Configuring and Navigating Chromatogram Window NIST26

Video/Associated Handout

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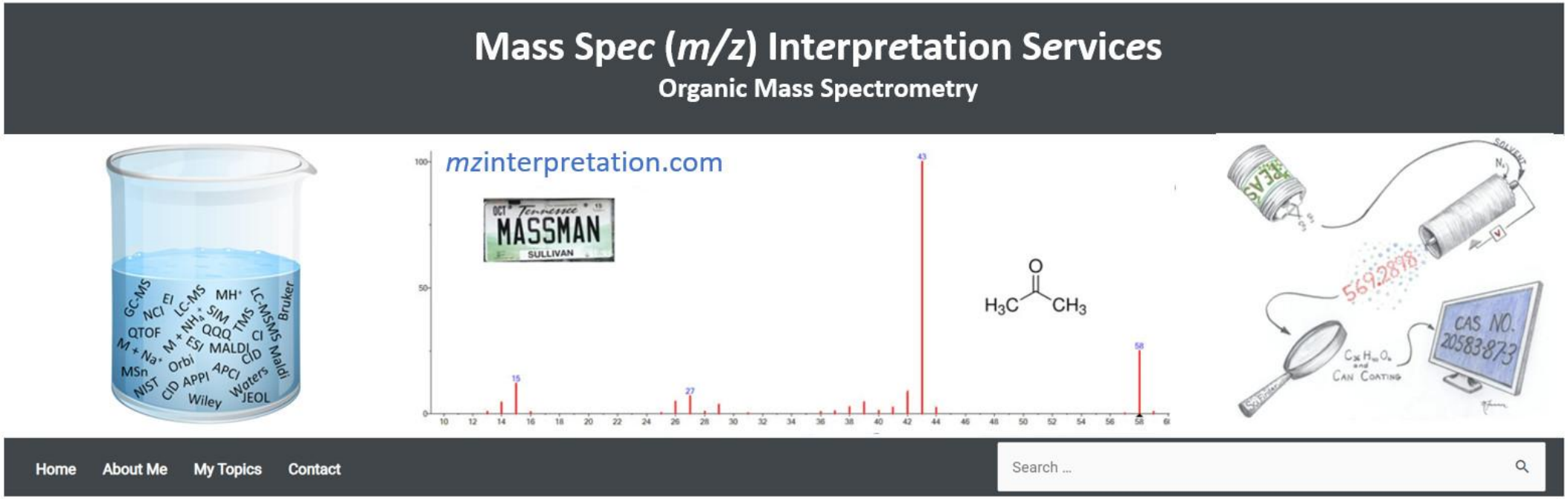
See *Full Course* on NIST26 with new *Integrated* Deconvolution/Library Searching for *EI GC-MS* and *LC-MS/MS*!



