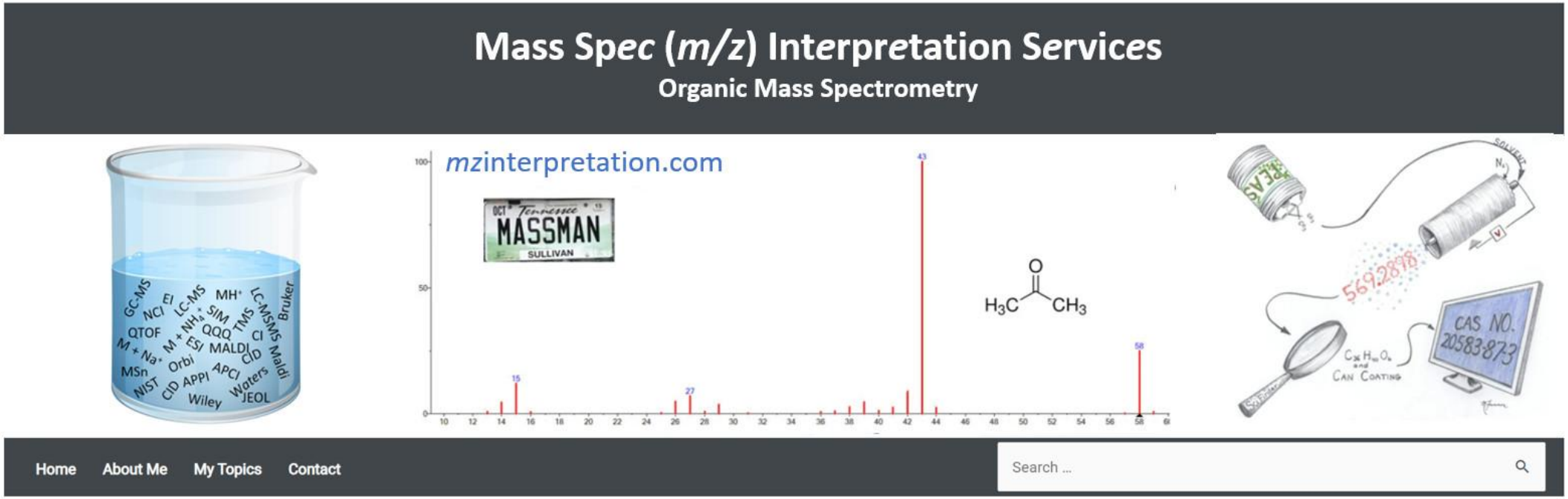
Processing EI GC-MS Data in Chromatogram Window NIST26

Video/Associated Handout

James Little
Mass Spec Interpretation Services
April 26, 2026
mzinterpretation.com

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



Important Skills

- Assume familiar with configuring and navigating Chromatogram NIST26
- ***If not***, review following video and associated handout

Configuring and Navigating Chromatogram Window NIST26

Video/Associated Handout

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April 24, 2026
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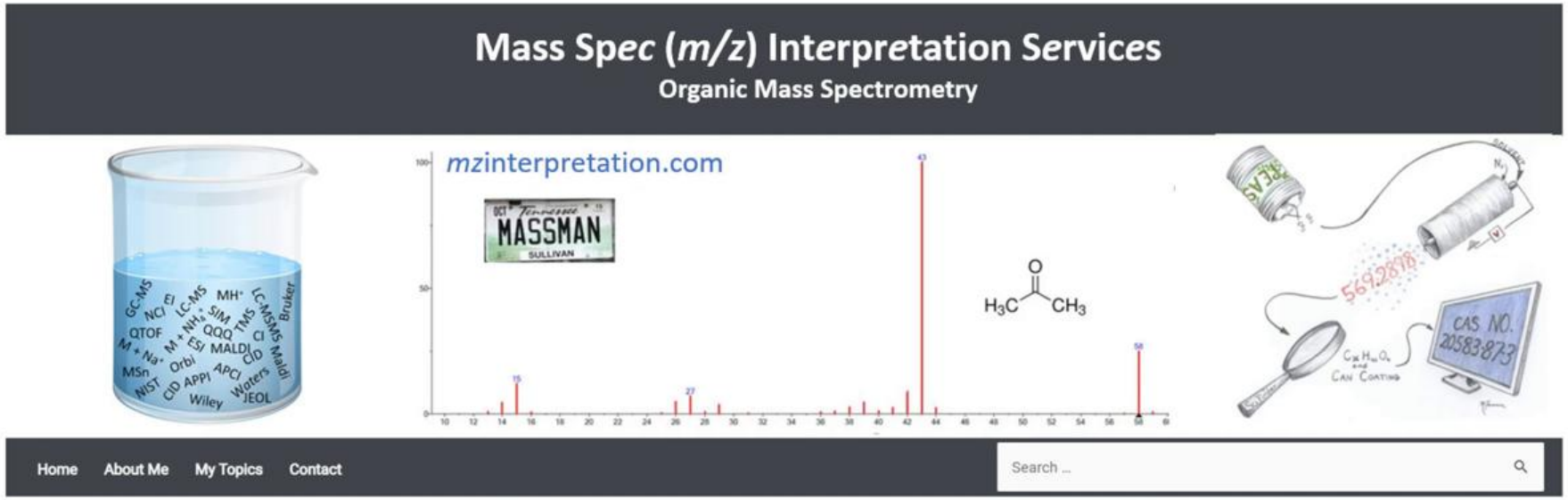


AMDIS in NIST26 Chromatogram Window vs. AMDIS Stand Alone Version

- AMDIS still available as stand-alone application offering multiple library hits per peak searched (no structures), comparison of two files looking for differences, *etc.*
- Extensive Documentation on stand-alone AMDIS on my webpage
- *Link to Website*

Home About Me My Topics Contact Search ...

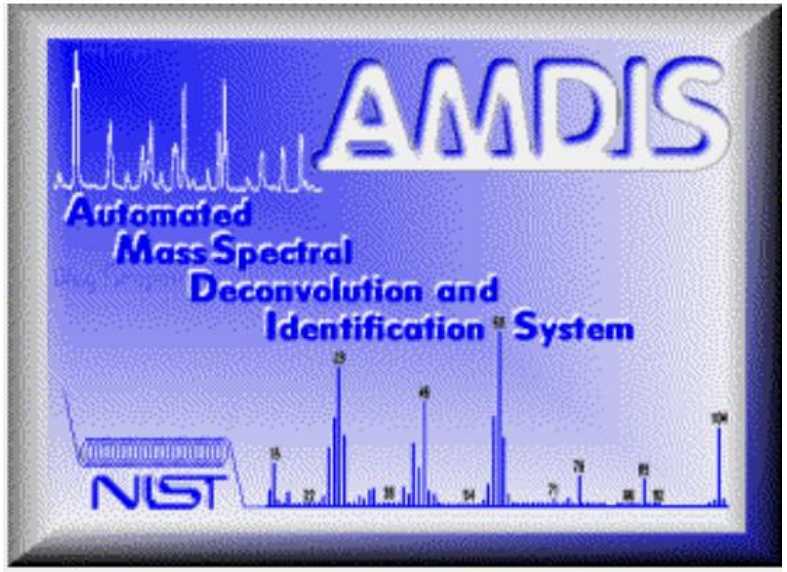
NIST Search of EI Mass Spectral Databases in Unknown Identifications

