

NIST/EPA/NIH EI-MS Library

2026 Release

35K NEW NIST MEASURED/EVALUATED COMPOUNDS

431K Electron Ionization (EI) Spectra

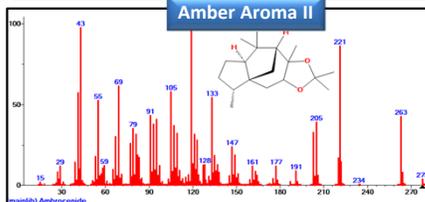
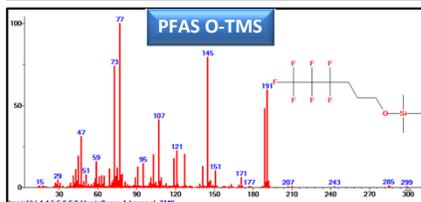
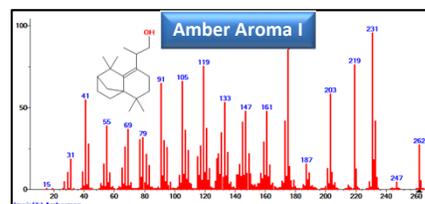
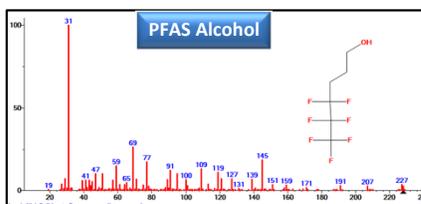
- 382,180 Compounds, 49,097 Replicate Spectra
- 35 K More Compounds than NIST 23

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

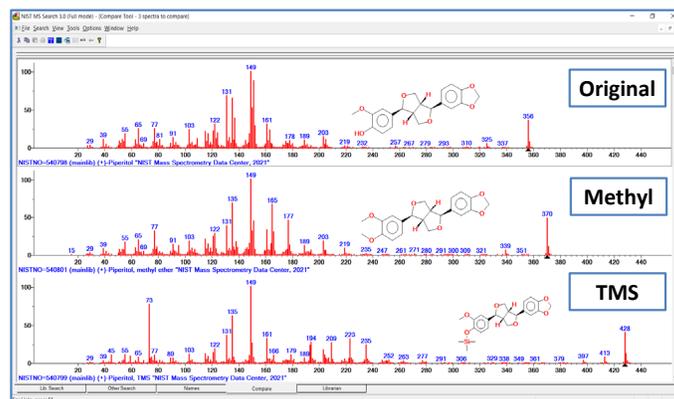
Name: Valeryl fentanyl
 Formula: C₂₄H₃₂N₂O
 MW: 364 Exact Mass: 364.251463 CAS#: 122882-90-0 NIST#: 463844 ID#: 18711
 Contributor: NIST Mass Spectrometry Data Center
 InChIKey: VCCPXHWAIYQWQR-UHFFFAOYSA-N Non-stereo
 Synonyms:
 1-Pentanamide, N-phenyl-N-[1-(2-phenylethyl)-4-piperidinyl]-; 2-N-Phenyl-N-[1-(2-phenylethyl)-4-piperidinyl]-
 Other DBs:
 -Wikipedia-
 wikipedia2021 via cheminfo_SMILES
 -Environmental-
 SUSDATFY22
 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

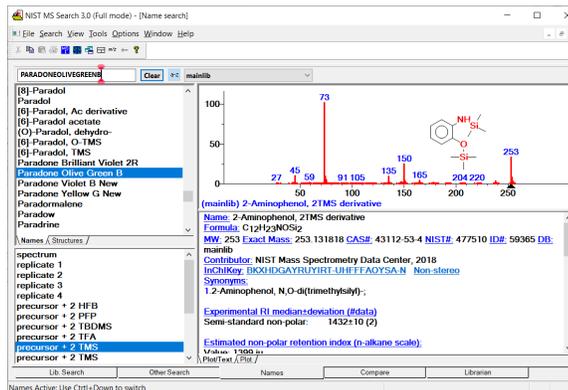
HIT LIST

COMPOUND/SPECTRUM LOOKUP

Retention Index For All Hits (Expt'l or AIRI*)	#	L	Match	R	Me	RI	Del...	S	DBs	Name
	1	R	999	995		1442	0	1		2-Aminophenol, 2TMS deriva
Select Columns Mass Difference, Reverse Score, Probability, ...	2	M	965	965		1930	-50	0		3-Amino-2-naphthol, N,O-bis
Prior Probability (OtherDBs)	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 der
	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(1
	11	M	938	946		1469	-17	1	7 EM	2-Mercaptophenol, 2TMS der
	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, 2TM
	15	M	929	929		1930	-50	0		2-Amino-1-naphthol, N,O-bisi

