NIST/EPA/NIH EI-MS LIBRARY

2023 Release

40K New NIST Measured/Evaluated Compounds

1.7

394K Electron Ionization (EI) Spectra

- 347,100 Compounds, 46,954 Replicate Spectra
- 40 K More Compounds than NIST 20

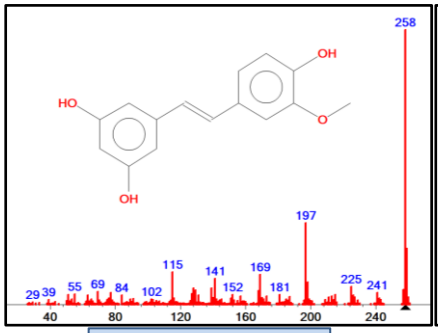
492K Retention Index (RI) Values

- 153K RI Compounds with EI, >40 K Increase
- AI-RI Estimates for All EI Compounds

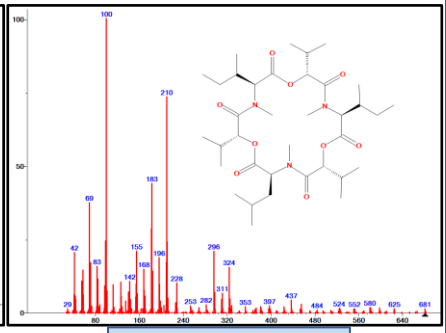
Compounds Selected for Analytical Relevance

Fully Evaluated with Derivatives, Retention Indices & Class Information

Citation	New	Total
Wikipedia	1570	6227
EPA Tox	2969	7117
Food DB	582	4273
EU Contaminants	6263	15149
Protein Data Bank	1194	4716
Human Metabolite DB	1992	9393
PFAS	161	749
Adams (Essential Oils)	2136	2136



Plant Stilbenoid



Myocotoxin ENN A

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-pi
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)

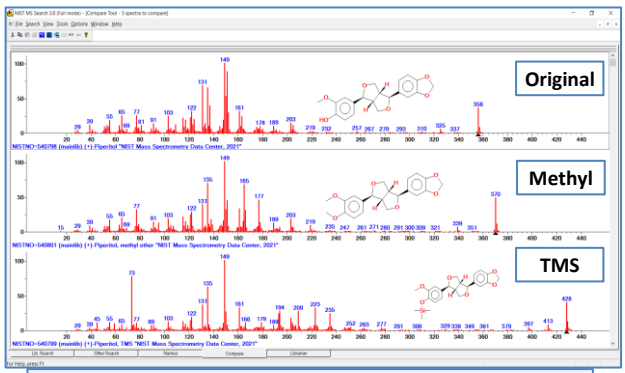
RI Averages →

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)

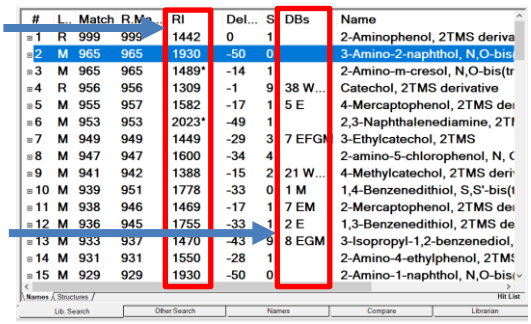
Enhancements

Hit List

New: Retention Index For All Hits (Expt'l or AI-RI*)

