

# Lib Search: Normal EI Search for Spectra Sent from Chromatogram Window Video/Handout

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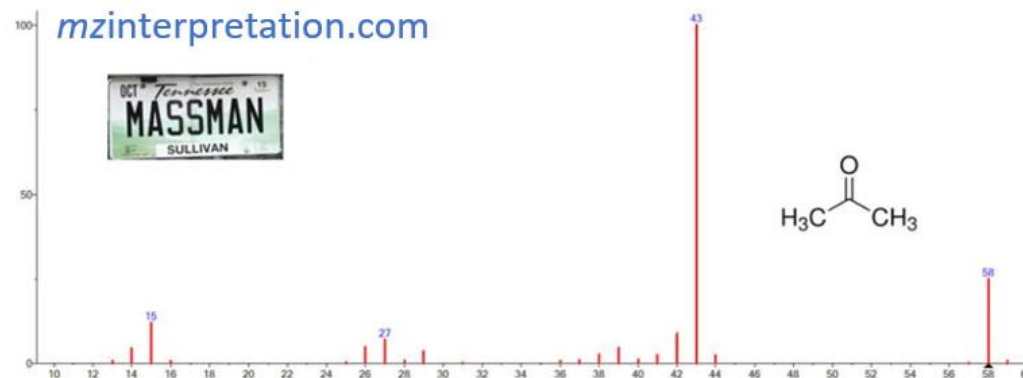
Mass Spec Interpretation Services

April 25, 2026

[mzinterpretation.com](http://mzinterpretation.com)

See **Full Course** on NIST26 with new **Integrated** Deconvolution/Library Searching for **EI GC-MS** and **LC-MS/MS**!

## Mass Spec ( $m/z$ ) Interpretation Services Organic Mass Spectrometry



# Lots of Previous Information on Lib Search and Other NIST Software on My Website

## NIST Search of EI Mass Spectral Databases in Unknown Identifications

- **Extensive** Resources on Lib Search and Other Programs within NIST Search
- See [Link](#)
- This video **only** discusses program **basics**
- No information on Chromatogram Window

### *Videos and Videos Zipped:*

Part 0: Changes in EI NIST23 Program (V3.0)

Part I: Spectral Searches with NIST MS Search

Part II: Structure Searches with MS Search and Using MS Interpreter

Part III: AMDIS (NIST) for Processing EI Mass Spectral Data Files

Part IV: Advanced NIST Hybrid Search of EI and MS/MS Spectra

Part V: Creating and Sharing User EI and MS/MS Libraries

Part VI: Creating and Using Retention Indices in NIST Software

Part VII: Tracking Complex Coelution with AMDIS and NIST Search

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### *Other Webinar Resources:*

# Main Reasons for Sending Results from Chromatogram to Lib Search Window

- The EI Normal Identity search results in Chromatogram **only** show the **best** result, *i.e.*, only one hit per unknown
- The same search in Lib Search Shows Large List of candidates
- Send to Lib Search by right clicking on component of interest then selecting “Library Search”