The webinars cover multiple versions of the software:

- V4.0 (2026): start with NIST26
- V3.0 (2023): start with Part 0
- V2.4: start with Part I

Videos and Videos Zipped:

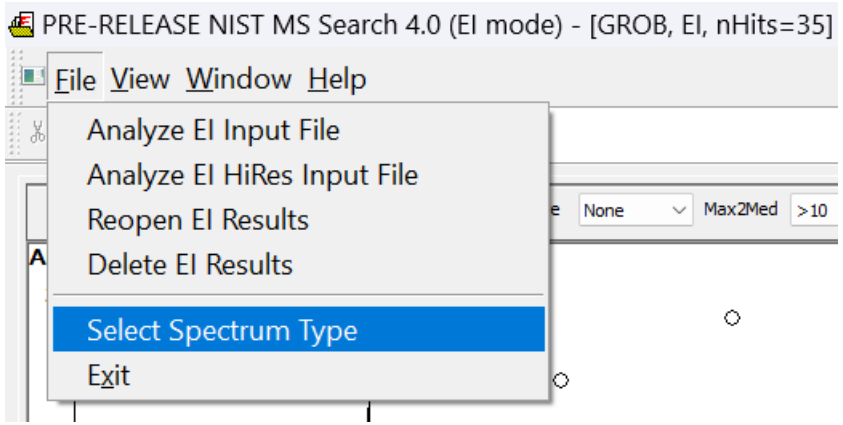
NIST26
Part 0: Changes in EI NIST23 Program (V3.0)
Part I: Spectral Searches with NIST MS Search
Part II: Structure Searches with MS Search and Using MS Interpreter
Part III: AMDIS (NIST) for Processing EI Mass Spectral Data Files
Part IV: Advanced NIST Hybrid Search of EI and MS/MS Spectra
Part V: Creating 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

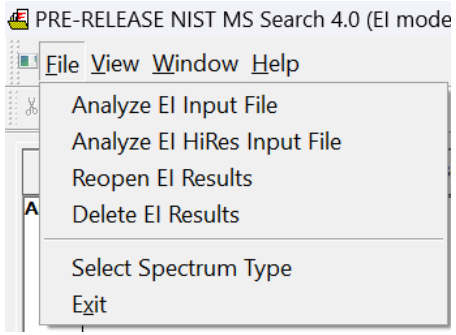


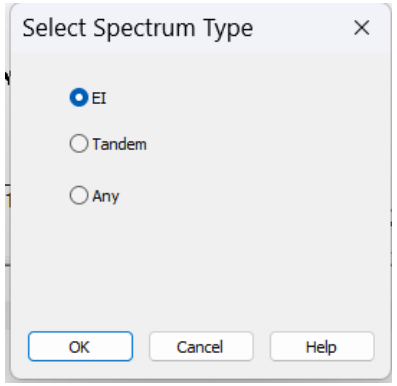
Selecting Process Mode and Saving Configuration

- Useful to select mode if both EI and Tandem NIST software installed
- ***After*** all ***program parameters*** set in ***all windows*** including Chromatogram, ***save the configuration***
- Makes easy to restore a configuration between different data processing requirements
- Software usually delivered by NIST with some default configurations (*.ini) files

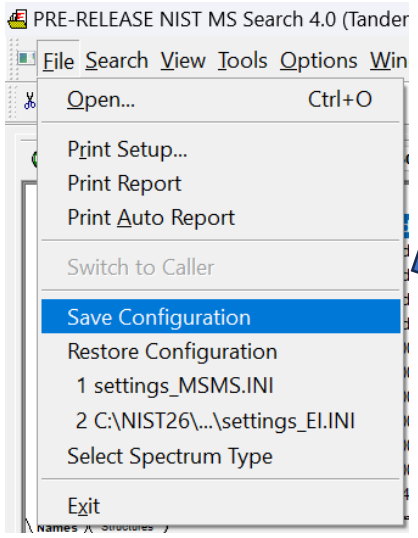
File Menu in Chromatogram window

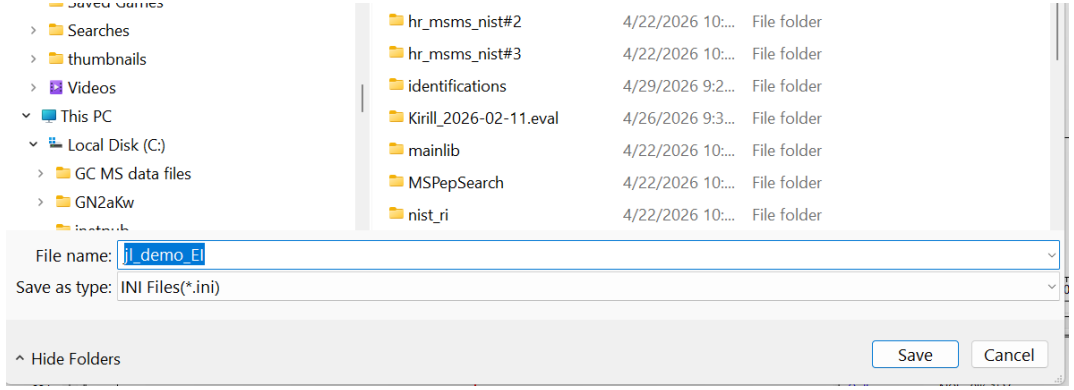




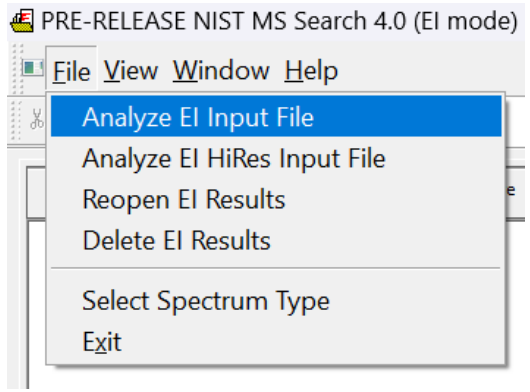


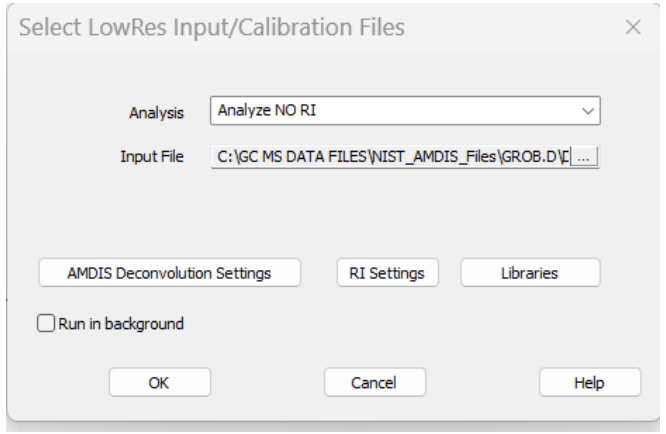
Saving/Restoring Configurations (*.ini) *Note* This Menu in Lib Search Tab