Names

Spectra
 Replicates
 Derivatives
 Stereo



NIST EI Library Software

2026 EI Release

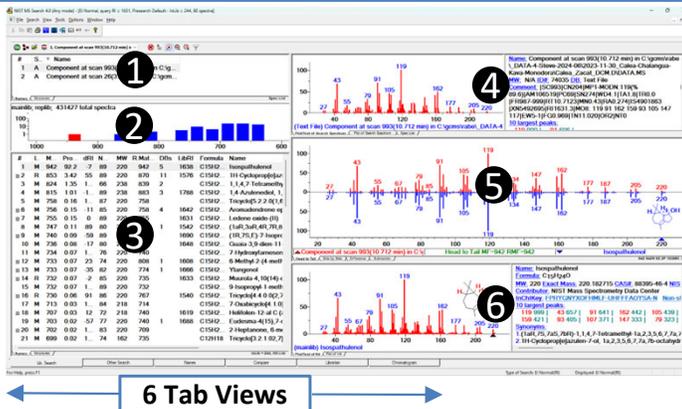
EI MS ANALYSIS TOOLS

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

6 Tab Views

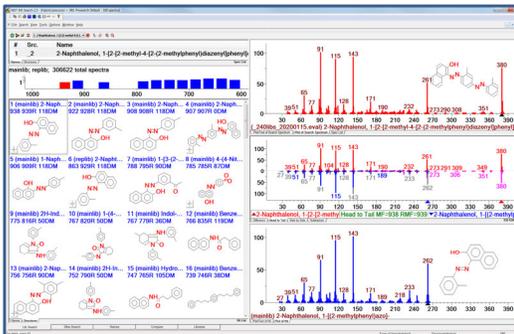
Hybrid Search

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

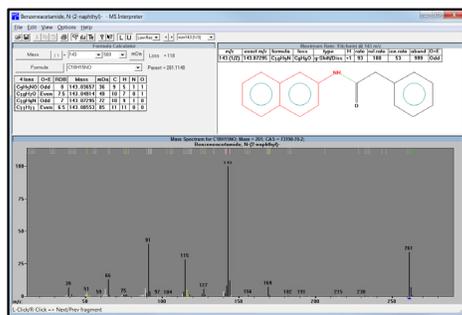


DMass	Replace or Insert
1	H->D, C->C13, NH->O, CH->N
2	CH2->O, C=C->C-C
12	CH2->C=CH2
14	X-Y->X-CH2-Y
16	X-Y->X-O-Y
17	NH->S
18	H->F
28	X-Y->X-CO-Y
30	H->CH3O-H
32	X-Y->X-S-Y
34	H->Cl
50	Phenyl->Naphthyl
76	H->Phenyl
162	H->Glucose

MS Interpreter

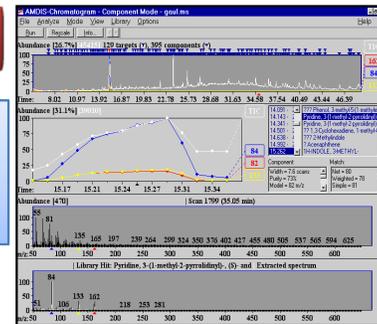
CONNECT PEAKS TO PLAUSIBLE FRAGMENTS (IN RED)

CONFIRM ID
COMPUTE FRAGMENT MASSES
CONNECT PEAKS TO STRUCTURES



AMDIS

'PURIFIES' SPECTRA AND CONNECTS TO NISTMS



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 v2.0f with a small demonstration library.

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_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>