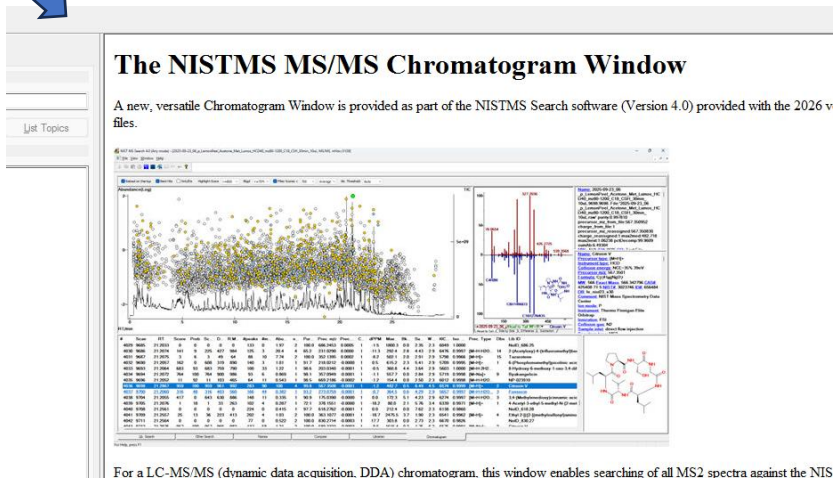
Setup for NIST26 Chromatogram Window

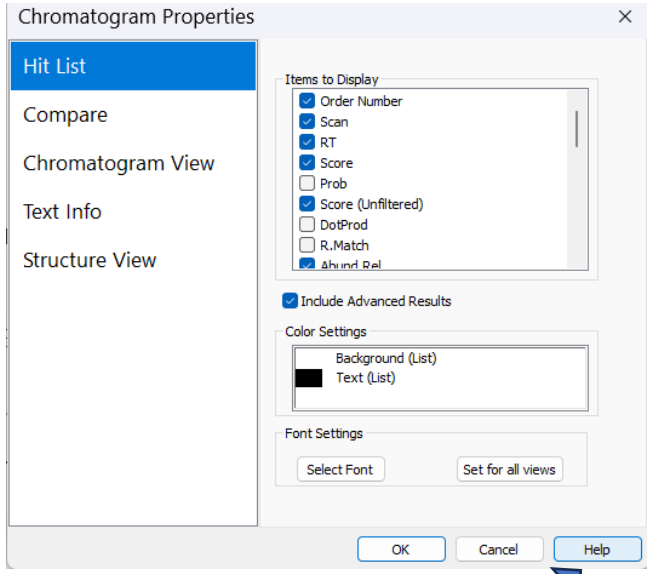
- Very windows compliant
- Consistent approach in Chromatogram and Other Windows within NIST Search
- Demonstrated for EI and MS/MS in MS/MS Chromatogram window
- Essentially same setup in EI and MS/MS conceptually
- Lots of In-program help and detailed Users' Manual

Help Options (1 of 3)

- Help right corner many windows
- V4.0 User's Manual

F1





User's Manual

Right corner Help

NIST Standard Reference Database 1A

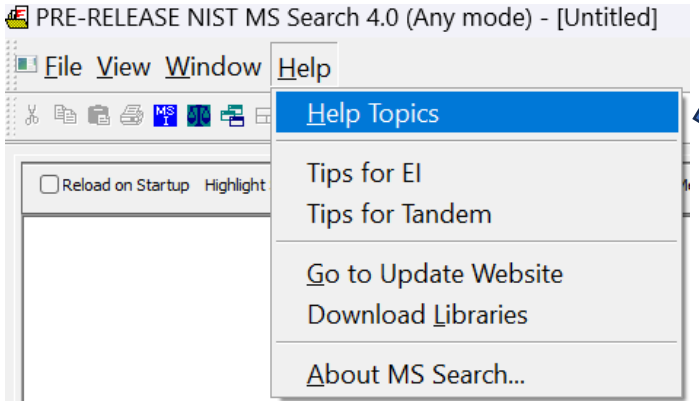
NIST Mass Spectral Search Program (Version 4.0)
Mass Spectral Libraries (NIST/EPA/NIH EI & NIST Tandem 2026)
For Use with Microsoft® Windows
User's Guide

This provides instructions for the use of NIST/EPA/NIH and Tandem Libraries, which are provided under separate Licenses, with MS Search v.4.0. Some sections are for individual Libraries and others are for use of both Libraries.

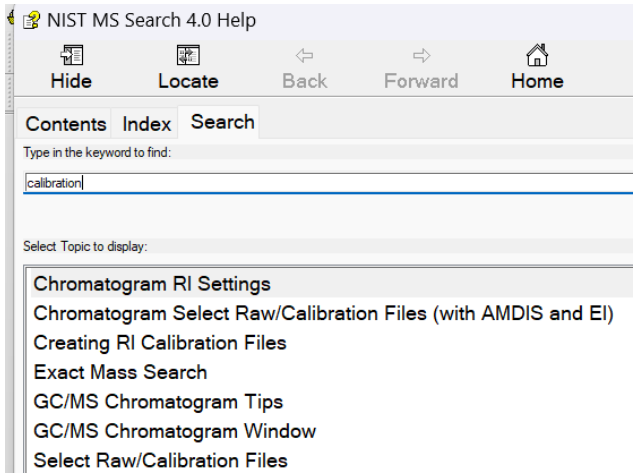
Contents

Help Options (*2 of 3*)

