

# NIST/EPA/NIH EI-MS LIBRARY

## 2023 Release

### 40K NEW NIST MEASURED/EVALUATED COMPOUNDS

#### 394K Electron Ionization (EI) Spectra

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

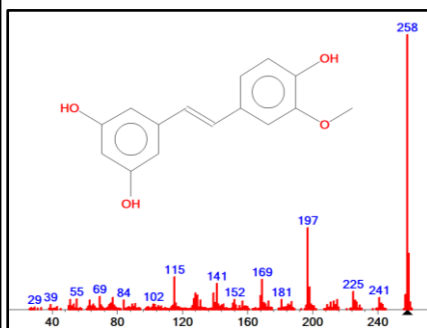
#### 492K Retention Index (RI) Values

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

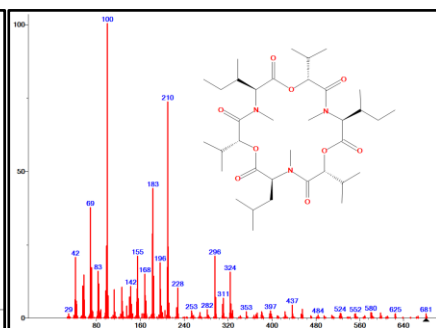
### COMPOUNDS SELECTED FOR ANALYTICAL RELEVANCE

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



Mycotoxin ENNA

#### Compound Data

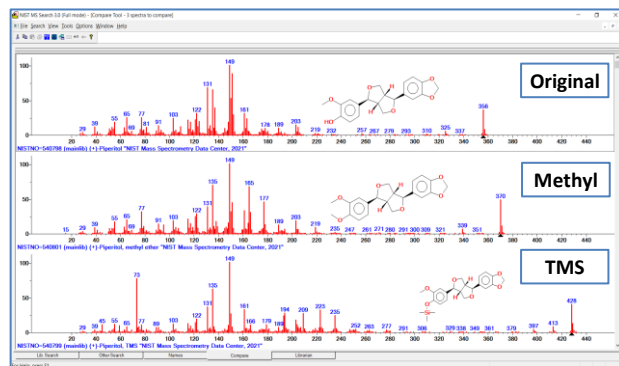
**Name:** Valeryl fentanyl  
**Formula:** C<sub>24</sub>H<sub>32</sub>N<sub>2</sub>O  
**MW:** 364 **Exact Mass:** 364.251463 **CAS#:** 122882-90-0 **NIST#:** 463844 **ID#:** 18711  
**Contributor:** NIST Mass Spectrometry Data Center  
**InChIKey:** VCCPXHWAJYWQMR-UHFFFAOYSA-N **Non-steric**  
**Synonyms:**  
 1 Pentanamide, N-phenyl-N-[1-(2-phenylethyl)-4-piperidinyl]-; 2 N-Phenyl-N-[1-(2-phenylethyl)-4-piperidinyl]-  
**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)

### ENHANCEMENTS

### Hit List

### Compound/Spectrum Lookup

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

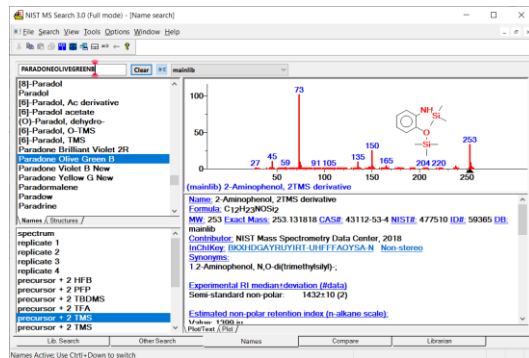
**Select Columns Mass Difference, Reverse Score, Probability, ...**

