

NIST/EPA/NIH EI-MS Library

2026 Release

35K NEW NIST MEASURED/EVALUATED COMPOUNDS

431K Electron Ionization (EI) Spectra

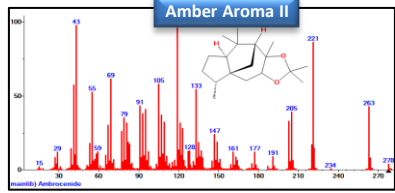
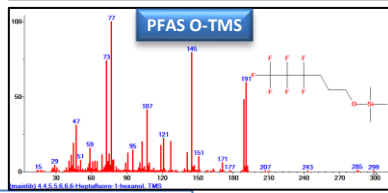
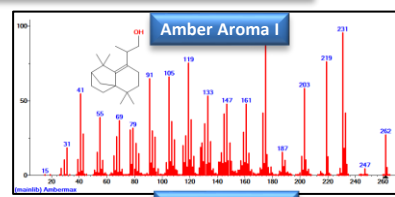
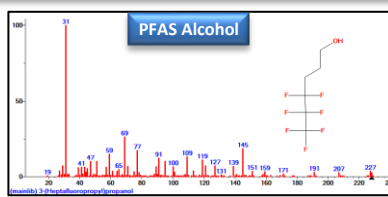
- 382,180 Compounds, 49,097 Replicate Spectra
- 35 K More Compounds than NIST 23

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

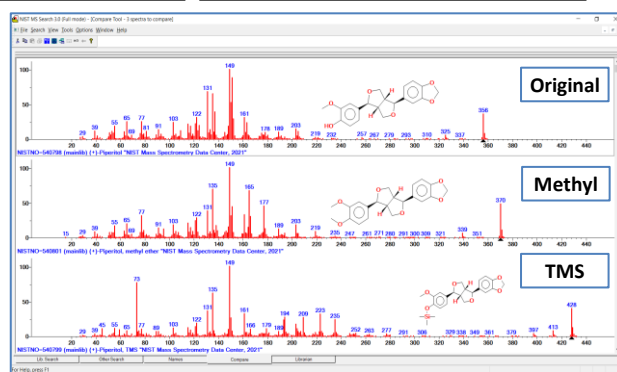
Name: Valeryl fentanyl
Formula: C₂₄H₃₂N₂O
MW: 364 **Exact Mass:** 364.251463 **CAS#:** 122882-90-0 **NIST#:** 463844 **ID#:** 18711
Contributor: NIST Mass Spectrometry Data Center
InChIKey: VCCPXHWAJYWQMR-UHFFFAOYSA-N **Non-stereo**
Synonyms:
 1 Pentanamide, N-phenyl-N-[1-(2-phenylethyl)-4-piperidinyl]-; 2 N-Phenyl-N-[1-(2-phenylethyl)-4-piperidinyl]-5-pentanamide
Other DBs:
 - Wikipedia
 - wikipedia2021_via_cheminfo_SMILES
 - Environmental
 - SUSDATAFY22
Experimental RI median±deviation (#data)
 Semi-standard non-polar: 2962±18 (2)
 Standard non-polar: 2958±N/A (1)
Estimated non-polar retention index (n-alkane scale):
 Value: 2938 iu
 Confidence interval (Nitrogen-containing): 83(50%) 356(95%) iu
Retention index:
 1. Value: 2980.5 iu
 Column Type: Capillary
 Column Class: Semi-standard non-polar
 Active Phase: HP-5MS
 Column Length: 30 m

Collections

RI Averages

AI-RI Estimates

RI Measured



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

RICH OUTPUT

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

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

Prior Probability
(OtherDBs)

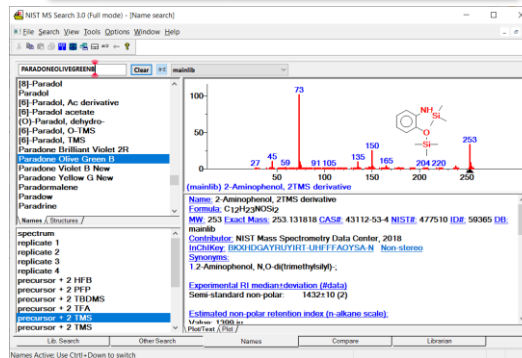
#	Library Match	R.M.	RI	Del.	S	DBs	Name
1	R	999	998	1442	0	1	2-Aminophenol, 2TMS deriva
2	M	965	965	1930	-50	0	3-Amino-2-naphthol, N,O-bis
3	M	965	965	1489*	-14	1	2-Amino-m-cresol, N,O-bis(tr
4	R	956	956	1309	-1	9	38 W...
5	M	955	957	1582	-17	1	5 E
6	M	953	953	2023*	-49	1	4-Mercaptophenol, 2TMS der
7	M	949	949	1449	-29	3	7 EFGN
8	M	947	947	1600	-34	4	2-amino-5-chlorophenol, N, C
9	M	941	942	1388	-15	2	21 W...
10	M	939	951	1778	-33	0	1 M
11	M	938	946	1469	-17	1	7 EM
12	M	936	945	1755	-33	1	2 E
13	M	933	937	1470	-43	9	8 EGM
14	M	931	931	1550	-28	1	2-Amino-4-ethylphenol, 2TM
15	M	929	929	1930	-50	0	2-Amino-1-naphthol, N,O-bisi