- Help from Menu bar
- Help topics
- Other useful topics accessed in Help Topics
- Tips for EI, Tips for Tandem, What's New

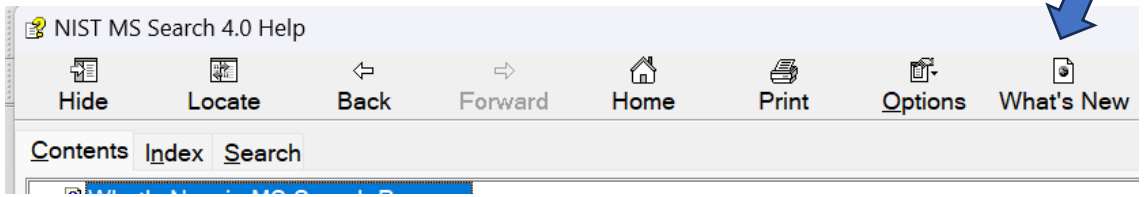


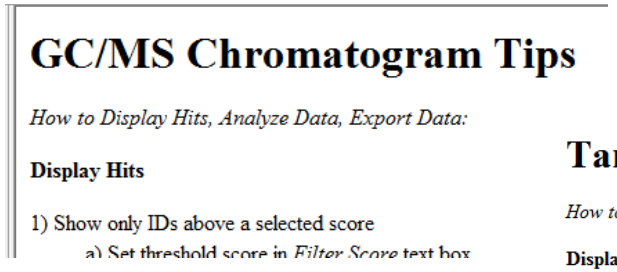
Help Bar Menu



- **Click on Help Topics can:**
- **Select contents for general categories**
- **Index for Pages**
- **Search for Key Words**

What's New





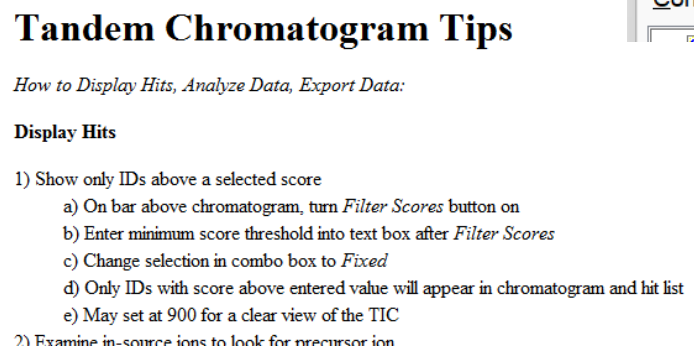
GC/MS Chromatogram Tips

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



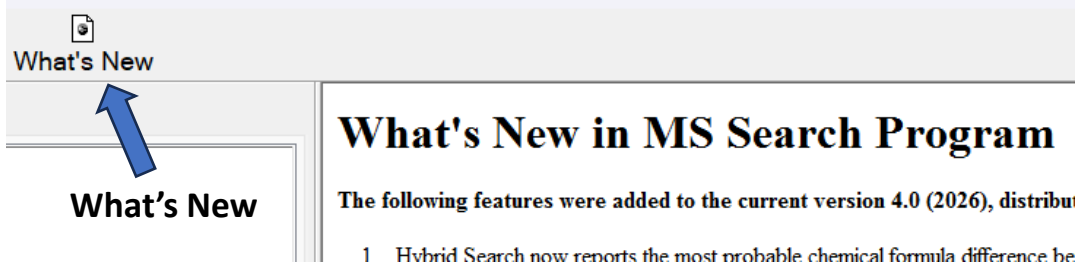
Tandem Chromatogram Tips

How to Display Hits, Analyze Data, Export Data:

Display Hits

1) Show only IDs above a selected score
   a) On bar above chromatogram, turn *Filter Scores* button on
   b) Enter minimum score threshold into text box after *Filter Scores*
   c) Change selection in combo box to *Fixed*
   d) Only IDs with score above entered value will appear in chromatogram and hit list
   e) May set at 900 for a clear view of the TIC

