

# 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

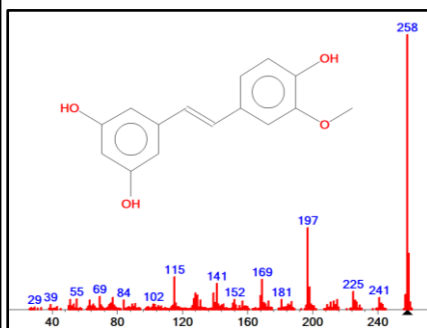
#### 492K Retention Index (RI) Values

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

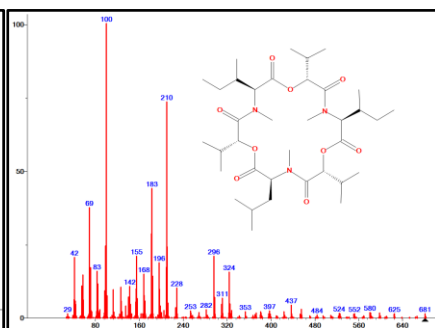
### COMPOUNDS SELECTED FOR ANALYTICAL RELEVANCE

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 ENN A

#### Compound Data

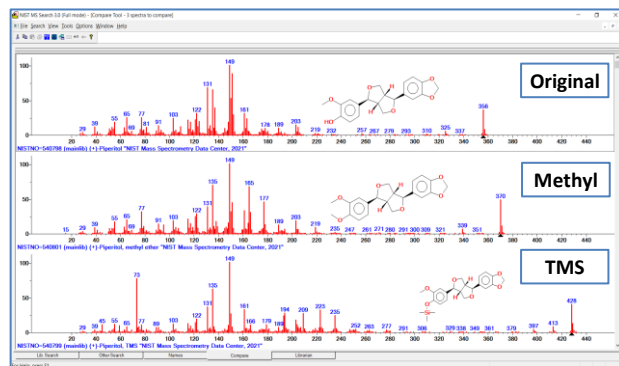
**Name:** Valeryl fentanyl  
**Formula:** C<sub>24</sub>H<sub>32</sub>N<sub>2</sub>O  
**MW:** 364 **Exact Mass:** 364.251463 **CAS#:** 122882-90-0 **NIST#:** 463844 **ID#:** 18711  
**Contributor:** NIST Mass Spectrometry Data Center  
**InChIKey:** VCCPXHWAJYWQMR-UHFFFAOYSA-N **Non-steric**  
**Synonyms:**  
 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\*)**

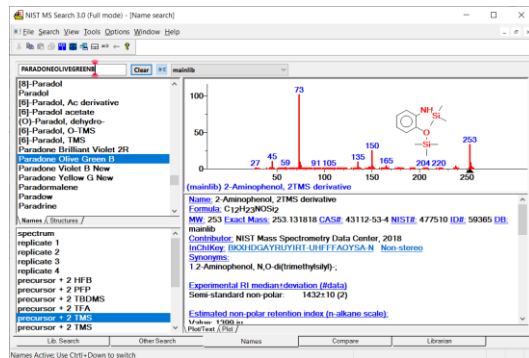
**Select Columns Mass Difference, Reverse Score, Probability, ...**

**New: Expanded Compound Classes**

#	Lib	Match	R.M.	RI	Del...	S	DBs	Name
1	R	999	999	1442	0	1		2-Aminophenol, 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...	Catechol, 2TMS derivative
5	M	955	957	1582	-17	1	5 E	4-Mercaptophenol, 2TMS deri
6	M	953	953	2023*	-49	1		2,3-Naphthalenediamine, 2TI
7	M	949	949	1449	-29	3	7 EFGN	3-Ethylcatechol, 2TMS
8	M	947	947	1600	-34	4		2-amino-5-chlorophenol, N, C
9	M	941	942	1388	-15	2	21 W...	4-Methylcatechol, 2TMS deri
10	M	939	951	1778	-33	0	1 M	1,4-Benzenedithiol, S,S'-bis(t
11	M	938	946	1469	-17	1	7 EM	2-Mercaptophenol, 2TMS de
12	M	936	945	1755	-33	1	2 E	1,3-Benzenedithiol, 2TMS de
13	M	933	937	1470	-43	9	8 EGM	3-Isopropyl-1,2-benzenediol,
14	M	931	931	1550	-28	1		2-Amino-4-ethylphenol, 2TMS
15	M	929	929	1930	-50	0		2-Amino-1-naphthol, N,O-bisi-

#### Names

#### Spectra Replicates Derivatives Stereo



# NIST EI LIBRARY SOFTWARE

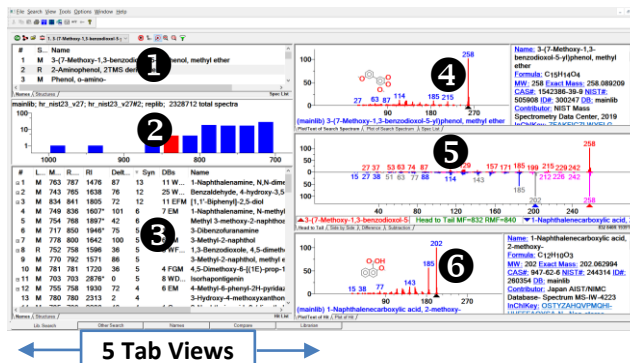
## 2023 EI Release EI MS ANALYSIS TOOLS

### 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

5 Tab Views

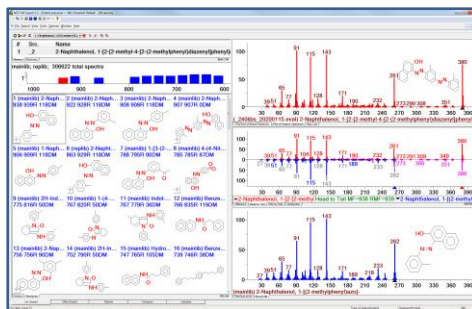
### Hybrid Search

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

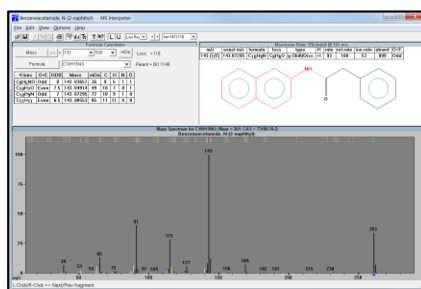


DMass	Replace or Insert
1	H->D, C->C13, NH->O, CH->N
2	CH2->O, C=C->C-C
12	CH2->C=CH2
14	X-Y->X-CH2-Y
16	X-Y->X-O-Y
17	NH->S
18	H->F
28	X-Y->X-CO-Y
30	H->CH3O-H
32	X-Y->X-S-Y
34	H->Cl
56	Phenyl->Naphthyl
70	H->Phenyl
162	H->Glucose

### MS Interpreter

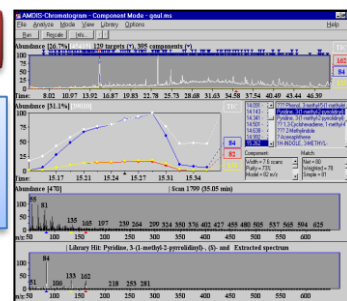
CONNECT PEAKS TO PLAUSIBLE FRAGMENTS (IN RED)

CONFIRM ID  
COMPUTE FRAGMENT MASSES  
CONNECT PEAKS TO STRUCTURES



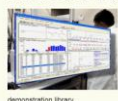
### AMDIS

'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 Web Search Program v2.0 with a small

#### 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 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



<http://chemdata.nist.gov>