HIT LIST

COMPOUND/SPECTRUM LOOKUP

Names

Spectra
Replicates
Derivatives
Stereo



NIST EI Library Software

2026 EI Release

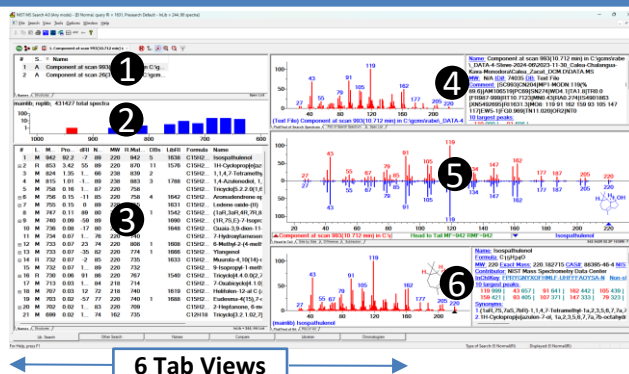
EI MS ANALYSIS TOOLS

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



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

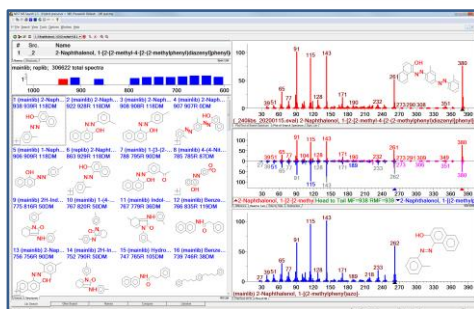
Hybrid Search

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

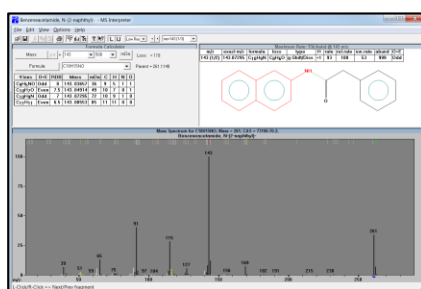


DMass	Replace or Insert
1	H->D, C->C13, NH->O, CH->N
2	CH2->O, C=C->C-C
12	CH2->C=CH2
14	X-Y->X-CH2-Y
16	X-Y->X-O-Y
17	NH->S
18	H->F
28	X-Y->X-CO-Y
30	H->CH3O-H
32	X-Y->X-S-Y
34	H->Cl
50	Phenyl->Naphthyl
76	H->Phenyl
162	H->Glucose

MS Interpreter

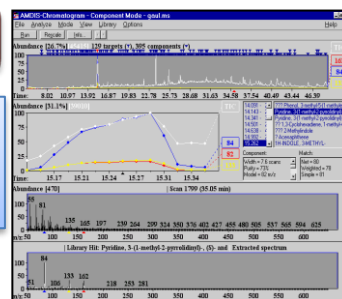
CONNECT PEAKS TO PLAUSIBLE FRAGMENTS (IN RED)

CONFIRM ID
COMPUTE FRAGMENT MASSES
CONNECT PEAKS TO STRUCTURES



AMDIS

'PURIFIES' SPECTRA AND CONNECTS TO NISTMS



FREELY AVAILABLE DATA AND SOFTWARE

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 v2.0.0 with a small demonstration library.

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_Plano (New, 2021) - A new software tool for annotating peaks in collision induced dissociation (CID) tandem mass spectra of peptides and N-glycopeptides.

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 methoximation 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 ethylxime for the non-acid carboxylic 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