#	RT	Score	Abund.Rel.	AbUncertPct	DotProd	R.Match	Prob	Max2Med	Formula	Dbs	LibRI	Lib ID
17	9.3950	812	3.02	15.1	827	812	92	7.4	C8H16O2	31	1123	Hexanoic acid, 2-ethyl-
18	9.8478	862	0.258	19.3	852	862	91	21.7	C10H3...	25	1175	Cyclopentasiloxane, decam
19	10.2450	938	8.62	2.8	958	941	29	20.4	C8H11N	25	1167	2,6-Xylidine
20	10.6012	913	52.4	0.2	899	913	40	50.0	C12H26	31	1200	Dodecane
21	12.0603	805	0.102	0.0	773						1212	m-Aminophenylacetylene
22	12.3013	730	0.548	31.9	664						1837	5-Amino-1-methyl-1H-pyraz
23	12.3756	928	24.7	0.8	927						1326	Decanoic acid, methyl ester
24	12.9496	641	0.0211	0.0	641						1432	2,2'-Trimethylenebis-1,3-dio
25	12.9736	770	0.158	36.7	752						1665	2,2-Dimethyl-propyl 2,2-dim
26	13.3580	919	83.4	0.1	920						1400	Tetradecane
27	13.6878	916	29.1	1.4	934						1427	Undecanoic acid, methyl es
28	13.9645	884	2.38	12.7	895						1442	Cyclohexanamine, N-cycloh
29	14.1132	616	0.0778	0.0	616						2522	4-Methyl-2,4-bis(p-hydroxyp
30	14.5198	738	0.838	13.4	602						1189	Pentasiloxane, dodecameth
31	14.5557	373	0.0222	21.1	373						2373	1-Triethylsilyloxyheptadeca
32	14.8820	924	3.76	2.8	942	924	71	43.4	C15H24O	40	1513	Butylated Hydroxytoluene
33	14.9265	924	28.5	0.9	927	924	85	76.8	C13H2...	33	1526	Dodecanoic acid, methyl es
34	15.1349	656	0.00717	30.2	656	656	80	1.4	C10H1...	1	1822	1,3-Dioxolane, 2-(3-bromo-5
35	15.4552	634	0.0512	48.8	634	634	29	2.3	C10H22	2	919	4,4-Dimethyl octane
36	15.5040	786	0.0649	21.5	836	786	19	3.6	C15H1...		2351	1H-Benzimidazole, 1-(2-phen
37	15.8021	922	93.1	0.1	923	922	32	76.8	C16H34	34	1600	Hexadecane
38	15.9841	499	0.0580	21.4	499	499	57	3.2	C7H22...		842	1,1,1,3,5,5,5-Heptamethyltris
39	16.4966	664	0.612	12.9	541	664	38	18.8	C16H4...		1767	2-(2',4',4',6',6',8',8'-Heptame
40	16.4966	741	0.407	16.8	614	741	34	17.2	C14H4...	4	1353	Hexasiloxane, tetradecameth
41	17.6943	732	0.0830	27.4	696	732	10	2.6	C11H24	2	963	Octane, 2,2,6-trimethyl-
42	17.9976	920	98.7	0.4	924	920	22	124.9	C18H38	28	1800	Octadecane

- Library Search
- Library Search Options
- Send To
- Copy Selected Hits to Clipboard
- Export Selected Hits to Text File
- Show Selected
- Show All
- Properties



#	Library	Match	Prob. (%)	DBs	Name
1	mainlib	923	39.5	31	Dodecane
2	mainlib	877	5.78	31	Tridecane
3	mainlib	867	4.20	30	Undecane
4	mainlib	860	3.36	33	Tetradecane
5	mainlib	859	3.25	33	Pentadecane
6	replib	846	2.15	29	Heptadecane
7	replib	846	2.15	34	Hexadecane
8	mainlib	843	1.95	2	Nonane, 4,5-dimethyl-
9	mainlib	830	1.29	7	Dodecane, 2,6,11-trimethyl-
10	replib	829	1.25	7	Undecane, 2-methyl-
11	mainlib	828	1.21	4	Dodecane, 4,6-dimethyl-
12	mainlib	827	1.17	4	Undecane, 4,7-dimethyl-
13	mainlib	825	1.10	3	Undecane, 2,6-dimethyl-
14	mainlib	825	1.10	1	Undecane, 3,5-dimethyl-
15	mainlib	825	1.10	4	Dodecane, 2,7,10-trimethyl-
16	mainlib	824	1.06	2	Undecane, 4,6-dimethyl-
17	mainlib	824	1.06	1	Undecane, 5-methyl-
18	mainlib	822	1.00	4	Decane, 2,6,8-trimethyl-
19	replib	822	1.00	23	Nonadecane
20	mainlib	821	0.96	3	Heptadecane, 2,6,10,14-tetramethyl-
21	replib	819	0.90	32	Decane
22	mainlib	818	0.88	18	Decane, 2-methyl-
23	mainlib	817	0.85	1	Dodecane, 2,5-dimethyl-
24	mainlib	815	0.80	4	Undecane, 3,6-dimethyl-
25	mainlib	814	0.77	5	Undecane, 3-methyl-
26	mainlib	813	0.75	4	Octane, 6-ethyl-2-methyl-
27	mainlib	813	0.75	5	Octane, 3,5-dimethyl-
28	mainlib	812	0.72	4	Decane, 3,7-dimethyl-

# Open Settings

PRE-RELEASE NIST MS Search 4.0 (Any mode) - [EI Normal, Pres

File Search View Tools Options Window Help

Go [Icons] 1. Component at scan 781(10.601 min) ii

#	Src.	T	W	Formula	Name
1	A	0			Component at scan 781(10.601 min)...
2	A	0			Component at scan 1287(14.927 mi...
3	A	0			Component at scan 1424(10.688 mi...
4	L	0			TESTMIX2_180504_MAS011_06_s...
5	L	0			TESTMIX2_180504_MAS011_06_s...
6	L	0			Checkout_TestMix_AMSMS.834.83...