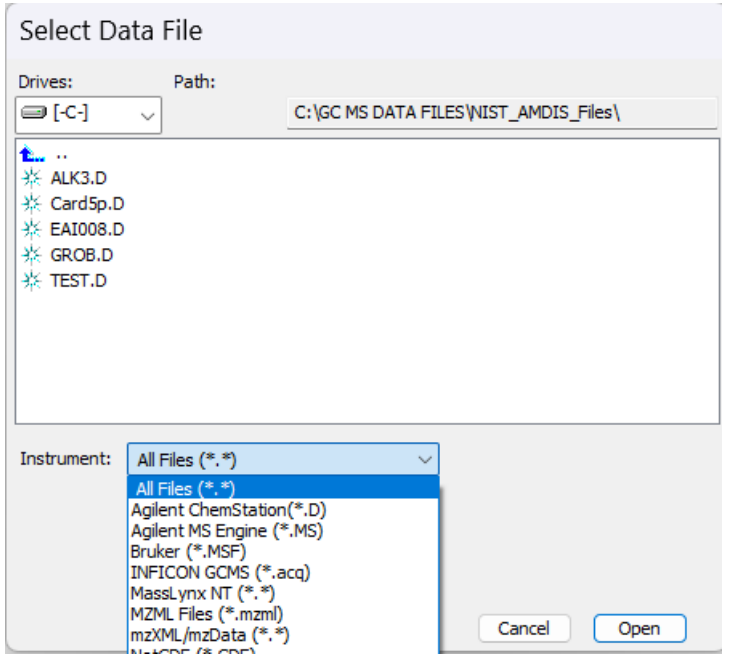


Open a GC/MS File for Processing in Chromatogram Window

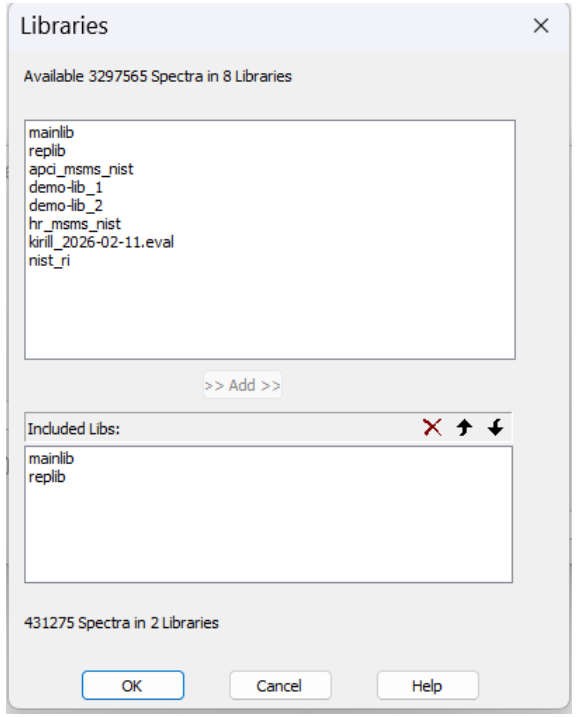




Many different file formats

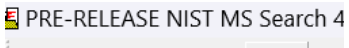


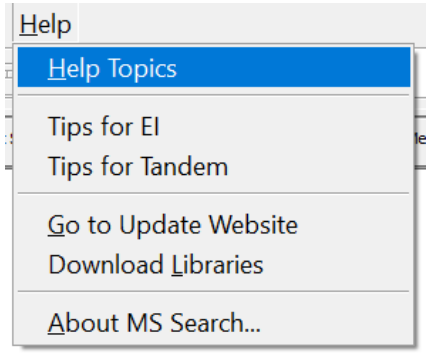
NIST libraries are mainlib and replib, but can search multiple other libraries suh as Wiley, user libraries, etc.

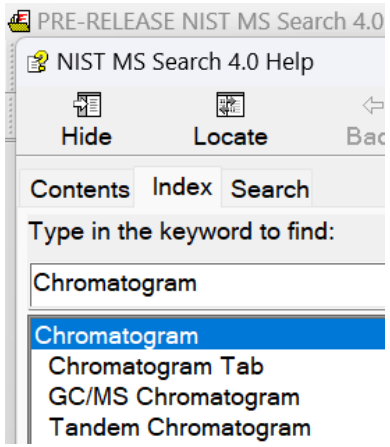


Excellent Help Information on New NIST26 Chromatogram Window

- To ***see all*** the useful information, go to Help on Menu and Select Help Topics
- Then ***Index*** and type in Chromatogram
- Click on Chromatogram Tab and the GC-MS Chromatogram Tips ***at the bottom*** of that page
- Also, in original index search, click on GC/MS Chromatogram







Chromatogram Tab

Depending on data type and available libraries, this display shows identifications of spectra from the input
bar that controls what is being shown below. Depending on libraries installed this window can describe sp
chromatogram. Data types will differ for the two types of data. The chromatogram is show on the left at th
active search spectrum (highlighted below) and library spectra are show at the upper right. This hit list at t
data for each identification. On its right is a structure of the identification.

GC/MS Control Bar

LC/MS-MS Control Bar

Link below at bottom of Chomatogram Tab

Show All (same as double click on chromatogram), Zoom rectangle options and Properties.

GC_MS_Chromatogram_Tips

Tandem_Chromatogram_Tips

GC/MS Chromatogram Tips

How to Display Hits, Analyze Data, Export Data:

Display Hits

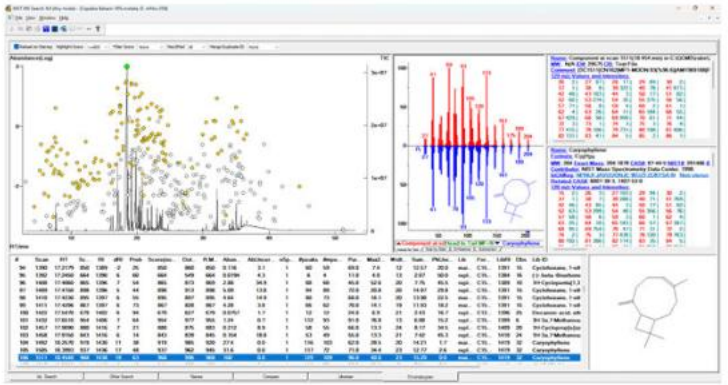
1) Show only IDs above a selected score
   a) Set threshold score in *Filter Score* text box
   b) Both chromatogram and hit list will show only these IDs
   c) Highlight score only determined colors if IDs