<http://chemdata.nist.gov>

NEW

Full GC/MS Chromatogram Analysis by NIST EI Library

Quick Filtering

All MS, Color Coded IDs, Zoom/Rezoom Display

Query and Best Library Match

Hit List with Optional High Level of Detail

#	Scan	RT	Score	dRI	Prob	St...	D...	R.M.	#peaks	#m...	Abu...	n...	Pur...	Max...	Widt...	St...	PKU...	Ab...	Db...	Lib	Formula	LibRI	Lib ID	
166	1987	18.8935									0.0336	1	20.0	9.8	10	2.68	66.7	15.6		mainlib	C14H30O3S	1886	Sulfurous acid, butyl decyl ester	
167	2000	18.9798									0.00...	1	11.0	4.6	10	1.25	66.7	19.7		mainlib	C14H27NO5	1852	L-Leucine, N-(2-methoxyethoxy)carbonyl ester	
168	2015	19.0729									1.50	1	56.0	66.6	11	5.23	42.4	6.5	4		mainlib	C17H34O2	1883	Pentadecanoic acid, 14-methyl-, methyl ester
169	2018	19.0935									1.97	1	72.0	124.9	10	4.73	33.9	2.9	4		replib	C17H34O2	1883	Pentadecanoic acid, 14-methyl-, methyl ester
170	2028	19.1504									100	1	96.0	159.8	11	4.61	0.0	0.0	31		mainlib	C17H34O2	1926	Hexadecanoic acid, methyl ester
171	2032	19.1772									0.0235	1	2.4	10.0	7	0.0235	11.0	3.9	12		mainlib	C17H34O2	1883	Pentadecanoic acid, 14-methyl-, methyl ester
172	2054	19.3166									0.0715	1	36.0	6.2	10	0.0715	11.0	3.9	12		mainlib	C17H34O2	1883	Pentadecanoic acid, 14-methyl-, methyl ester
173	2062	19.3653									0.0209	1	11.0	3.9	12	0.0209	11.0	3.9	12		mainlib	C17H34O2	1883	Pentadecanoic acid, 14-methyl-, methyl ester
174	2103	19.6247									0.00...	1	6.2	4.7	10	0.00...	11.0	3.9	12		mainlib	C17H34O2	1883	Pentadecanoic acid, 14-methyl-, methyl ester
175	2138	19.8415									0.00...	1	3.6	5.3	15	0.00...	11.0	3.9	12		mainlib	C17H34O2	1883	Pentadecanoic acid, 14-methyl-, methyl ester
176	2145	19.8827									0.0223	1	18.0	14.7	12	0.0223	11.0	3.9	12		mainlib	C17H34O2	1883	Pentadecanoic acid, 14-methyl-, methyl ester
177	2156	19.9471									0.00...	1	8.7	4.8	11	0.00...	11.0	3.9	12		mainlib	C17H34O2	1883	Pentadecanoic acid, 14-methyl-, methyl ester
178	2183	20.1214									0.265	1	49.0	55.5	17	0.265	11.0	3.9	12		mainlib	C17H34O2	1883	Pentadecanoic acid, 14-methyl-, methyl ester
179	2187	20.1477									0.125	1	46.0	17.8	13	0.125	11.0	3.9	12		mainlib	C17H34O2	1883	Pentadecanoic acid, 14-methyl-, methyl ester
180	2210	20.2896									0.0953	1	38.0	3.5	10	0.0953	11.0	3.9	12		mainlib	C20H32O2	2058	(E)-Valerenyl isovalerate
181	2218	20.3408									0.0933	1	33.0	3.9	12	0.0933	11.0	3.9	12		mainlib	C16H30O4	2054	Dimethyl tetradecanedioate
182	2229	20.4064	451	2045	-6	66	451	420	641	16	6	0.00...	1	7.3	3.1	13	5.96	75.0	62.3		mainlib	C12H11O3	2051	1-Acetyl-2,6-naphthalenediol

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

Reopen EI Results

C:\GMS\RABE\2024-05-14-Hemp_Key-Gene\Hemp-fower-DCM-conc.D\DATA.MS

Banisteriopsis-muricata_DCM-R2
Hemp-fower-DCM-conc

Oban_14_EI_1_...
Oban_14_EI_1_...
Val_14_70eV_4a_01
PMAG1559
N-Methylperfluorooctane sulfonamide-mod2
N-Methylperfluorooctane sulfonamide-mzml
Orbitrap_01
Copaliba Balam 10%,mzdata
8169_3_07
Coffee_SPME
1.1
30cm 1