2) Examine in-source ions to look for precursor ion

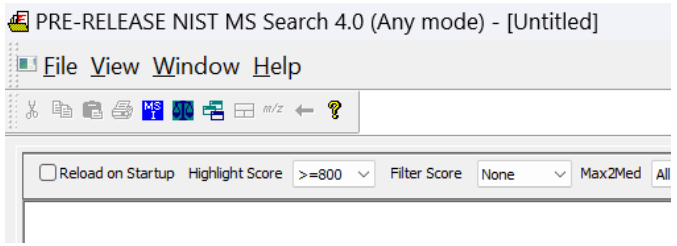


What's New

Help Options (3 of 3)

- Within Chromatogram and other functions
- F1 on keyboard will display very useful help files
- When Chromatogram opened with no results shown, see Fig. 1
- When open with an EI File results shown, Fig. 2
- When open with a MS/MS File shown, Fig. 3
- Fig. 2 and 3 show more specific information, Fig. 1 more general!

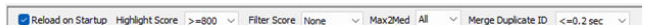
Fig. 1



Chromatogram Tab

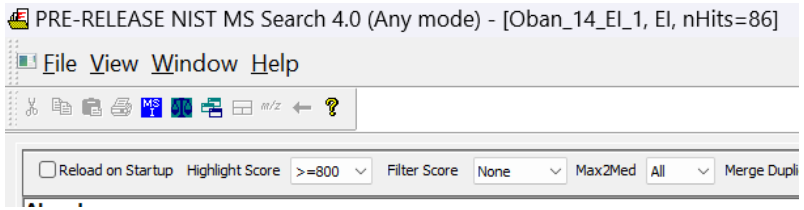
Depending on data type and available libraries, this display shows identifications of spectra from the input data fi
bar that controls what is being shown below. Depending on libraries installed this window can describe spectra i
chromatogram. Data types will differ for the two types of data. The chromatogram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

GC/MS Control Bar



No File Results when program opens

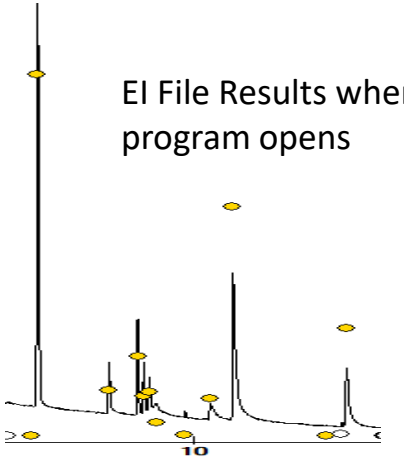
Fig. 2



The NISTMS GC/MS Chromatogram Window

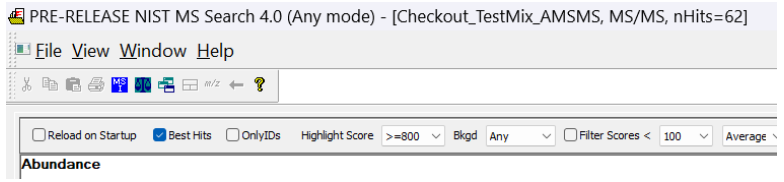
A new, versatile Chromatogram Window is provided as part of the NISTMS Search software (Version 4.0) p
version of the NIST Mass Spectral Libraries. It enables library search processing of a full data file using an enh
used AMDIS deconvolution program while enabling further processing of individual spectra using the extensive
NISTMS software. Both low- and high-resolution data can be processed.