**New: Expanded Compound Classes**

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

#### Names

#### Spectra Replicates Derivatives Stereo



# NIST EI LIBRARY SOFTWARE

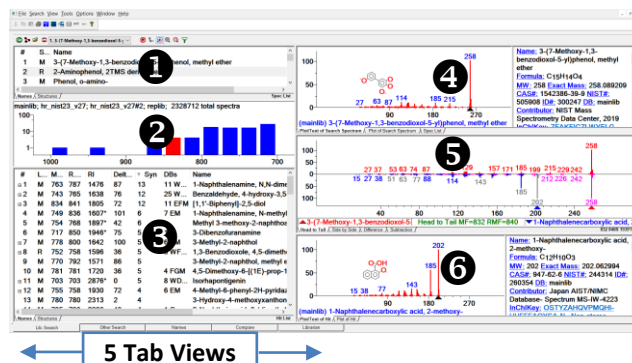
## 2023 EI Release EI MS ANALYSIS TOOLS

### NISTMS

FULL FEATURED MS LIBRARY SEARCH/DISPLAY PROGRAM

MULTIPLE SEARCH TYPES & DISPLAY MODES

5 VIEWS: SPECTRUM SEARCH, FEATURE SEARCH, COMPARE, NAME/SPECTRUM, USER LIBRARY



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

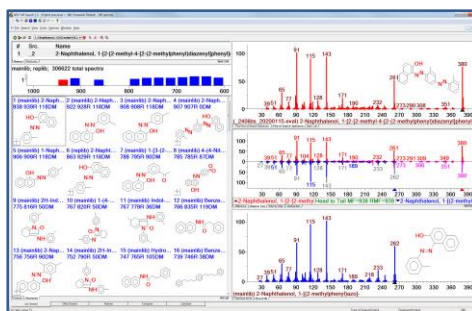
### Hybrid Search

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

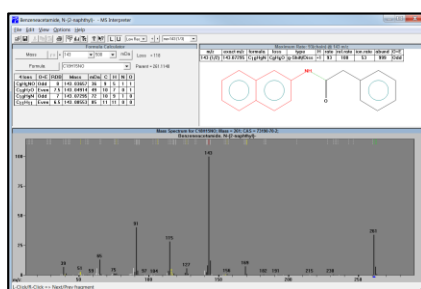


DMass	Replace or Insert
1	H->D, C->C13, NH->O, CH->N
2	CH2->O, C=C->C-C
12	CH2->C=CH2
14	X-Y->X-CH2-Y
16	X-Y->X-O-Y
17	NH->S
18	H->F
28	X-Y->X-CO-Y
30	H->CH3O-H
32	X-Y->X-S-Y
34	H->Cl
56	Phenyl->Naphthyl
70	H->Phenyl
162	H->Glucose

### MS Interpreter

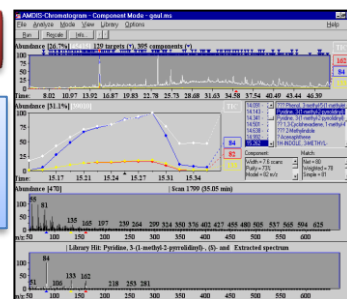
CONNECT PEAKS TO PLAUSIBLE FRAGMENTS (IN RED)

CONFIRM ID  
COMPUTE FRAGMENT MASSES  
CONNECT PEAKS TO STRUCTURES



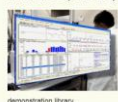
### AMDIS

'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 molecules and peptides), 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's MS Search Program v3.29 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\_Piano (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>

# NIST Tandem Mass Spectral Library

## 2023 Release

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

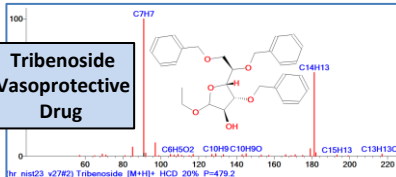
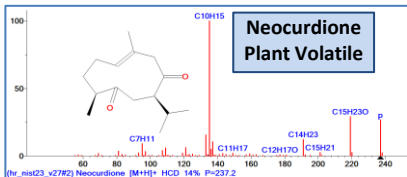
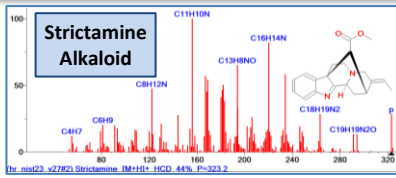
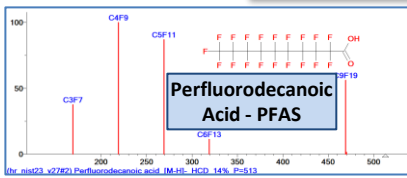
### Fragmentation Methods

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<sup>4</sup>)  
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

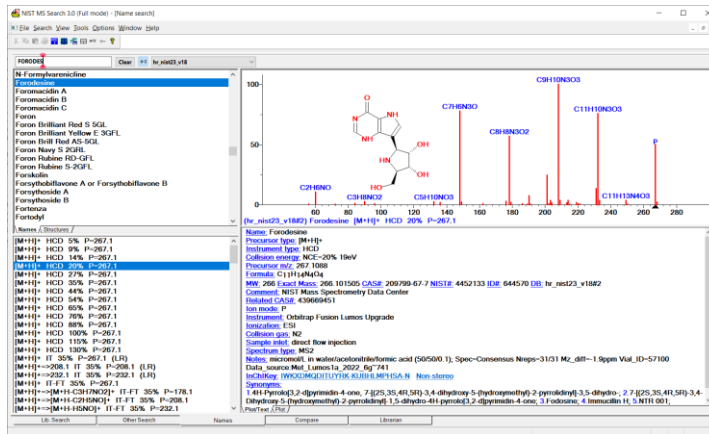


Citation	New	Total
Wikipedia	1618	6424
EPA Tox	3181	8146
Food DB	602	4491
EU Contaminants	6553	15818
Protein Data Bank	1246	4945
Human Metabolite DB	2071	9686
PFAS	90	116