NEW Full GC/MS Chromatogram Analysis by NIST EI Library

Quick Filtering

All MS2, Color Coded IDs, Zoom/Rezoom Display

Query and Best Library Match

Hit List with Optional High Level of Detail

#	Scan	RT	Score	RI	dRI	Prob	Sc...	D...	R.M...	#peaks	#m...	Abu...	n...	Pur...	Max...	Widt...	Su...	PKJ...	Ab...	Dbs	Lib	Formula	Lib-RI	Lib ID
166	1987	18.8935	0.0336	1	20.0	9.8	10	2.58	66.7	15.6	6	0.0235	1	2.4	10.0	7	6.92	54.6	16.6	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	6	0.0715	1	36.0	6.2	10	5.93	45.0	22.4	5	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	0.0209	1	11.0	3.9	12	5.93	45.0	22.4	5	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	0.00...	1	3.6	5.3	15	5.96	75.0	62.3	mainlib	C17H34O2	1883	Pentadecanoic acid, 14-methyl-, methyl ester	
170	2028	19.1504	100	1	96.0	199.8	11	4.61	0.0	0.0	31	0.0235	1	2.4	10.0	7	5.96	75.0	62.3	mainlib	C17H34O2	1926	Hexadecanoic acid, methyl ester	
171	2032	19.1772	0.0235	1	2.4	10.0	7	6.92	54.6	16.6	6	0.0715	1	36.0	6.2	10	5.93	45.0	22.4	5	mainlib	C18H36O2	1910	1,13-Dichlorododecane, 2-phenylborane, 2-phenyl ester
172	2054	19.3166	0.0715	1	36.0	6.2	10	5.93	45.0	22.4	5	0.0209	1	11.0	3.9	12	5.93	45.0	22.4	5	mainlib	C18H36O2	1910	1,13-Dichlorododecane, 2-phenylborane, 2-phenyl ester
173	2062	19.3653	0.0209	1	11.0	3.9	12	5.93	45.0	22.4	5	0.00...	1	6.2	4.7	10	5.93	45.0	22.4	5	mainlib	C18H36O2	1910	1,13-Dichlorododecane, 2-phenylborane, 2-phenyl ester
174	2103	19.5247	0.00...	1	6.2	4.7	10	5.93	45.0	22.4	5	0.0235	1	2.4	10.0	7	5.93	45.0	22.4	5	mainlib	C18H36O2	1910	1,13-Dichlorododecane, 2-phenylborane, 2-phenyl ester
175	2138	19.8415	0.00...	1	3.6	5.3	15	5.93	45.0	22.4	5	0.0223	1	18.0	14.7	12	5.93	45.0	22.4	5	mainlib	C18H36O2	1910	1,13-Dichlorododecane, 2-phenylborane, 2-phenyl ester
176	2145	19.8827	0.0223	1	18.0	14.7	12	5.93	45.0	22.4	5	0.00...	1	8.7	4.8	11	5.93	45.0	22.4	5	mainlib	C18H36O2	1910	1,13-Dichlorododecane, 2-phenylborane, 2-phenyl ester
177	2155	19.9471	0.00...	1	8.7	4.8	11	5.93	45.0	22.4	5	0.265	1	49.0	55.5	17	5.93	45.0	22.4	5	mainlib	C20H32O2	2058	(E)-Valereryl isovalerate
178	2183	20.1214	0.265	1	49.0	55.5	17	5.93	45.0	22.4	5	0.0933	1	33.0	3.9	12	5.93	45.0	22.4	5	mainlib	C16H30O4	2054	Dimethyl tetradecanedioate
179	2187	20.1477	0.0933	1	33.0	3.9	12	5.93	45.0	22.4	5	0.00...	1	7.3	3.1	13	5.96	75.0	62.3	mainlib	C12H10O3	2051	1-Acetyl-2-naphthalenediol	
180	2210	20.2896	0.00...	1	7.3	3.1	13	5.96	75.0	62.3	13													
181	2218	20.3408																						
182	2229	20.4064																						

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:\GCMs\labe\2024-05-14-Hemp_Key-Gene\Hemp-flower-DCM-conc.D\DATA.MS

Banisteriopsis-muricata_DCM-R2
 Hemp-flower-DCM-conc
 Oban_14_EI_1
 Oban_14_EI_1
 Vial_14_70eV_4ua_01
 PMAG1559
 N-Methylperfluorooctane sulfonamide-mod2
 N-Methylperfluorooctane sulfonamide-nzm1
 Orbitrap_01
 Copaiba Balsam 10%.mzdata
 B169_3_07
 Coffee_SPME
 1_1
 30cm 1