- Select Libraries
- Commercial Libraries *e.g.* Wiley
- User Libraries, *etc.*
- Results combined

Library Search Options

Available 3292820 Spectra in 5 Libraries

Search

MS/MS

**Libraries**

Automation

Limits

Constraints

RI (GC)

mainlib  
replib  
apci\_msms\_nist  
hr\_msms\_nist  
nist\_ri

>> Add >>

Included Libs:  
mainlib  
replib

- Identity Radio Button selected
- EI Normal is the same search performed in Chromatogram Window
- Full Spectrum Search

Library Search Options

**Search**

MS/MS

Libraries

Automation

Limits

Constraints

RI (GC)

Spectrum Search Type

Identity  Similarity

EI Normal

Precursor MW

In spectrum

Spectrum Scoring Options

Method Full Spectrum Search (Score)

Compound Ubiquity Correction

Presearch

Default  Fast  Off  Mass(Da) 1

InChIKey

blank = match search spectrum InChIKey

Other Options

Automation  Auto Report

- Save configuration
- Settings, Font and window sizes, etc.

PRE-RELEASE NIST MS Search 4.0 (EI

File Search View Tools Options V

Open... Ctrl+O

Print Setup...

Print Report

Print Auto Report

Switch to Caller

**Save Configuration**

Restore Configuration

1 jl\_ei\_normal+others.ini

2 jl\_hybrid.ini

3 settings\_MSMS.INI

4 settings\_EI.INI

Select Spectrum Type

Exit

# EI Normal Identity Search

- Note no. of spectra top bar
- Note Type of Search, bottom right bar
- Type of information displayed bottom right bar

PRE-RELEASE NIST MS Search 4.0 (EI mode) - [EI Normal, Presearch Default - InLib = 133, 100 spectra]

File Search View Tools Options Window Help

1. Component at scan 781(10.601 min)

#	Src.	MW	Formula	Name
1	L	0		Component at scan 781(10.601 min)...
2	L	0		

(History) Component at scan 781(10.601 min) in C:\GC-MS DATA FILES\NIST\_AMDIS\_Files\GROB.D\DATA.MS

Names: Structures / Spec List

mainlib; replib; 431275 total spectra

Component at scan 781(10.601 min) in C:\GC-MS DATA FILES\NIST\_AMDIS\_Files\GROB.D\DATA.MS

Head to Tail MF=923 RMF=923 Dodecane 923 923R 39.5F

#	Lib.	Match	Prob. (%)	DBs	Name
1	M	923	39.5	31	Dodecane
2	R	911	39.5	31	Dodecane
3	R	908	39.5	31	Dodecane
4	R	885	39.5	31	Dodecane
5	M	877	5.78	31	Tridecane
6	R	870	5.78	31	Tridecane
7	M	867	4.20	30	Undecane
8	R	865	39.5	31	Dodecane
9	R	864	5.78	31	Tridecane
10	M	860	3.36	33	Tetradecane
11	M	859	3.25	33	Pentadecane
12	R	855	5.78	31	Tridecane
13	R	854	5.78	31	Tridecane
14	R	852	3.36	33	Tetradecane
15	R	849	4.20	30	Undecane
16	R	847	5.78	31	Tridecane
17	R	846	2.15	29	Heptadecane
18	R	846	2.15	34	Hexadecane
19	R	845	3.36	33	Tetradecane
20	R	844	4.20	30	Undecane
21	R	844	3.36	33	Tetradecane
22	M	843	1.95	2	Nonane, 4,5-dimethyl-
23	R	842	2.15	34	Hexadecane
24	R	839	3.25	33	Pentadecane
25	R	838	4.20	30	Undecane
26	M	832	2.15	34	Hexadecane