2) Examine all identifications of a compound (or precursor mass)

The NISTMS GC/MS Chromatogram Window

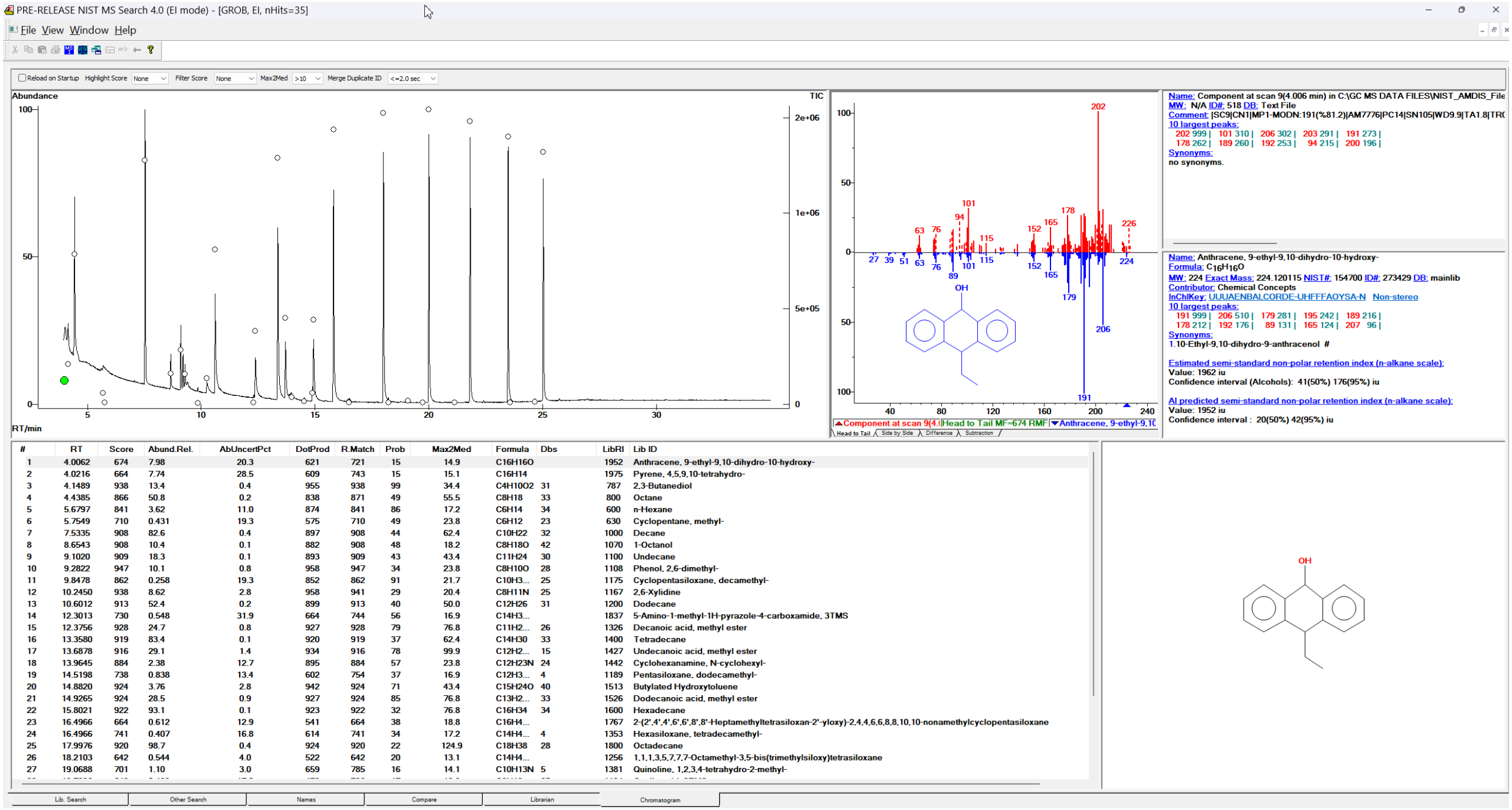
A new, versatile Chromatogram Window is provided as part of the NISTMS Search software (Version 4.
version of the NIST Mass Spectral Libraries. It enables library search processing of a full data file using an
used AMDIS deconvolution program while enabling further processing of individual spectra using the exten
NISTMS software. Both low- and high-resolution data can be processed.

Low Resolution



High Resolution

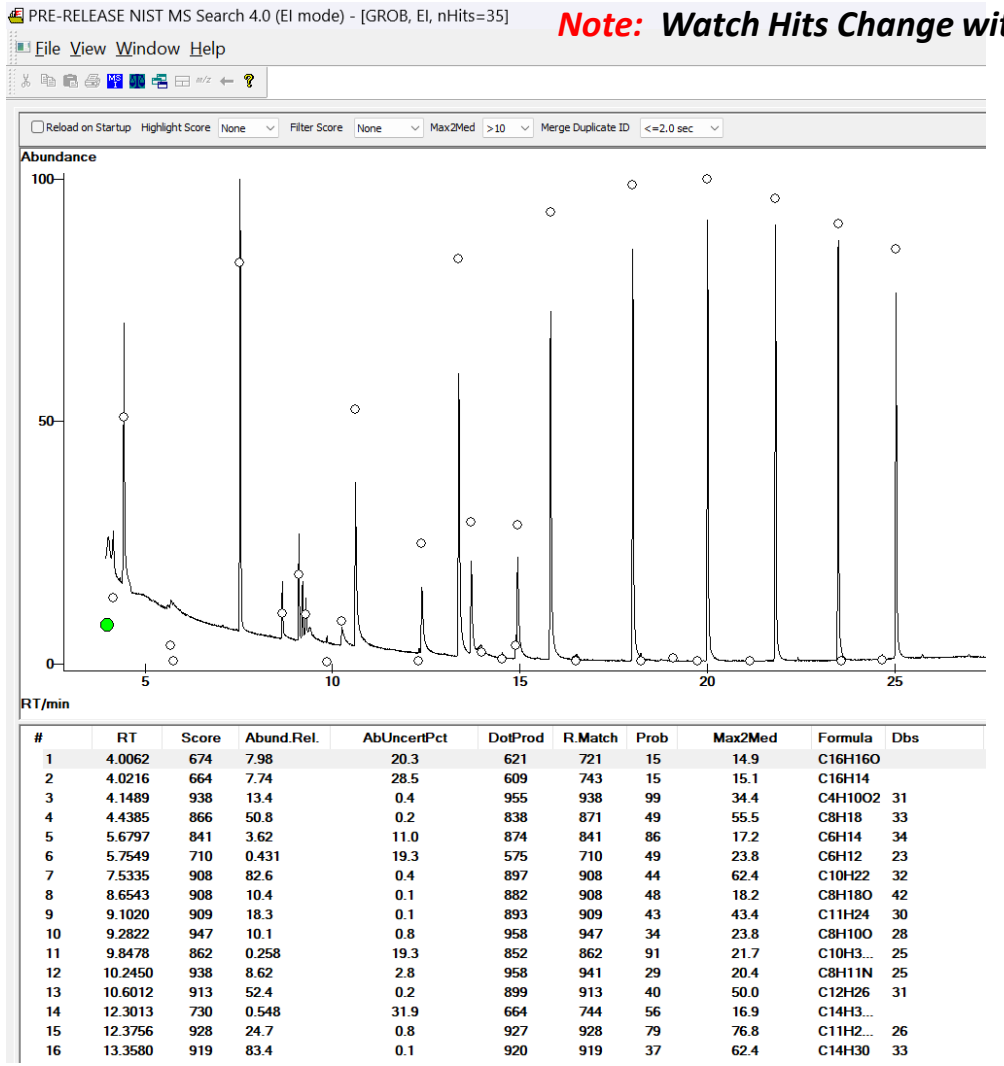
In Video, Showing Initial Results and Demonstrating Some Window Changes *plus* Abundance Linear vs. Log