Low Resolution



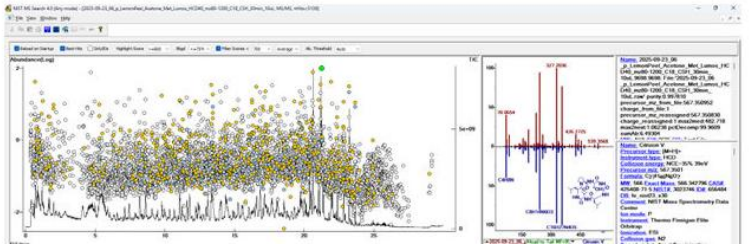
EI File Results when program opens

Fig. 3

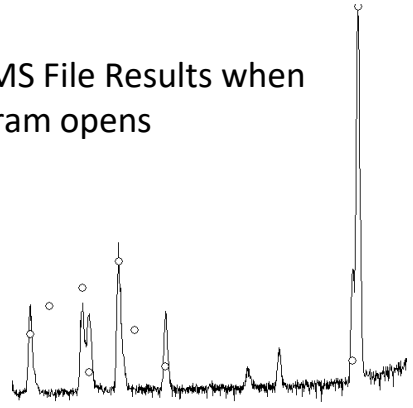


The NISTMS MS/MS Chromatogram Window

A new, versatile Chromatogram Window is provided as part of the NISTMS Search software (Version 4.0)
version of the NIST Mass Spectral Libraries. It enables library search processing of complete LC-MS/MS