Select Columns Mass Difference, Reverse Score, Probability, …

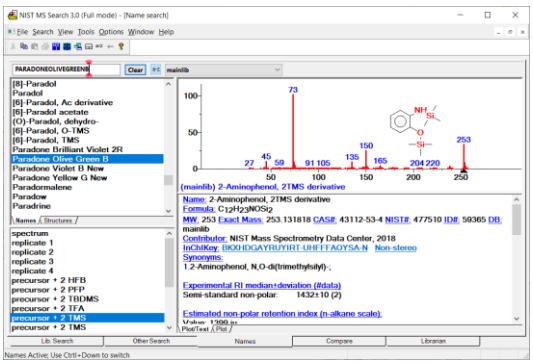
New: Expanded Compound Classes



Compound/Spectrum Lookup

Names

Spectra
Replicates
Derivatives
Stereo



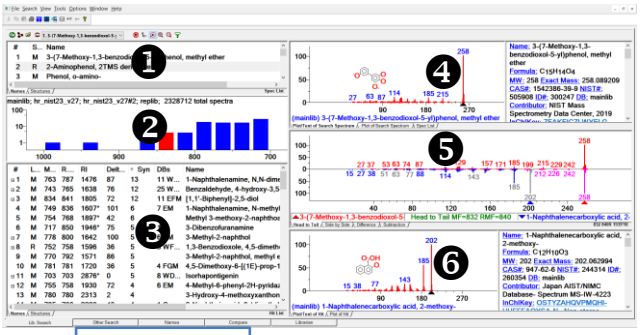
NIST EI LIBRARY SOFTWARE

2023 EI Release

EI MS Analysis Tools

NISTMS

- Full Featured MS Library Search/Display Program
- Multiple Search Types & Display Modes
- 5 Views: Spectrum Search, Feature Search, Compare, Name/Spectrum, User Library



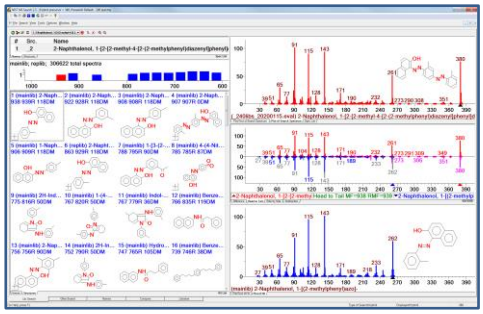
5 Tab Views

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 Found in Library & ID Confirmation
- Finds 'Modified' Library IDs and Masses of Modifications With Their Shifted Peaks
- Uses MW Estimate

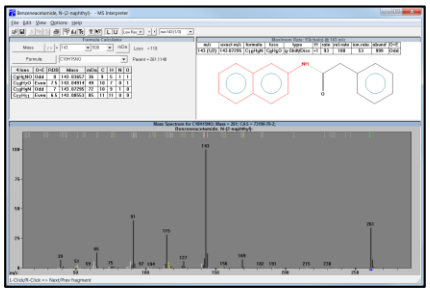
Delta Mass => Chemical Formula



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

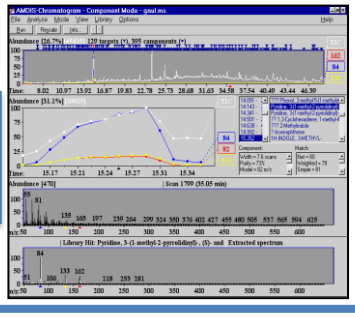
MS Interpreter

- 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.

NIST Tandem Mass Spectral Library

2023 Release

51,501 Compounds, 60% More than 2020
400 K Precursor Ions – 2.4 M Spectra

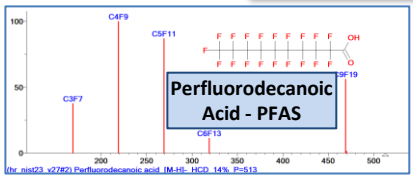
Fragmentation Methods

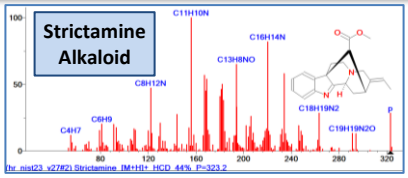
- 49,590 HRAM (High Res Accurate Mass) Compounds
- 50,071 QTOF, HCD, IT-HRAM, QqQ Compounds
- 49,561 Ion Trap Compounds (Low Res., up to MS^4)
- 561 APCI HRAM Compounds

