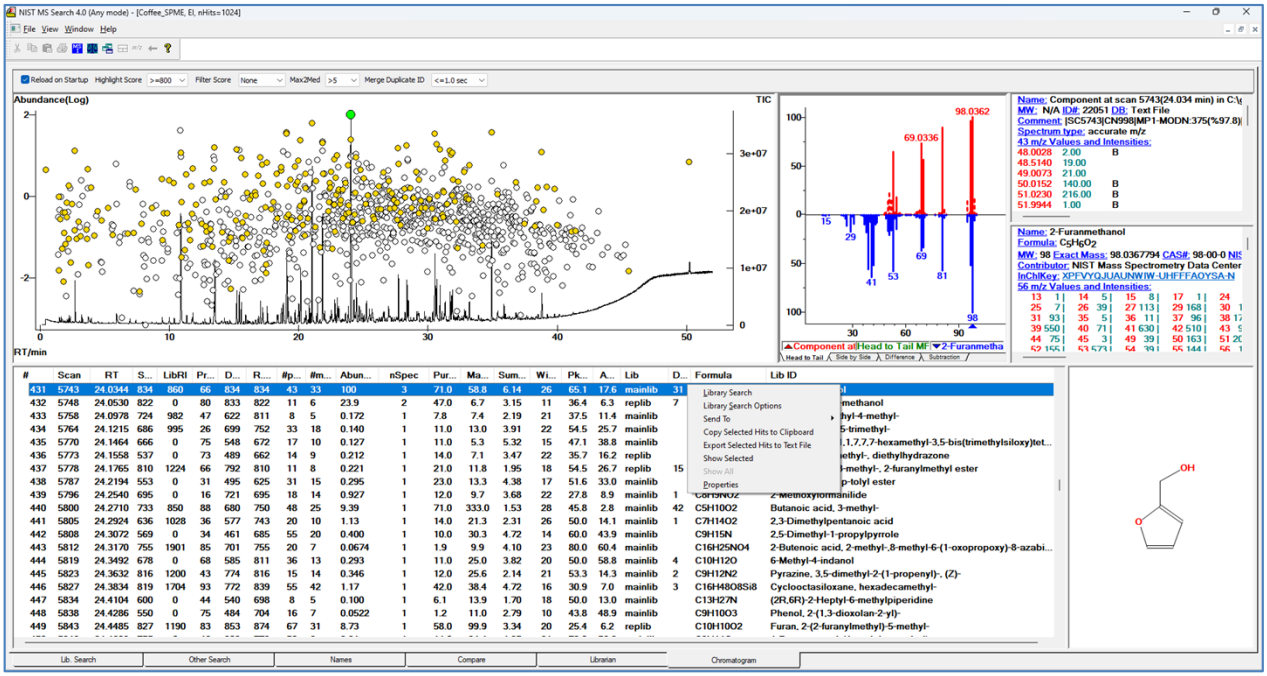


Send to MS Interpreter for Spectrum Analysis

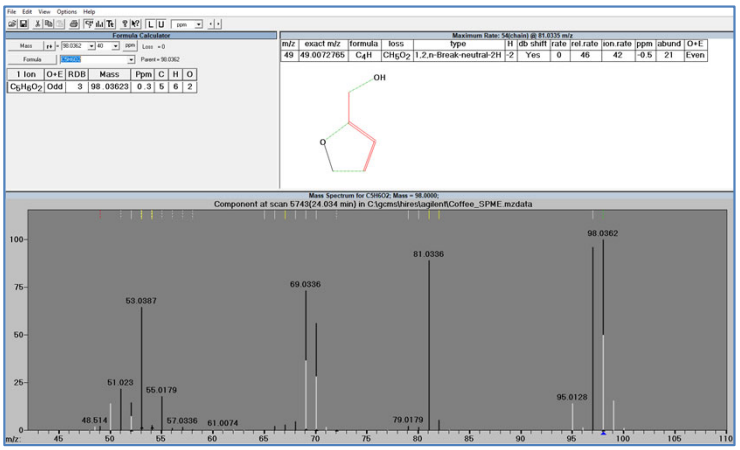


Easily Re-examine Results

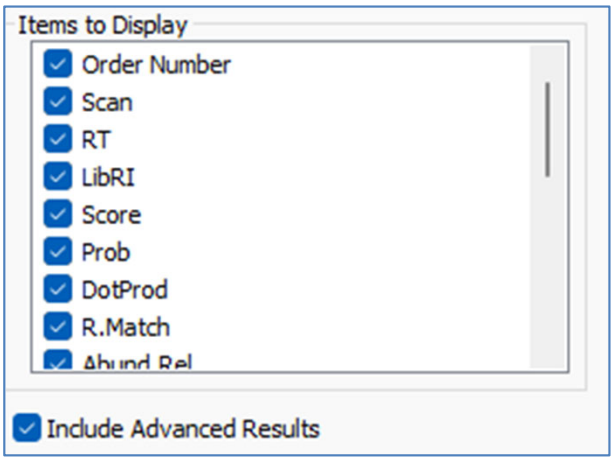
High Resolution GC/MS with AMDIS Deconvolution



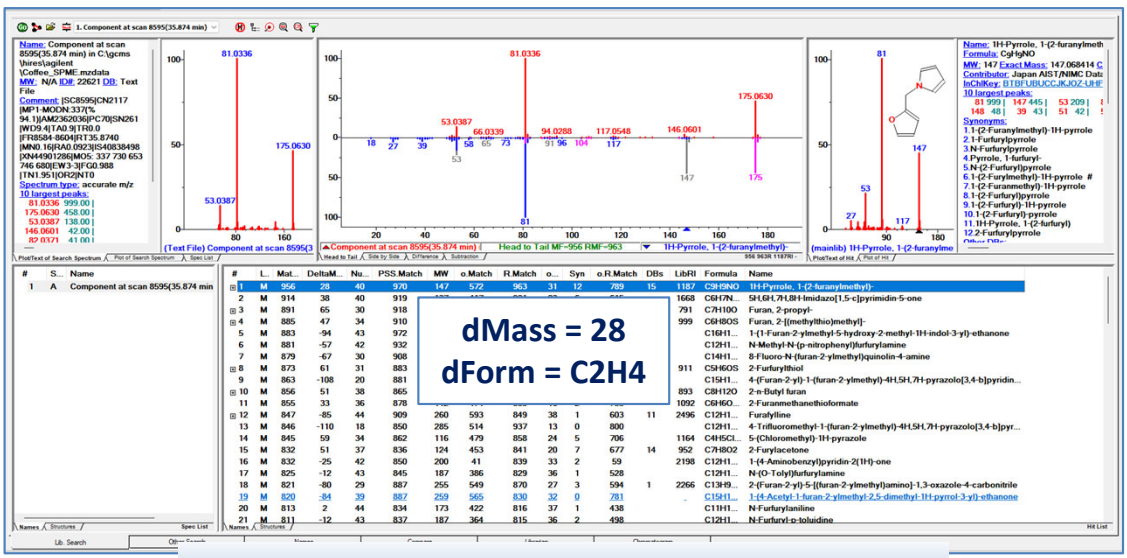
MS Interpreter - high or low resolution



Extensive Data



Hybrid Search - high or low resolution



Original Score = 700 –> Hybrid Score = 956