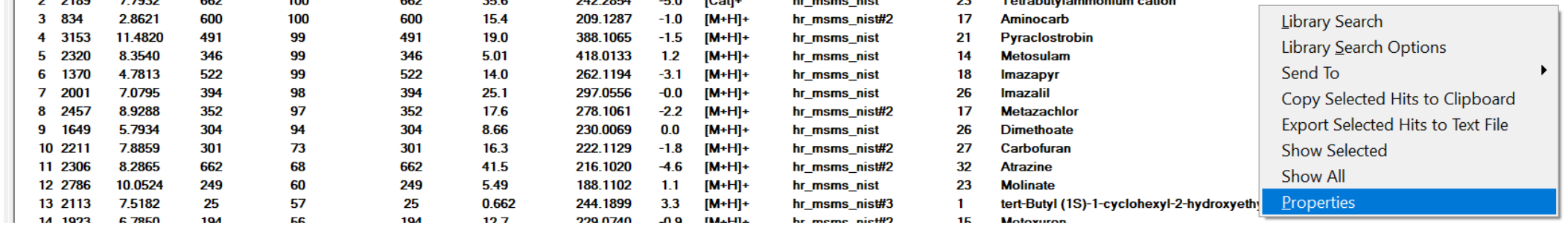


MS/MS File Results when program opens

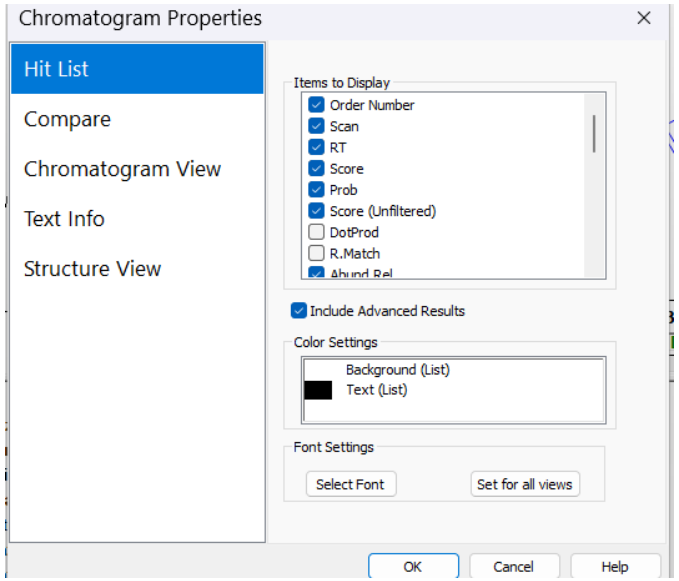


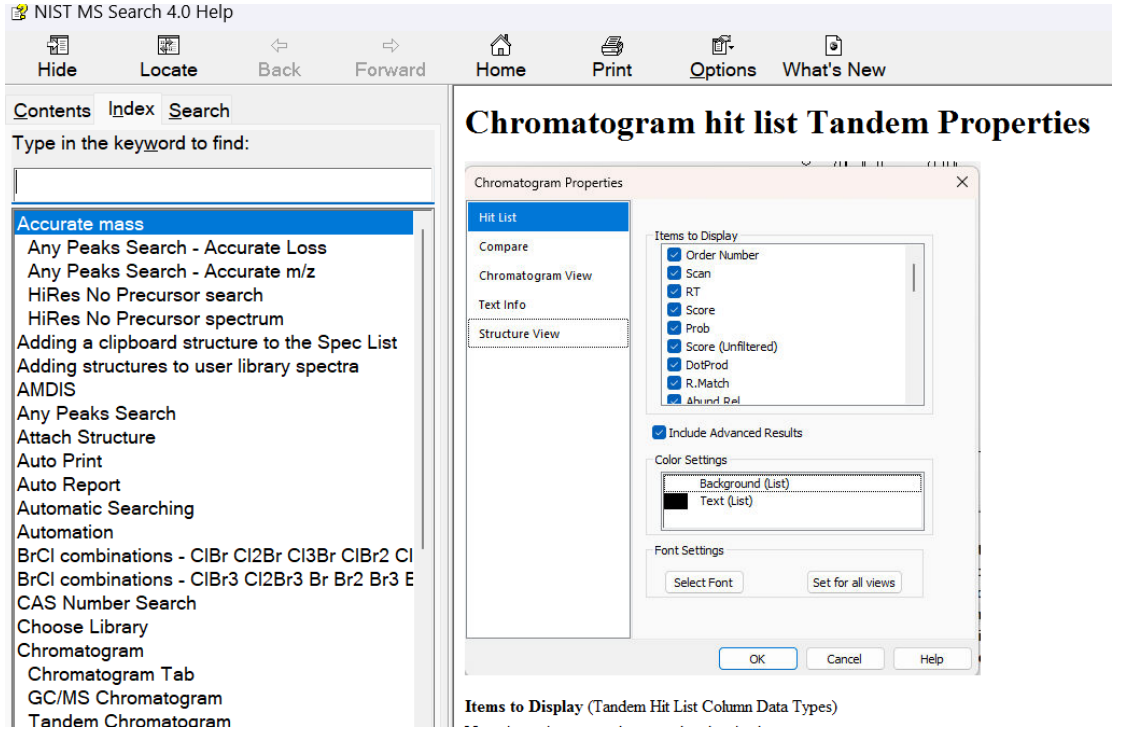
- **Suggested Properties, *Many Others* by Right Clicking on Bottom Window and Selecting Properties**
- ***All windows* offer additional processing options with Right Click**

#	Scan	RT	Score	Prob	Score (Unfiltered)	Abund.Rel.	Prec. m/z	dPPM	Prec. Type	Lib	Dbs	Lib ID
1	3171	11.5521	754	100	754	100	305.1091	-2.9	[M+H]+	hr_msms_nist#2	32	Diazinon
2	2189	7.7932	662	100	662	35.6	242.2854	-5.0	[Cat]+	hr_msms_nist	23	Tetrabutylammonium cation
3	834	2.8621	600	100	600	15.4	209.1287	-1.0	[M+H]+	hr_msms_nist#2	17	Aminocarb
4	3153	11.4820	491	99	491	19.0	388.1065	-1.5	[M+H]+	hr_msms_nist	21	Pyraclostrobin
5	2320	8.3540	346	99	346	5.01	418.0133	1.2	[M+H]+	hr_msms_nist	14	Metosulam
6	1370	4.7813	522	99	522	14.0	262.1194	-3.1	[M+H]+	hr_msms_nist	18	Imazapyr
7	2001	7.0795	394	98	394	25.1	297.0556	-0.0	[M+H]+	hr_msms_nist	26	Imazalil
8	2457	8.9288	352	97	352	17.6	278.1061	-2.2	[M+H]+	hr_msms_nist#2	17	Metazachlor
9	1649	5.7934	304	94	304	8.66	230.0069	0.0	[M+H]+	hr_msms_nist	26	Dimethoate
10	2211	7.8859	301	73	301	16.3	222.1129	-1.8	[M+H]+	hr_msms_nist#2	27	Carbofuran
11	2306	8.2865	662	68	662	41.5	216.1020	-4.6	[M+H]+	hr_msms_nist#2	32	Atrazine
12	2786	10.0524	249	60	249	5.49	188.1102	1.1	[M+H]+	hr_msms_nist	23	Molinate
13	2113	7.5182	25	57	25	0.662	244.1899	3.3	[M+H]+	hr_msms_nist#3	1	tert-Butyl (1S)-1-cyclohexyl-2-hydroxyeth
14	1923	6.7850	194	56	194	12.7	229.0740	-0.9	[M+H]+	hr_msms_nist#2	15	Metoxuron