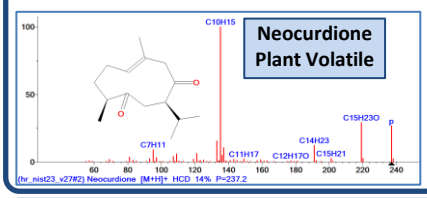
Precursor Ion Types

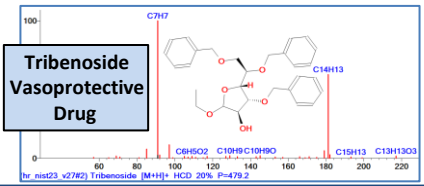
- 44,191 Protonated
- 19,620 Deprotonated
- 14,318 Water/Ammonia Loss
- 44,547 Other In-Source Generated

All Compounds Selected for Relevance
Measured at NIST, Thoroughly Evaluated







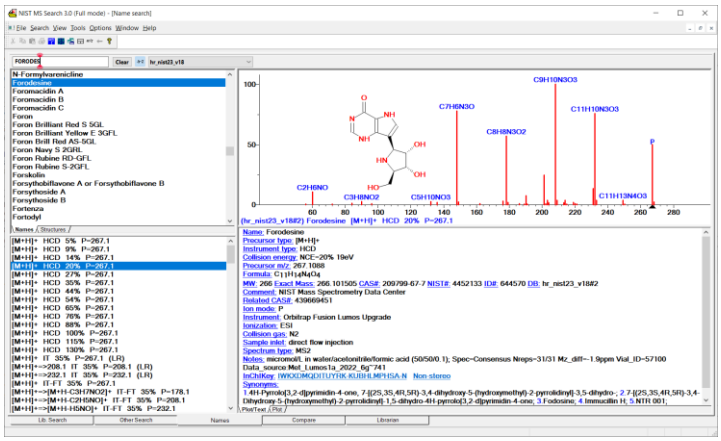


Citation	New	Total
Wikipedia	1618	6424
EPA Tox	3181	8146
Food DB	602	4491
EU Contaminants	6553	15818
Protein Data Bank	1246	4945
Human Metabolite DB	2071	9686
PFAS	90	116

All Spectra Shown for Each Compound

1. Compound Name Many Synonyms

2. All Related Spectra All Energies Fragmentation Types In-Source Ions, …



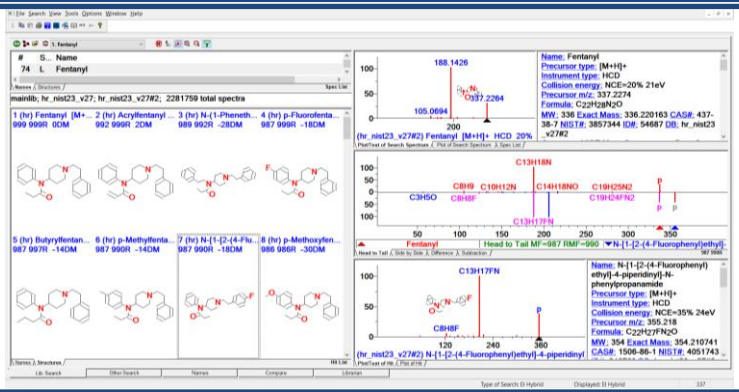
Full Spectrum Selected from List at Lower Left

All Spectrum Text Information

Hybrid Search
Recommended for All Tandem MS Searches

Find Related Compounds Even if Query is not in Library

Differences in masses are 'Modifications'