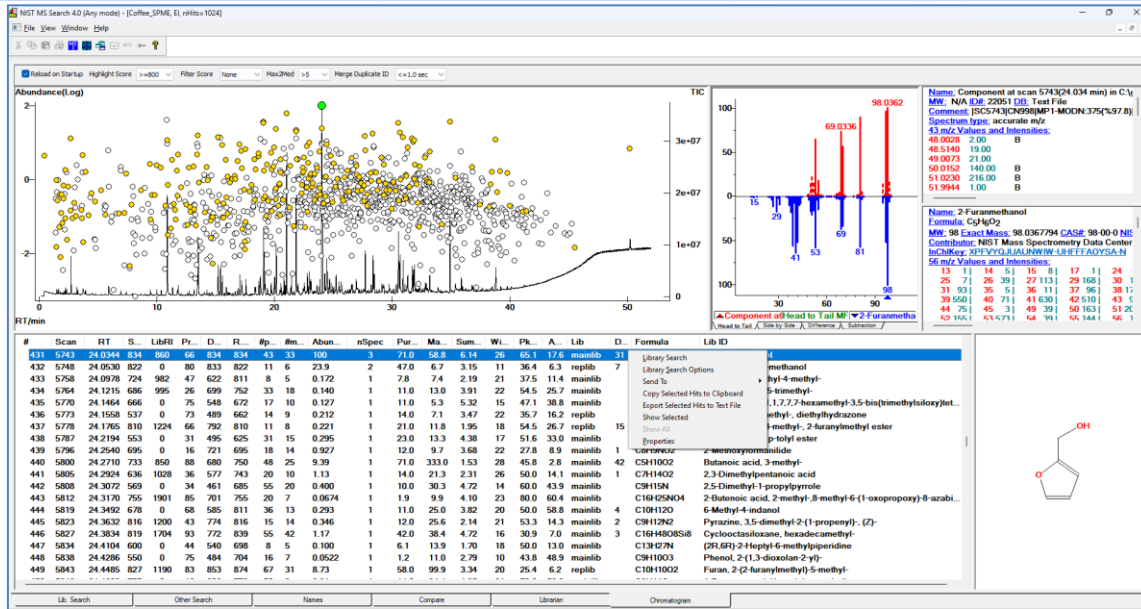
Run Options

Mode: LowRes
Calibration file: C:\gms\ra\be\2024-05-14-Hemp_Key-Gene\2024-05-14-HEMP_KEY-GENE.cal
RI tolerance: 20
RI penalty rate: Average
Component width: 20
Adjacent peak subtraction: One
Resolution: Medium
Sensitivity: Medium
Shape requirements: Medium
Combine scans: None
Min m/z: 1
Libraries: mainlib; replib
Date: December 21, 2025

OK Cancel Help

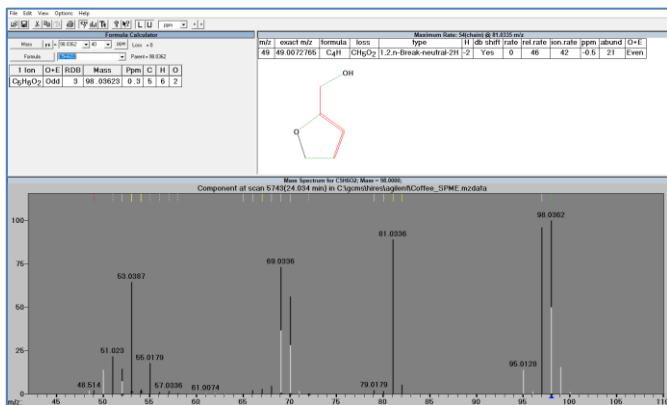
Easily Re-examine Results

High Resolution GC/MS with AMDIS Deconvolution



MS Interpreter - high or low resolution

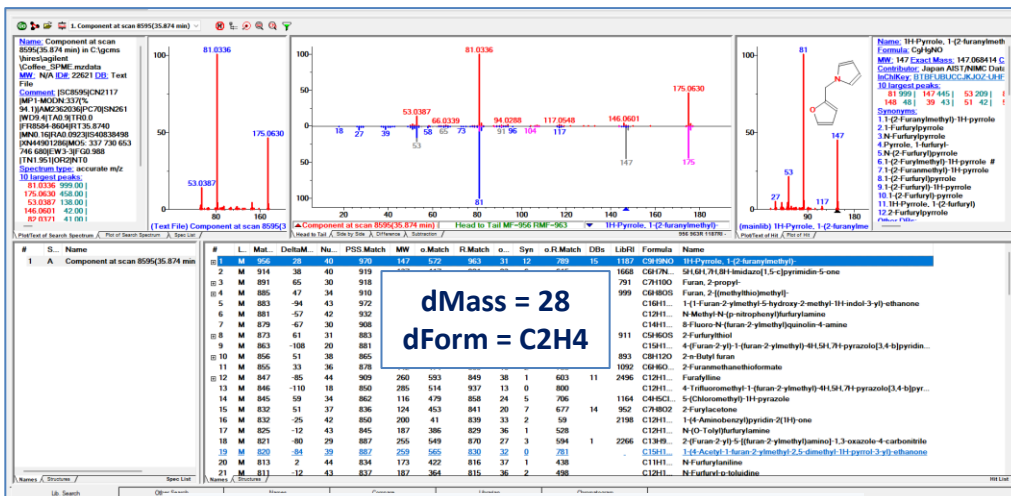
Extensive Data



Items to Display

- Order Number
- Scan
- RT
- LibRI
- Score
- Prob
- DotProd
- R.Match
- Abund Rel
- Include Advanced Results

Hybrid Search - high or low resolution



Original Score = 700 → Hybrid Score = 956