- **Select “Include Advanced Results”**
- **keyboard F1 or Help for definitions**





Move Position of Properties Displayed by Left Click and Drag

#	Scan	RT	Score	Prob	Abund.Rel.	Prec. m/z	dPPM	Prec. Type	Lib	Dbs	Lib ID
1	3171	11.5521	754	100	100	305.1091	-2.9	[M+H]+	hr_msms_nist#2	32	Diazinon
2	2189	7.7932	662	100	35.6	242.2854	-5.0	[Cat]+	hr_msms_nist	23	Tetrabutylammonium cation
3	834	2.8621	600	100	15.4	209.1287	-1.0	[M+H]+	hr_msms_nist#2	17	Aminocarb
4	3153	11.4820	491	99	19.0	388.1065	-1.5	[M+H]+	hr_msms_nist	21	Pyraclostrobin

#	Scan	RT	Score	Abund.Rel.	Prec. m/z	Prob	dPPM	Prec. Type	Lib	Dbs	Lib ID
1	3171	11.5521	754	100	305.1091	100	-2.9	[M+H]+	hr_msms_nist#2	32	Diazinon
2	2189	7.7932	662	35.6	242.2854	100	-5.0	[Cat]+	hr_msms_nist	23	Tetrabutylammonium cation

"Stretch Columns" by left click and drag, see double arrow to grab side of a column

d.Rel.	Prec. m/z	Prob	dPPM	Pre
	305.1091	100	-2.9	[M-
	242.2854	100	-5.0	[Ca
	209.1287	100	-1.0	[M-

Prec. m/z	Prob	dPPM	Pr
305.1091	100	-2.9	[M
242.2854	100	-5.0	[C

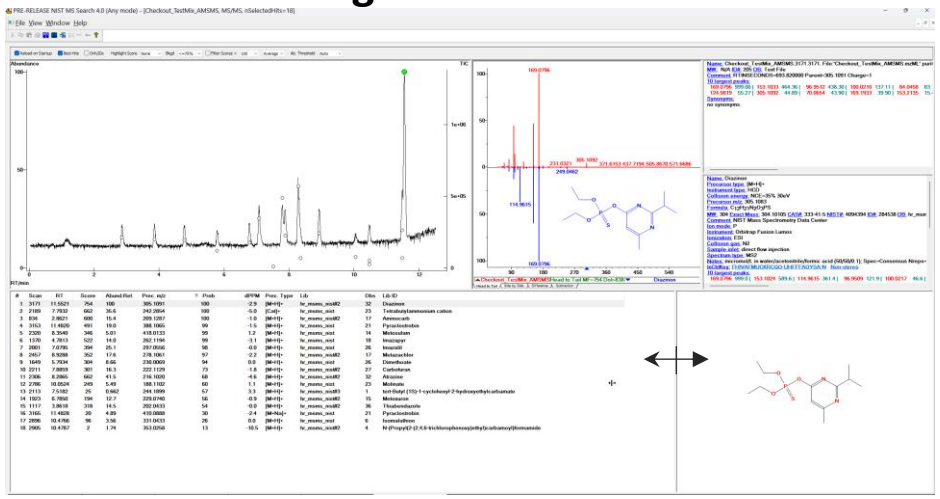
Left Clicking on column sorts results by that property, click twice to change from high to low value