Names: Structures / InLib = 133, Hit List

PlotText of Search Spectrum / Plot of Search Spectrum / Spec List /

PlotText of Hit / Plot of Hit /

Name: Dodecane  
Formula: C<sub>12</sub>H<sub>26</sub>  
MW: 170 Exact Mass: 170.203451 CAS#: 112-40-3 NIST#: 291499 ID#: 32271 DB: mainlib  
Contributor: NIST Mass Spectrometry Data Center, 1998.  
InChIKey: SNRUBQQJBEYML-UHFFFAOYSA-N Non-stereo  
59 m/z Values and Intensities:  
15 1 26 3 27 69 29 137 30 3  
38 1 39 74 40 141 41 380 42 1071  
43 683 44 23 50 1 51 41 52 21  
53 26 54 19 55 187 56 176 57 999  
58 43 59 1 63 1 65 41 66 1  
67 13 68 10 69 66 70 124 71 536  
72 29 73 1 77 2 79 3 81 2  
82 8 83 30 84 76 85 329 86 21  
87 1 91 1 96 2 97 14 98 62  
99 59 100 4 111 3 112 42 113 40  
114 3 126 20 127 30 128 3 140 8  
141 15 142 2 170 53 171 7  
Synonyms:  
1 n-Dodecane  
2 Adakane 12  
3 Ba 51-090453  
4 CH3(CH2)10CH3  
5 Dihexyl  
6 Dihexyl  
7 Duodecane

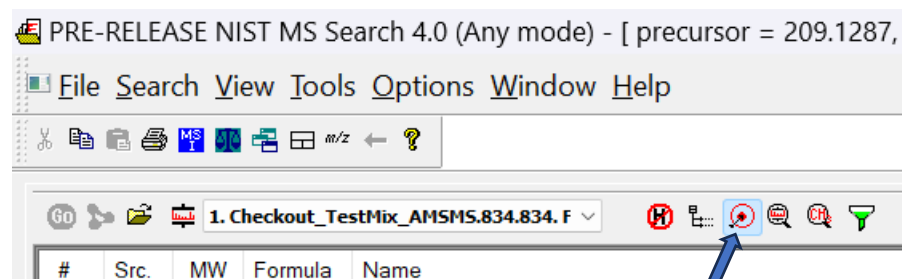
Lib. Search Other Search Names Compare Librarian Chromatogram

For Help, press F1

Type of Search: EI Normal Displayed: EI Normal

## Useful Filter Best Matching Only

- Best matching Only
- When selected, it removes most duplicate search results
- Makes reviewing data easier
- Toggle on and off by depressing button
- Done after the Presearch, thus reversible
- These filters applied *after* Presearch, and can be *easily reversed*



Best Matching Only

## Other Options Besides Standard Full Spectrum Search (Score)

Library Search Options

Search

MS/MS

Libraries

Automation

Limits

Constraints

RI (GC)

Spectrum Search Type

Identity  Similarity

EI Normal

Precursor MW

In spectrum

Spectrum Scoring Options

Method

Full Spectrum Search (Score)

Full Spectrum Search (Score)

Impurity Tolerant Search (Rev-Dot)

Partial Spectrum Search (PSS-Dot)

Compound

Presearch

Default  Fast  Off  Mass(Da) 1

InChIKey

blank = match search spectrum InChIKey

Other Options

Automation  Auto Report

Apply Limits  Use Constraints

Use RI

TMS mode Off

Structure Similarity Search Options

Match Number of Rings  Show Homologues

OK Cancel Help

### Method Selected:

- Full spectrum matching compares entire spectra and works best for clean data. Reverse matching focuses on whether key library peaks are present, making it robust to chemical noise.
- In other words, Reverse-Dot search does not penalize for extra peaks in spectrum that are not present in library spectrum
- The Wiley Library contains many partial spectra from the literature
- Thus, the Reverse Search (Impurity Tolerant Search, Rev-Dot) gives better search results against an unknown pure spectrum for these partial library reference spectra
- Can sort by left clicking on R.Match in results for full spectrum search, but entries that are filtered out in Presearch **will not be found** in results
- Thus, might need to **specify the method before** Presearch
- **Presearch** employed to **greatly increases speed** of final search
- Partial Spectrum search (PSS-Dot) more useful in tandem applications

## Manipulating Search Results in Lib Search Results

#	Lib.	Match	Prob. (%)	DBs	R.Match	Name
1	M	923	39.5	31	923	Dodecane
2	M	877	5.78	31	889	Tridecane
3	M	867	4.20	30	884	Undecane
4	M	860	3.36	33	861	Tetradecane
5	M	859	3.25	33	860	Pentadecane

- Additional column above added for R. Match
- Normally Match is best value to sort the results
- Can sort after the Full Spectrum search by left click on R.Match, but some values for R. Match might not be present after presearch
- Thus, for best R.Match results, do a "Impurity Tolerant Search (Rev-Dot)
- Then review results

