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

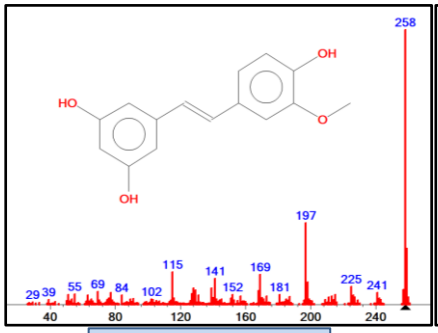
492K Retention Index (RI) Values

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

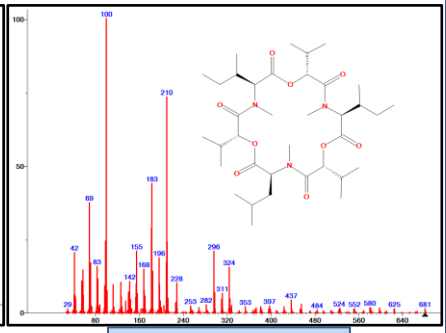
Compounds Selected for Analytical Relevance

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

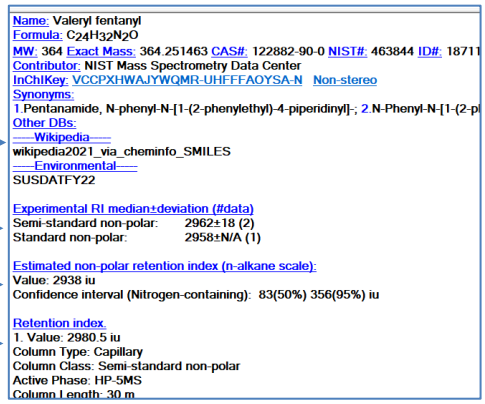


Plant Stilbenoid



Myocotoxin ENN A

Compound Data

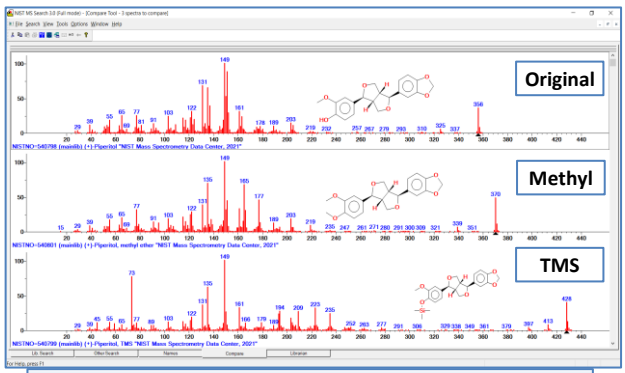


Collections →

RI Averages →

AI-RI Estimates →

RI Measured →



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

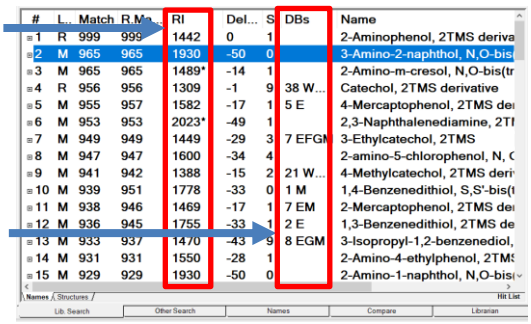
Enhancements

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

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

New: Expanded Compound Classes

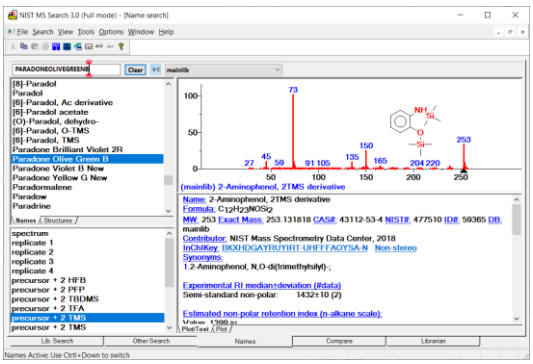
Hit List



Compound/Spectrum Lookup

Names

Spectra
Replicates
Derivatives
Stereo



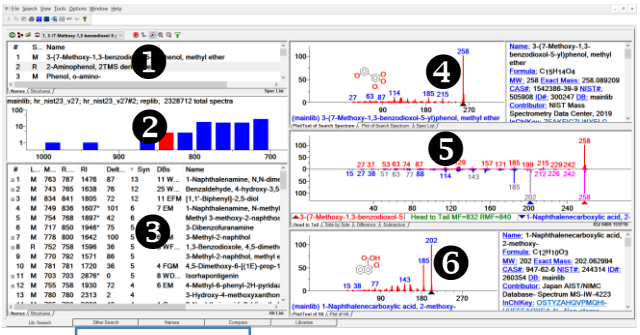
NIST EI LIBRARY SOFTWARE

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



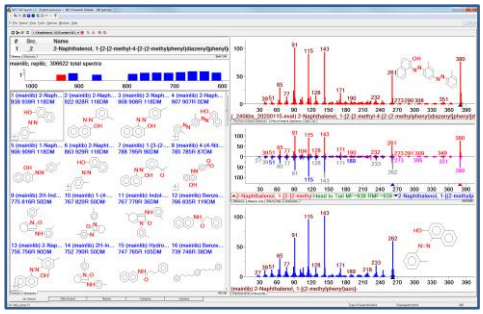
5 Tab Views

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

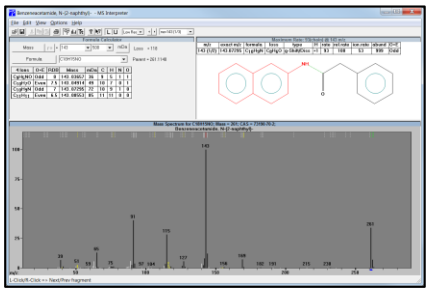
Delta Mass => Chemical Formula



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

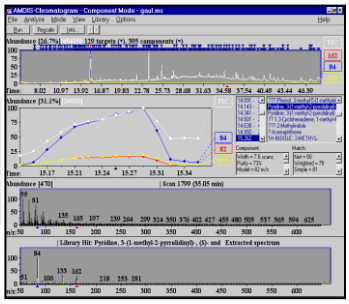
MS Interpreter

- 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.