#	RT	Score	Abund.Rel.	AbUncertPct	DotProd	R.Match	Prob	Max2Med	Formula	Dbs	LibRI	Lib ID
1	4.0062	674	7.98	20.3	621	721	15	14.9	C16H16O		1952	Anthracene, 9-ethyl-9,10-dihydro-10-hydroxy-
2	4.0216	664	7.74	28.5	609	743	15	15.1	C16H14		1975	Pyrene, 4,5,9,10-tetrahydro-
3	4.1489	938	13.4	0.4	955	938	99	34.4	C4H10O2	31	787	2,3-Butanediol
4	4.4385	866	50.8	0.2	838	871	49	55.5	C8H18	33	800	Octane
5	5.6797	841	3.62	11.0	874	841	86	17.2	C6H14	34	600	n-Hexane
6	5.7549	710	0.431	19.3	575	710	49	23.8	C6H12	23	630	Cyclopentane, methyl-
7	7.5335	908	82.6	0.4	897	908	44	62.4	C10H22	32	1000	Decane
8	8.6543	908	10.4	0.1	882	908	48	18.2	C8H18O	42	1070	1-Octanol
9	9.1020	909	18.3	0.1	893	909	43	43.4	C11H24	30	1100	Undecane
10	9.2822	947	10.1	0.8	958	947	34	23.8	C8H10O	28	1108	Phenol, 2,6-dimethyl-
11	9.8478	862	0.258	19.3	852	862	91	21.7	C10H3...	25	1175	Cyclopentasiloxane, decamethyl-
12	10.2450	938	8.62	2.8	958	941	29	20.4	C8H11N	25	1167	2,6-Xylidine
13	10.6012	913	52.4	0.2	899	913	40	50.0	C12H26	31	1200	Dodecane
14	12.3013	730	0.548	31.9	664	744	56	16.9	C14H3...		1837	5-Amino-1-methyl-1H-pyrazole-4-carboxamide, 3TMS
15	12.3756	928	24.7	0.8	927	928	79	76.8	C11H2...	26	1326	Decanoic acid, methyl ester
16	13.3580	919	83.4	0.1	920	919	37	62.4	C14H30	33	1400	Tetradecane
17	13.6878	916	29.1	1.4	934	916	78	99.9	C12H2...	15	1427	Undecanoic acid, methyl ester
18	13.9645	884	2.38	12.7	895	884	57	23.8	C12H23N	24	1442	Cyclohexanamine, N-cyclohexyl-
19	14.5198	738	0.838	13.4	602	754	37	16.9	C12H3...	4	1189	Pentasiloxane, dodecamethyl-
20	14.8820	924	3.76	2.8	942	924	71	43.4	C15H24O	40	1513	Butylated Hydroxytoluene
21	14.9265	924	28.5	0.9	927	924	85	76.8	C13H2...	33	1526	Dodecanoic acid, methyl ester
22	15.8021	922	93.1	0.1	923	922	32	76.8	C16H34	34	1600	Hexadecane
23	16.4966	664	0.612	12.9	541	664	38	18.8	C16H4...		1767	2-(2',4',4',6',6',8',8'-Heptamethyltetrasiloxan-2'-yloxy)-2,4,4,6,6,8,8,10,10-nonamethylcyclopentasiloxane
24	16.4966	741	0.407	16.8	614	741	34	17.2	C14H4...	4	1353	Hexasiloxane, tetradecamethyl-
25	17.9976	920	98.7	0.4	924	920	22	124.9	C18H38	28	1800	Octadecane
26	18.2103	642	0.544	4.0	522	642	20	13.1	C14H4...		1256	1,1,1,3,5,7,7,7-Octamethyl-3,5-bis(trimethylsiloxy)tetrasiloxane
27	19.0688	701	1.10	3.0	659	785	16	14.1	C10H13N	5	1381	Quinoline, 1,2,3,4-tetrahydro-2-methyl-

In Video, Demonstrate Effects of Various Changes in Filters on Top Menu

Video Demonstrates all such as Filter Score, *Max2Med, Merge Duplicates, Best Hits, etc.



Note: ***Watch Hits Change with filter changes!***

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1	4.0062	674	7.98	20.3	621	721	15	14.9	C16H16O	
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3	4.1489	938	13.4	0.4	955	938	99	34.4	C4H10O2	31
4	4.4385	866	50.8	0.2	838	871	49	55.5	C8H18	33
5	5.6797	841	3.62	11.0	874	841	86	17.2	C6H14	34
6	5.7549	710	0.431	19.3	575	710	49	23.8	C6H12	23
7	7.5335	908	82.6	0.4	897	908	44	62.4	C10H22	32
8	8.6543	908	10.4	0.1	882	908	48	18.2	C8H18O	42
9	9.1020	909	18.3	0.1	893	909	43	43.4	C11H24	30
10	9.2822	947	10.1	0.8	958	947	34	23.8	C8H10O	28
11	9.8478	862	0.258	19.3	852	862	91	21.7	C10H3...	25
12	10.2450	938	8.62	2.8	958	941	29	20.4	C8H11N	25
13	10.6012	913	52.4	0.2	899	913	40	50.0	C12H26	31
14	12.3013	730	0.548	31.9	664	744	56	16.9	C14H3...	
15	12.3756	928	24.7	0.8	927	928	79	76.8	C11H2...	26
16	13.3580	919	83.4	0.1	920	919	37	62.4	C14H30	33