# Impurity Tolerant Search (Reverse, Rev-dot) with Results Sorted by R. Match

- No. of hits shown on top bar
- The type of search noted and the type displayed on right bottom bar
- Note, Rev for Reverse, Impurity Tolerant Search, on bottom right corner
- Results are sorted by R Match
- Can reset for standard results by left clicking on Match

PRE-RELEASE NIST MS Search 4.0 (EI mode) - [EI Normal, Impurity Tolerant Search, Presearch Default - 62 spectra]

File Search View Tools Options Window Help

1. Component at scan 781(10.601 min)

#	Src.	MW	Formula	Name
1	L	0		Component at scan 781(10.601 min)...
2	L	0		

Name: Component at scan 781(10.601 min) in C:\GC MS DATA FILES\NIST\_AMDIS\_Files\GROB.D\DATA.MS  
 MW: N/A ID#: 1 DB: Spec. List  
 Comment: [SC781]CN41[MP1-MODN.57(%92.6)AM132130]PC85[SN309]WD4.7\TA3.2\TR0.0\FR777-790\RT.10.6012[MNO.11]RA1.30[S29]  
 40 m/z Values and Intensities:

42	122
43	847
44	28
53	23
54	17
55	160
56	166
57	999
58	44
65	3
66	2
67	13
68	10
69	60
70	113
71	502

mainlib: replib: 431275 total spectra

#	Lib.	Match	DBs	R.Match	Name
1	M	923	31	923	Dodecane
2	M	877	31	889	Tridecane
3	M	867	30	884	Undecane
4	M	860	33	861	Tetradecane
5	R	846	29	861	Heptadecane
6	M	859	33	860	Pentadecane
7	R	846	34	857	Hexadecane
8	M	843	2	857	Nonane, 4,5-dimethyl-
9	M	824	2	850	Undecane, 4,6-dimethyl-
10	M	827	4	849	Undecane, 4,7-dimethyl-
11	M	825	3	846	Undecane, 2,6-dimethyl-
12	R	819	32	846	Decane
13	M	822	4	846	Decane, 2,6,8-trimethyl-
14	M	809	3	846	Octane, 2,3,7-trimethyl-
15	M	825	1	845	Undecane, 3,5-dimethyl-
16	M	813	4	844	Octane, 6-ethyl-2-methyl-
17	M	828	4	841	Dodecane, 4,6-dimethyl-
18	M	818	18	839	Decane, 2-methyl-
19	R	829	7	839	Undecane, 2-methyl-
20	R	822	23	836	Nonadecane
21	M	825	4	836	Dodecane, 2,7,10-trimethyl-
22	M	804	4	836	Decane, 2,5,6-trimethyl-
23	M	803	3	835	Decane, 2,4,6-trimethyl-
24	M	821	3	833	Heptadecane, 2,6,10,14-tetramethyl-
25	M	830	7	832	Dodecane, 2,6,11-trimethyl-
26	M	815	4	832	Undecane, 3,6-dimethyl-

Name: Dodecane  
 Formula: C<sub>12</sub>H<sub>26</sub>  
 MW: 170 Exact Mass: 170.203451 CAS#: 112-40-3 NIST#: 291499 ID#: 32271 DB: mainlib  
 Contributor: NIST Mass Spectrometry Data Center, 1998  
 InChIKey: SNRUBGQJBEFMMJUHFFFAOYSA-N Non-stereo  
 59 m/z Values and Intensities:

15	1	26	31	27	69	29	137	30	3
38	1	39	74	40	14	41	380	42	107
43	683	44	23	50	1	51	4	52	2
53	26	54	19	55	187	56	176	57	999
58	43	59	11	63	11	65	4	66	1
67	13	68	10	69	66	70	124	71	536
72	29	73	1	77	2	79	3	81	2
82	8	83	30	84	76	85	329	86	21
87	1	91	1	96	2	97	14	98	62
99	59	100	4	111	3	112	42	113	40
114	3	126	20	127	30	128	3	140	8
141	15	142	2	170	53	171	7		

Synonyms:  
 1 n-Dodecane  
 2 Adakane 12  
 3 Ba 51-090453  
 4 CH<sub>3</sub>(CH<sub>2</sub>)<sub>10</sub>CH<sub>3</sub>  
 5 Bihexyl  
 6 Dihexyl  
 7 Duodecane

Type of Search: EI Normal Displayed: EI Normal Rev