Query Spectrum

Shifted Library Peaks (gray->red) Contain Modification

Library Spectrum

NIST TANDEM LIBRARY SOFTWARE

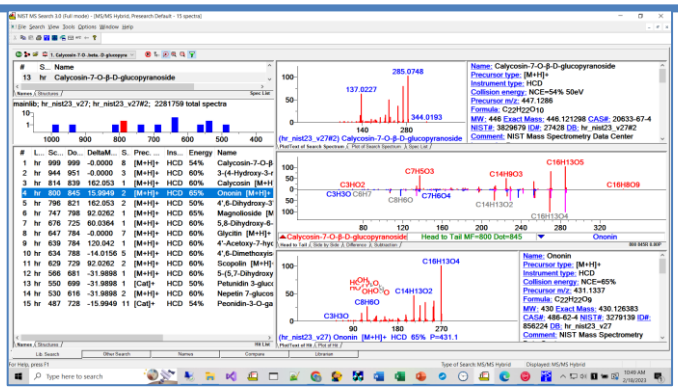
2023 Tandem Release

Tandem (MS/MS) Analysis Tools

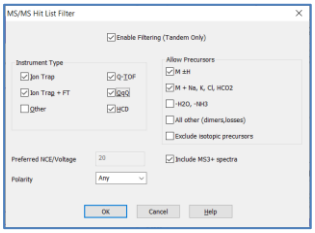
NISTMS

All Spectra for Each Compound in One List

Multiple Energies Ion Modes Fragmentation Type In Source Ions



Filter IDs by Spectrum Type



Hybrid Search

-Finds Compounds Not in Library and Confirms IDs
-Uses Peaks and Losses
-Shows Shifted Peaks

Recommended For Routine Use

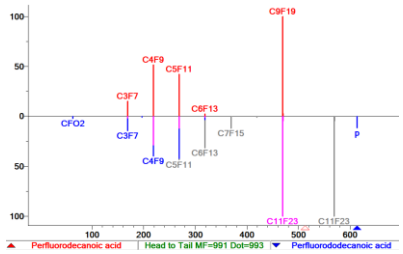
#	L..	S...	D...	DeltaMa...	DBs	Prec. ...	Inst...	En...	Name
1	hr	935	999	-0.0000	20 EGM	[M-H]-	HCD	20%	Perfluoroheptanoic acid [M-H]-
2	hr	891	976	-49.9968	27 WC...	[M-H]-	HCD	20%	Perfluorooctanoic acid [M-H]-
3	hr	866	938	-99.9936	24 WC...	[M-H]-	HCD	14%	Perfluorononanoic acid [M-H]-
4	hr	511	796	-249.984	18 CE...	[M-H]-	HCD	27%	Perfluorododecanoic acid [M-H
5	hr	466	714	-149.990	22 WC...	[M-H]-	HCD	9%	Perfluorodecanoic acid [M-H]-
6	hr	460	828	-199.987	18 CE...	[M-H]-	HCD	44%	Perfluoroundecanoic acid [M-H

1 (hr) Perfluorodecanoic acid [...
999 999R 0.00P -0.0000DM

2 (hr) Perfluorododecanoic acid...
991 993R 0.00P -99.9937DM

3 (hr) Perfluoroundecanoic acid
985 985R 0.00P -49.9968DM

PFAS Illustration: Applicable to Many Classes



MS Interpreter

Direct Access From NISTMS

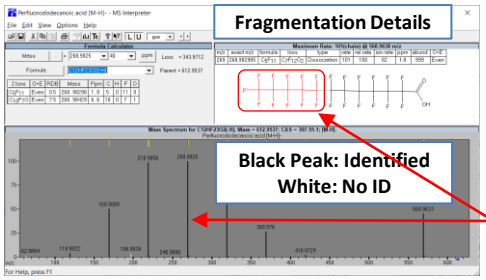
Connect Peaks to Structure

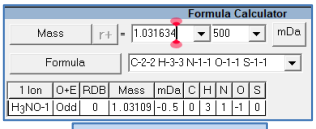
Chemical Formula Calculator

Isotope Calculator

Any resolution +/- Charge

Multiple Display Options





Find Formula from Delta Mass

NIST Website Chemdata.nist.gov

Freely Available Libraries and Software

Downloadable Libraries

Annotated Recurrent Unidentified Spectra
Urine, Plasma/Serum (ARUS)
Tryptic Peptides (Human, ...)
Oligosaccharide Libraries (Milk)
Glycopeptides (mAb, Glycan Distributions)
Acyl Carnitines

Software

NISTMS (2019)
MS Piano (Peptide a\Annotation)
MS Pepsearch – General Search Utility for NIST Libraries
MS Interpreter
Lib2NIST – Library Conversion

http://chemdata.nist.gov

NIST National Institute of Standards and Technology U.S. Department of Commerce