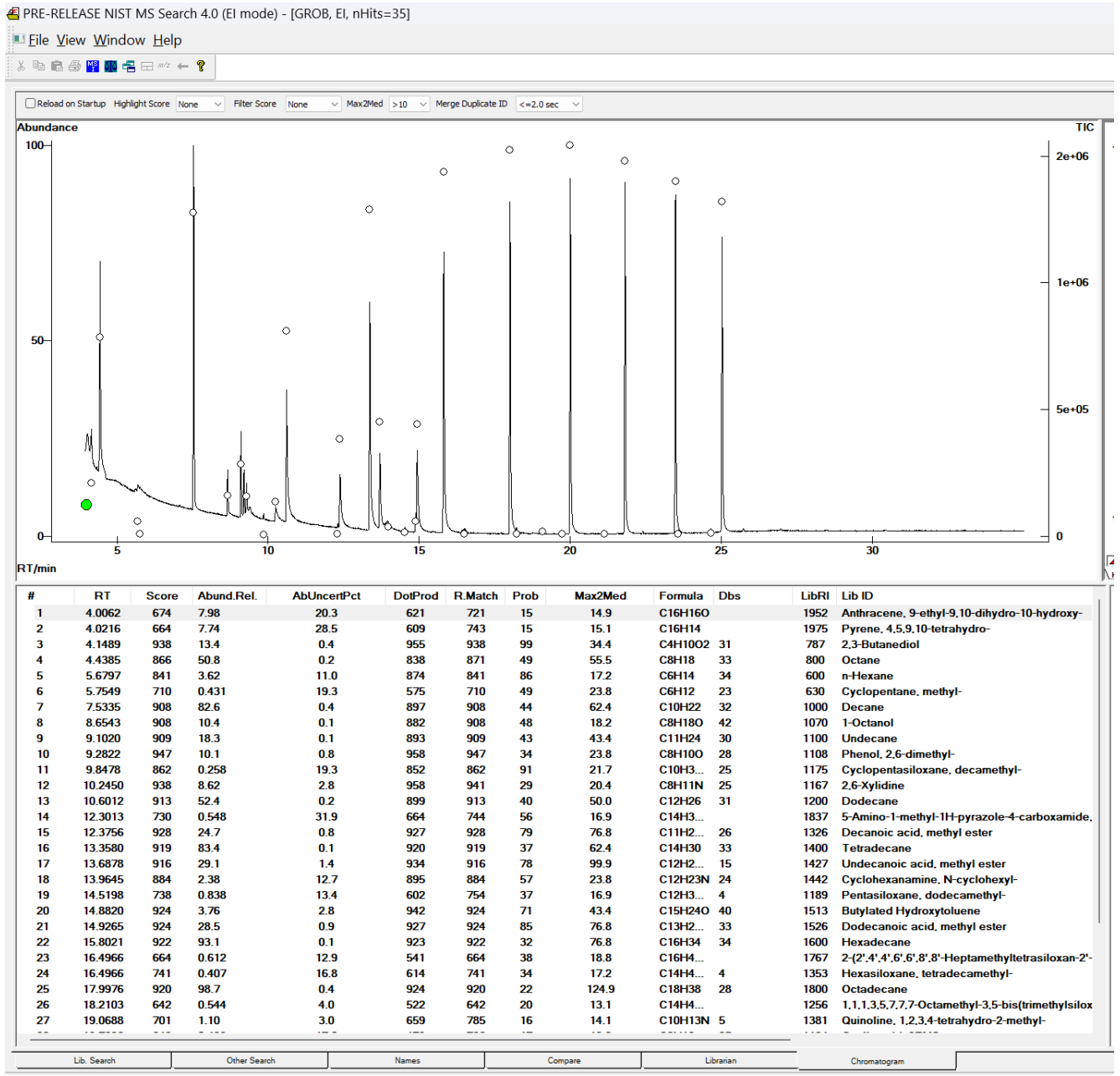
**Max2Med* – Maximum abundance divided by median abundance of query spectrum

Rule of thumb, library search results tend to be less reliable when Max2Med approaches 10

In Video, Demonstrate Sorting/Selecting Components of Interest from Results List

Operations Demonstrated in Video such as:

- Clicking to sort a column
- Selecting entries using keyboard Shift and Ctrl with left mouse click
- Sending selected to smaller list
- Almost endless numbers of approaches!
- Very flexible workflow to meet diverse user needs



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6	5.7549	710	0.431	19.3	575	710	49	23.8	C6H12	23	630	Cyclopentane, methyl-
7	7.5335	908	82.6	0.4	897	908	44	62.4	C10H22	32	1000	Decane
8	8.6543	908	10.4	0.1	882	908	48	18.2	C8H18O	42	1070	1-Octanol
9	9.1020	909	18.3	0.1	893	909	43	43.4	C11H24	30	1100	Undecane
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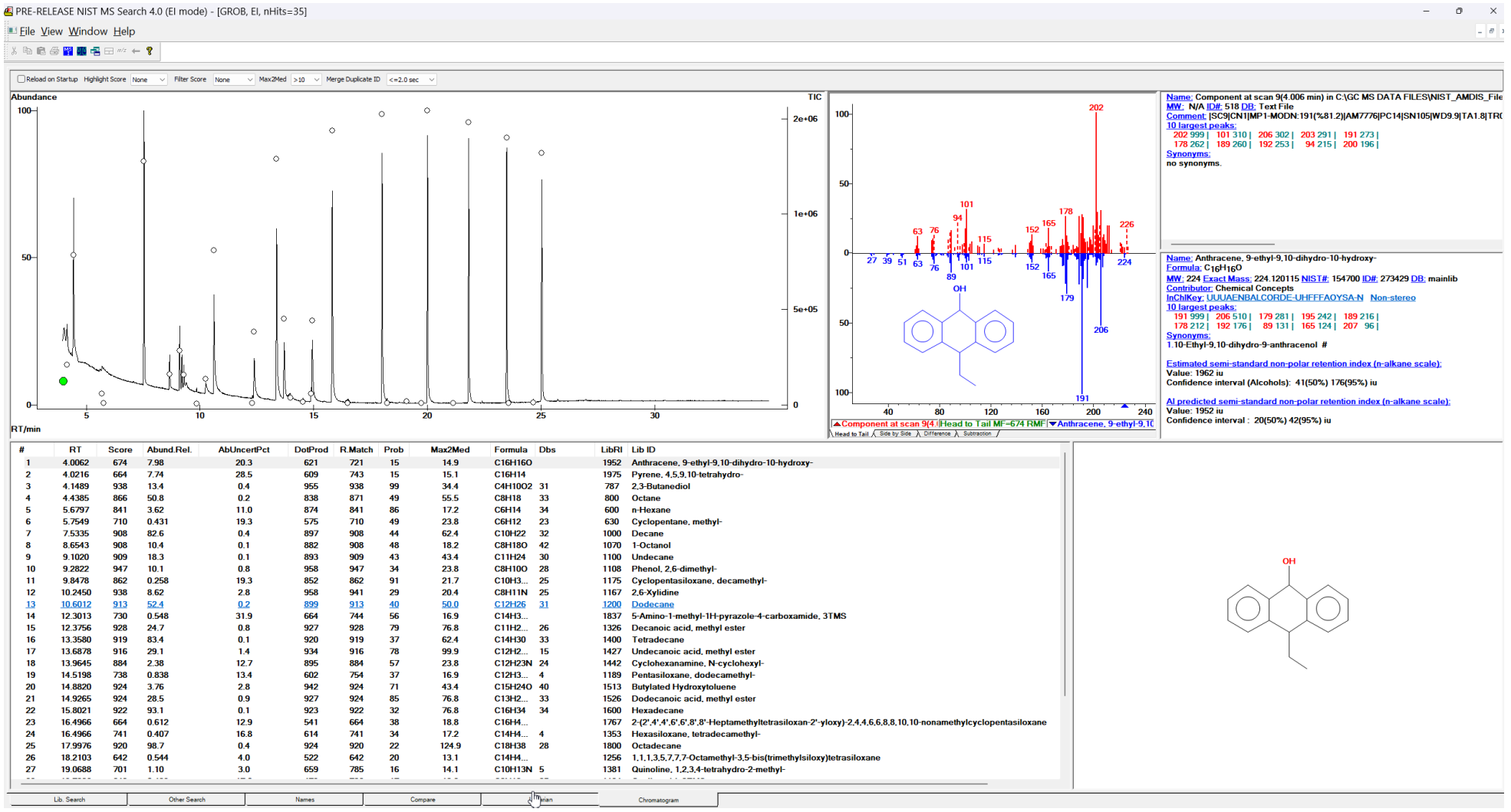
After User List of Interest Defined, Review