### 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

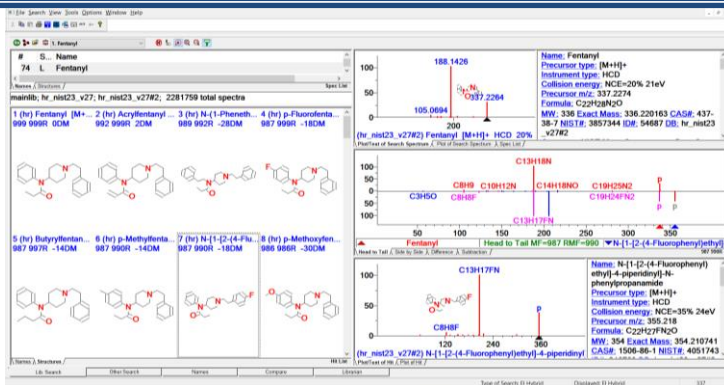
All Spectrum Text  
Information

### 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

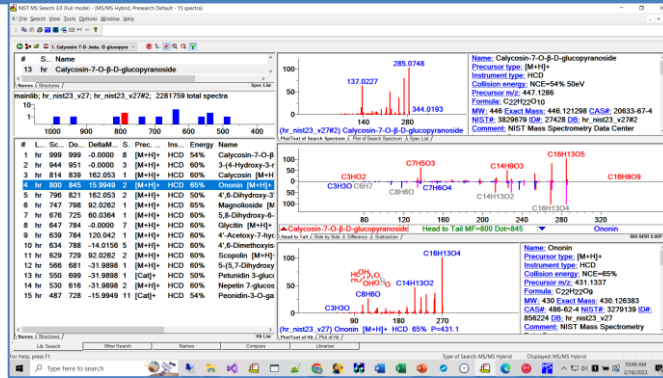
## 2023 Tandem Release

### 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

M/SMS Hit List Filter

Enable Filtering (Tandem Only)

Instrument Type:  Ion Trap,  Ion Trap + FT,  Other

Allow Precursors:  C16-H,  C16-H + Na, K, Cl, HCO2,  H2O, H4O,  All other (demon/losses),  Exclude isotopic precursors

Preferred HCE/Voltage: 20

Polarity: Any

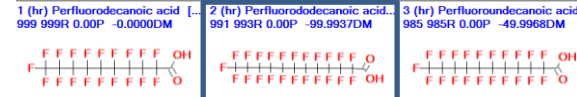
Buttons: OK, Cancel, Help

#### Hybrid Search

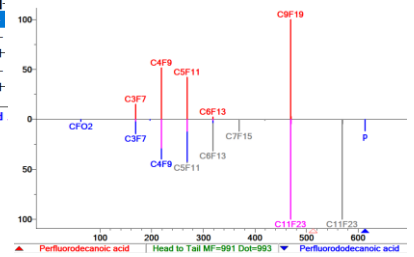
-FINDS COMPOUNDS NOT IN  
LIBRARY AND CONFIRMS IDS  
-USES PEAKS AND LOSSES  
-SHOWS SHIFTED PEAKS

RECOMMENDED FOR  
ROUTINE USE

#	L.	S.	D.	DeltaMa...	DBs	Prec. ...	Inst...	En...	Name
1	hr	935	999	-0.0000	20 EGM	[M-H] <sup>-</sup>	HCD	20%	Perfluoroheptanoic acid [M-H] <sup>-</sup>
2	hr	891	976	-49.9968	27 WC...	[M-H] <sup>-</sup>	HCD	20%	Perfluoro-octanoic acid [M-H] <sup>-</sup>
3	hr	866	938	-99.9936	24 WC...	[M-H] <sup>-</sup>	HCD	14%	Perfluoro-nonoic acid [M-H] <sup>-</sup>
4	hr	511	796	-249.984	18 CE...	[M-H] <sup>-</sup>	HCD	27%	Perfluoro-dodecanoic acid [M-H] <sup>-</sup>
5	hr	466	714	-149.990	22 WC...	[M-H] <sup>-</sup>	HCD	9%	Perfluoro-decanoic acid [M-H] <sup>-</sup>
6	hr	460	828	-199.987	18 CE...	[M-H] <sup>-</sup>	HCD	44%	Perfluoro-undecanoic acid [M-H] <sup>-</sup>



PFAS ILLUSTRATION: APPLICABLE TO MANY CLASSES



#### MS Interpreter

DIRECT ACCESS  
FROM NISTMS

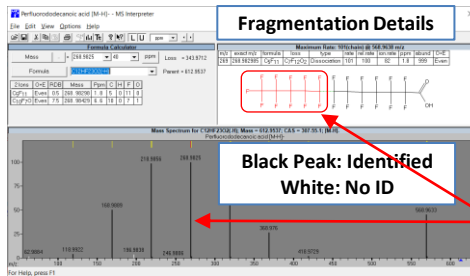
CONNECT PEAKS  
TO STRUCTURE

Chemical Formula  
Calculator

Isotope Calculator

Any resolution  
+/- Charge

Multiple Display  
Options



Formula Calculator

Mass: 1.031634, mDa: 500

Formula: C2-2 H-3 N-1 O-1 S-1

1 Ion	O+E	RDB	Mass	mDa	C	H	N	O	S
H3NO-1	Odd	0	1.03109	-0.5	0	3	1	1	0

Find Formula from  
Delta Mass

Select Peak  
Show Structure  
Fragment

#### 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>