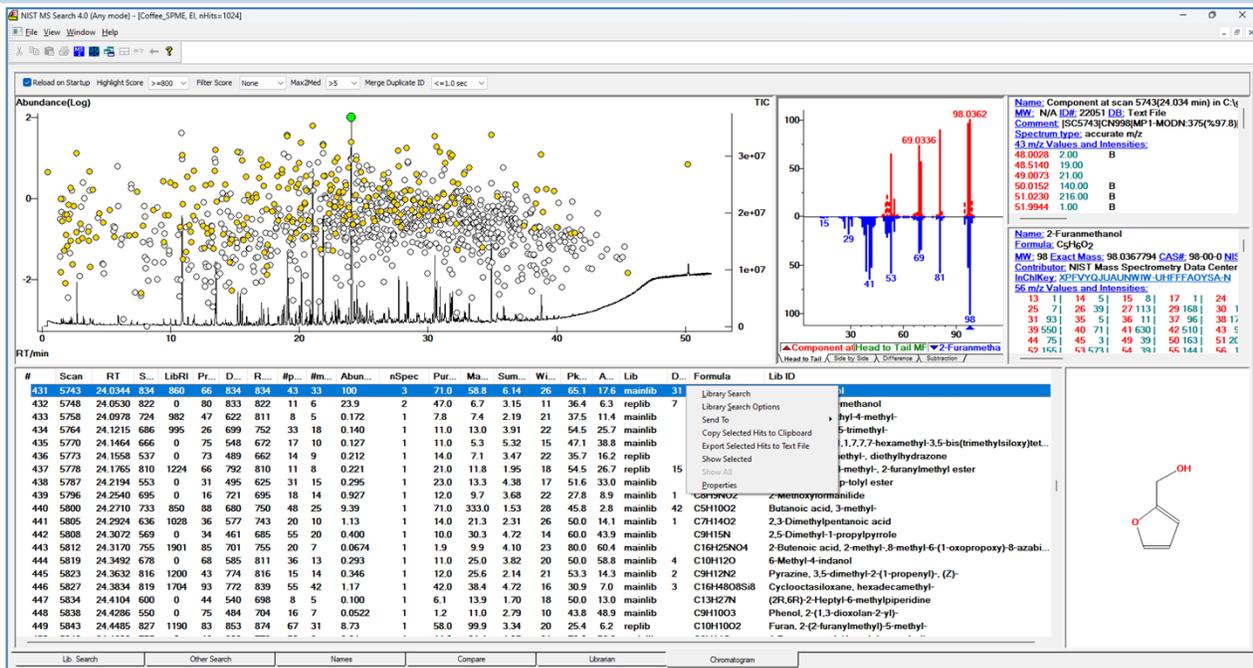
Run Options

Mode: LowRes
 Calibration file: C:\gms\labe\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

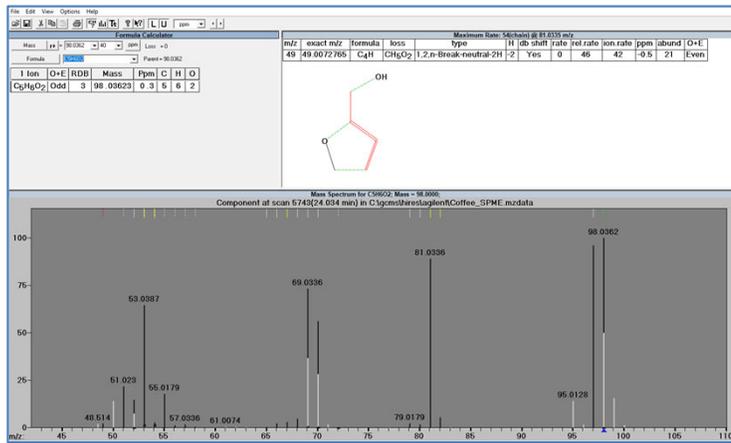
Easily Re-examine Results

High Resolution GC/MS with AMDIS Deconvolution



MS Interpreter - high or low resolution

Extensive Data

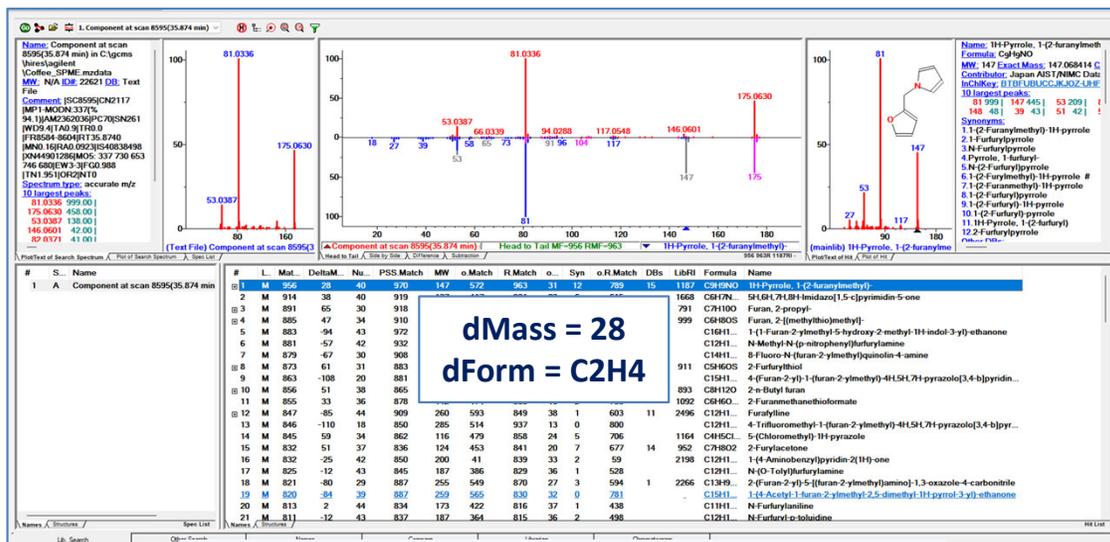


Items to Display

- 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