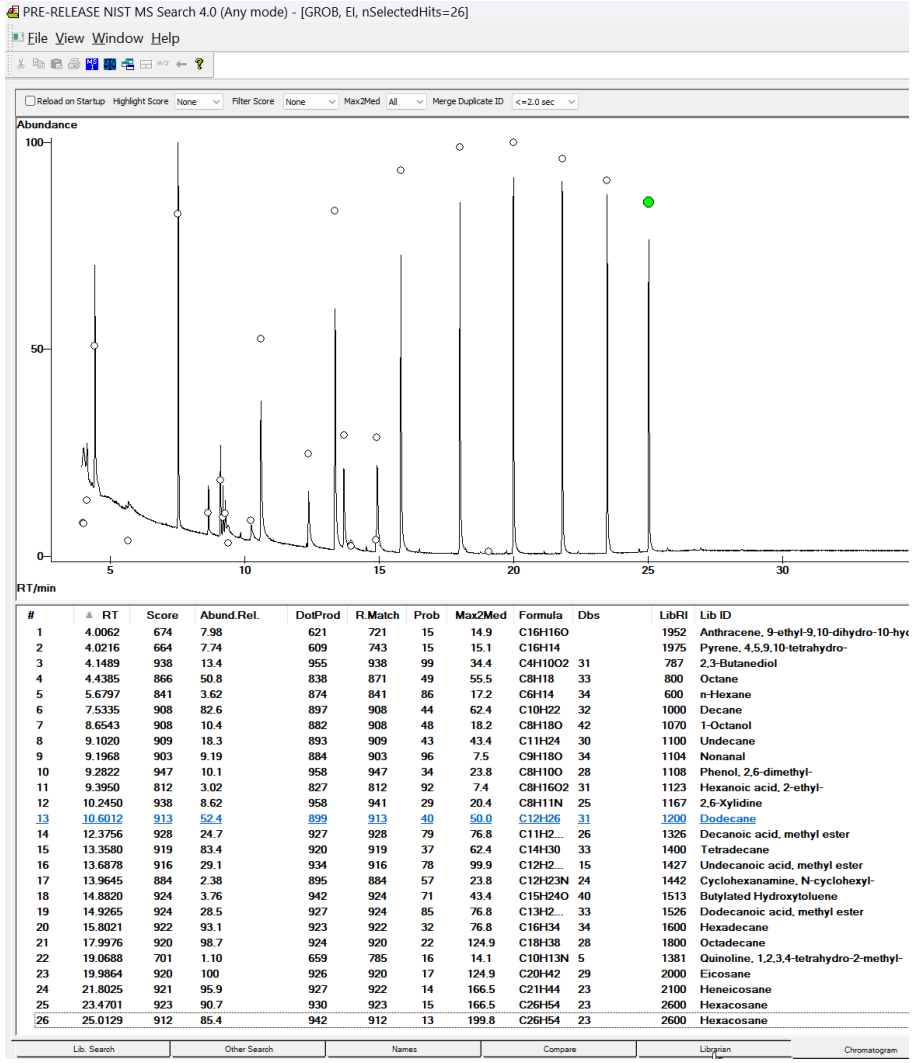
Video Demonstration of Reviewing Selected List:

- Usually sort by RT, retention time
- Left click on first hit in list to highlight
- Use up and down arrows on keyboard to step through list
- Carefully examine the butterfly display in top right box to decide if to include in final report
- Demonstrate ctrl and shift keys to modify components to report
- *etc.*



Creating a Report in Excel

- Select Entries of Interest, I created a list of all components >1% abundance
- Resorted by low to high retention tim
- Right click and Select “Copy Selected Hits to Clipboard”
- Can Then Paste into Excel



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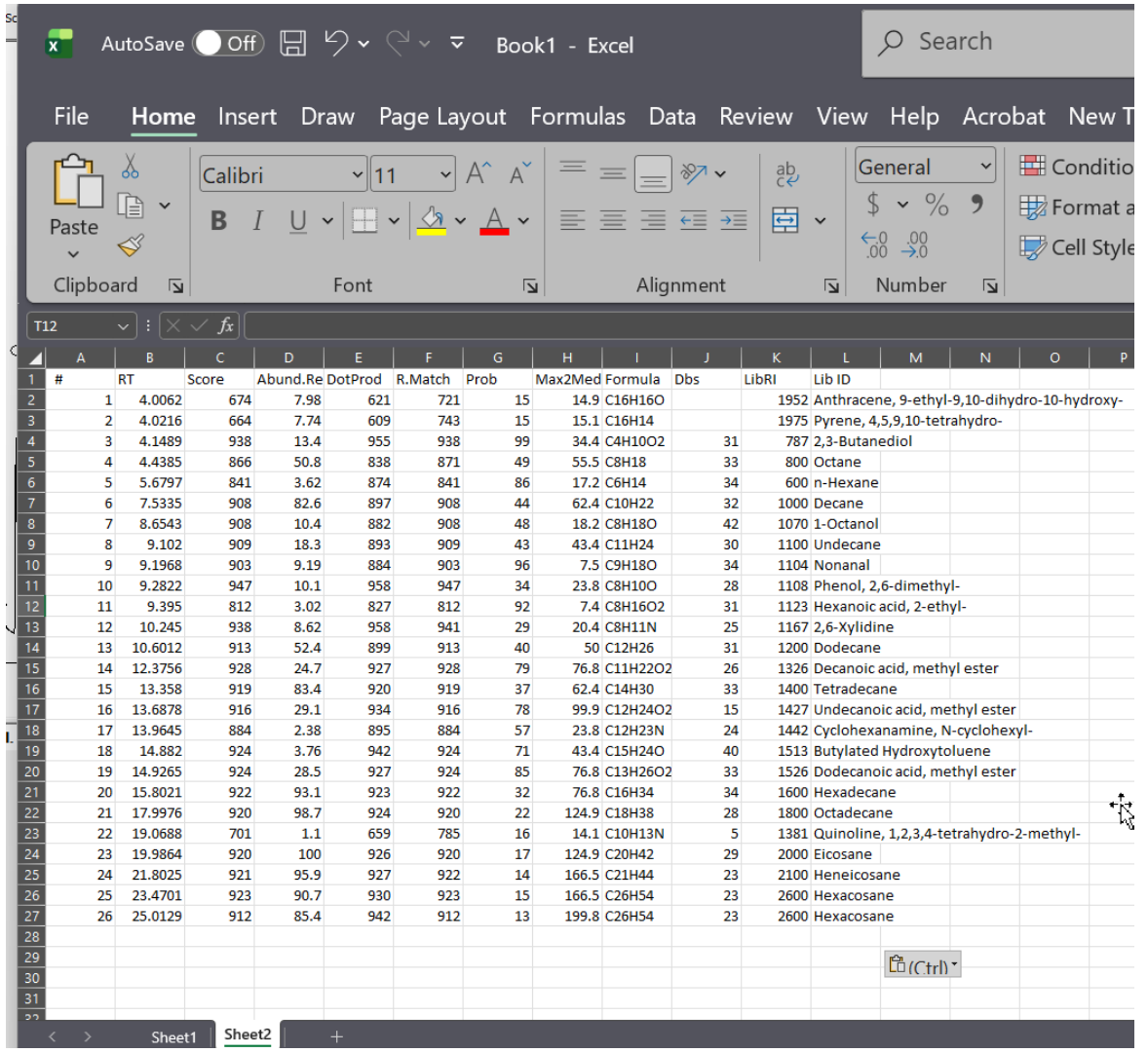
7	8.6543	908	10.4	882	908	48	18.2	C8H18O	42	1070	1-Octanol
8	9.1020	909	18.3	893	909	43	43.4	C11H24	30	1100	Undecane
9	9.1968	903	9.19	884	903	96	7.5	C9H18O	34	1104	Nonanal
10	9.2822	947	10.1	958	947	34	23.8	C8H10O	28	1108	Phenol, 2,6-dimethyl-
11	9.3950	812	3.02	827	812	92	7.4	C8H16O2	31	1123	Hexanoic acid, 2-ethyl-
12	10.2450	938	8.62	958	941	29	20.4	C8H11N	25	1167	2,6-Xylidine
13	10.6012	913	52.4	899	913	40	50.0	C12H26	31	1200	Dodecane
14	12.3756	928	24.7	927	928	79	76.8	C11H2...	26	1326	Decanoic acid, methyl ester
15	13.3580	919	83.4	920	919	37	62.4	C14H30	33	1400	Tetradecane
16	13.6878	916	29.1	934	916	78	99.9	C12H2...	15	1427	Undecanoic acid, methyl ester
17	13.9645	884	2.38	895	884	57	23.8	C12H23N	24	1442	Cyclohexanamine, N-cyclohexyl-
18	14.8820	924	3.76	942	924	71	43.4	C15H24O	40	1513	Butylated Hydroxytoluene
19	14.9265	924	28.5	927	924	85	76.8	C13H2...	33	1526	Dodecanoic acid, methyl ester
20	15.8021	922	93.1	923	922	32	76.8	C16H34	34	1600	Hexadecane
21	17.9976	920	98.7	924	920	22	124.9	C18H38	28	1800	Octadecane
22	19.0688	701	1.10	659	785	16	14.1	C10H13N	5	1381	Quinoline, 1,2,3,4-tetrahydro-2-methyl-
23	19.9864	920	100	926	920	17	124.9	C20H42	29	2000	Eicosane
24	21.8025	921	95.9	927	922	14	166.5	C21H44	23	2100	Heneicosane
25	23.4701	923	90.7	930	923	15	166.5	C26H54	23	2600	Hexacosane
26	25.0129	912	85.4	942	912	13	199.8	C26H54	23	2600	Hexacosane



#	RT	Score	Abund.Re	DotProd	R.Match	Prob	Max2Med	Formula	Dbs	LibRI	Lib ID
1	4.0062	674	7.98	621	721	15	14.9	C16H16O		1952	Anthracene, 9-ethyl-9,10-dihydro-10-hydroxy-
2	4.0216	664	7.74	609	743	15	15.1	C16H14		1975	Pyrene, 4,5,9,10-tetrahydro-
3	4.1489	938	13.4	955	938	99	34.4	C4H10O2	31	787	2,3-Butanediol
4	4.4385	866	50.8	838	871	49	55.5	C8H18	33	800	Octane
5	5.6797	841	3.62	874	841	86	17.2	C6H14	34	600	n-Hexane
6	7.5335	908	82.6	897	908	44	62.4	C10H22	32	1000	Decane
7	8.6543	908	10.4	882	908	48	18.2	C8H18O	42	1070	1-Octanol
8	9.102	909	18.3	893	909	43	43.4	C11H24	30	1100	Undecane
9	9.1968	903	9.19	884	903	96	7.5	C9H18O	34	1104	Nonanal
10	9.2822	947	10.1	958	947	34	23.8	C8H10O	28	1108	Phenol, 2,6-dimethyl-
11	9.395	812	3.02	827	812	92	7.4	C8H16O2	31	1123	Hexanoic acid, 2-ethyl-
12	10.245	938	8.62	958	941	29	20.4	C8H11N	25	1167	2,6-Xylidine
13	10.6012	913	52.4	899	913	40	50	C12H26	31	1200	Dodecane
14	12.3756	928	24.7	927	928	79	76.8	C11H22O2	26	1326	Decanoic acid, methyl ester
15	13.358	919	83.4	920	919	37	62.4	C14H30	33	1400	Tetradecane
16	13.6878	916	29.1	934	916	78	99.9	C12H24O2	15	1427	Undecanoic acid, methyl ester
17	13.9645	884	2.38	895	884	57	23.8	C12H23N	24	1442	Cyclohexanamine, N-cyclohexyl-
18	14.882	924	3.76	942	924	71	43.4	C15H24O	40	1513	Butylated Hydroxytoluene
19	14.9265	924	28.5	927	924	85	76.8	C13H26O2	33	1526	Dodecanoic acid, methyl ester
20	15.8021	922	93.1	923	922	32	76.8	C16H34	34	1600	Hexadecane
21	17.9976	920	98.7	924	920	22	124.9	C18H38	28	1800	Octadecane
22	19.0688	701	1.1	659	785	16	14.1	C10H13N	5	1381	Quinoline, 1,2,3,4-tetrahydro-2-methyl-
23	19.9864	920	100	926	920	17	124.9	C20H42	29	2000	Eicosane
24	21.8025	921	95.9	927	922	14	166.5	C21H44	23	2100	Heneicosane
25	23.4701	923	90.7	930	923	15	166.5	C26H54	23	2600	Hexacosane
26	25.0129	912	85.4	942	912	13	199.8	C26H54	23	2600	Hexacosane