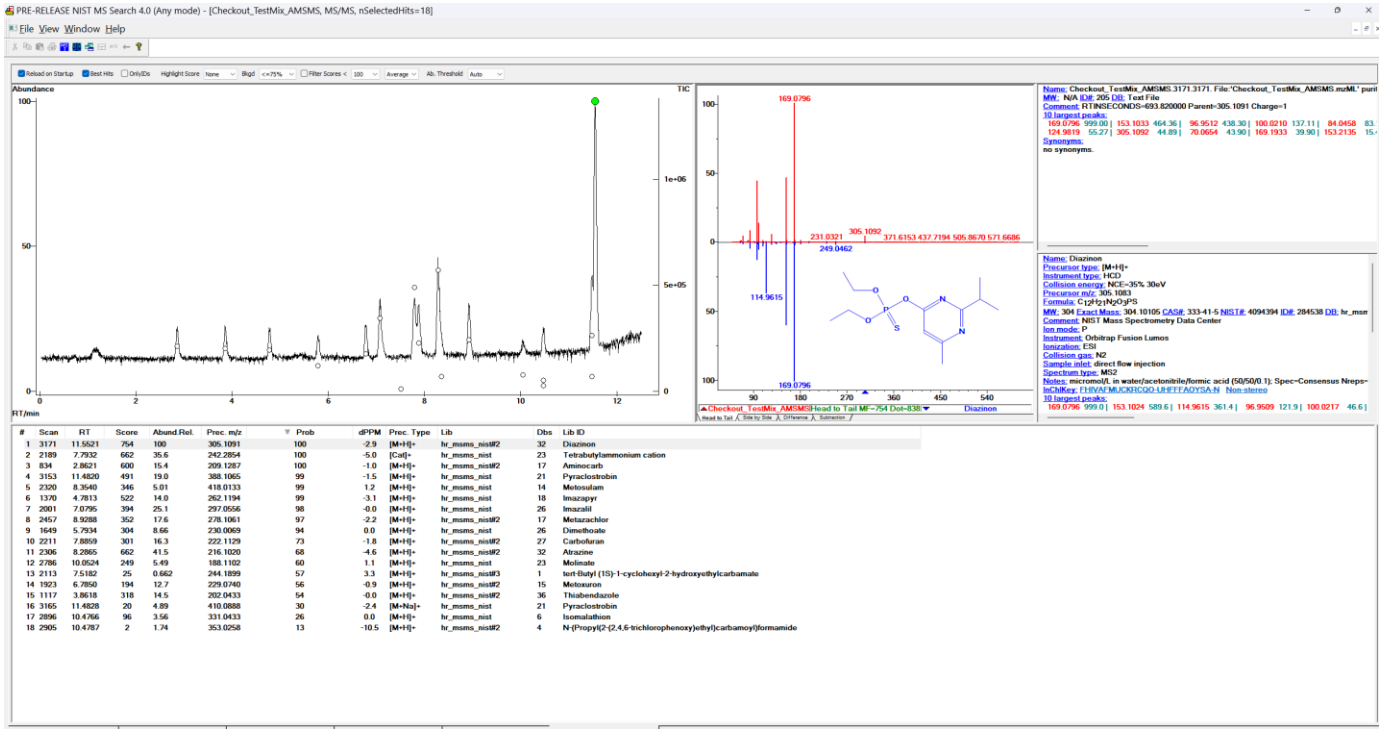
#	Scan	RT	Score	Abund.Rel.	Prec. m/z
3	3153	11.4820	491	19.0	388.1065
4	2905	10.4787	2	1.74	353.0258
5	2904	10.4768	4	1.44	348.0706
6	2896	10.4766	96	3.56	331.0433

#	Scan	RT	Score	Abund.Rel.	Prec. m/z
3	2189	7.7932	662	35.6	242.2854
4	834	2.8621	600	15.4	209.1287
5	1370	4.7813	522	14.0	262.1194
6	3153	11.4820	491	19.0	388.1065
7	2001	7.0795	394	25.1	297.0556
8	2457	8.9288	352	17.6	278.1061

#	Scan	RT	Score	Abund.Rel.	Prec
3	2075	7.3610	0	0.00579	295.
4	2197	8.1060	0	0.0152	222.
5	2634	9.5386	0	0.784	371.
6	2017	7.1496	2	2.16	311.
7	2494	8.9283	2	4.27	279.
8	2905	10.4787	2	1.74	353.

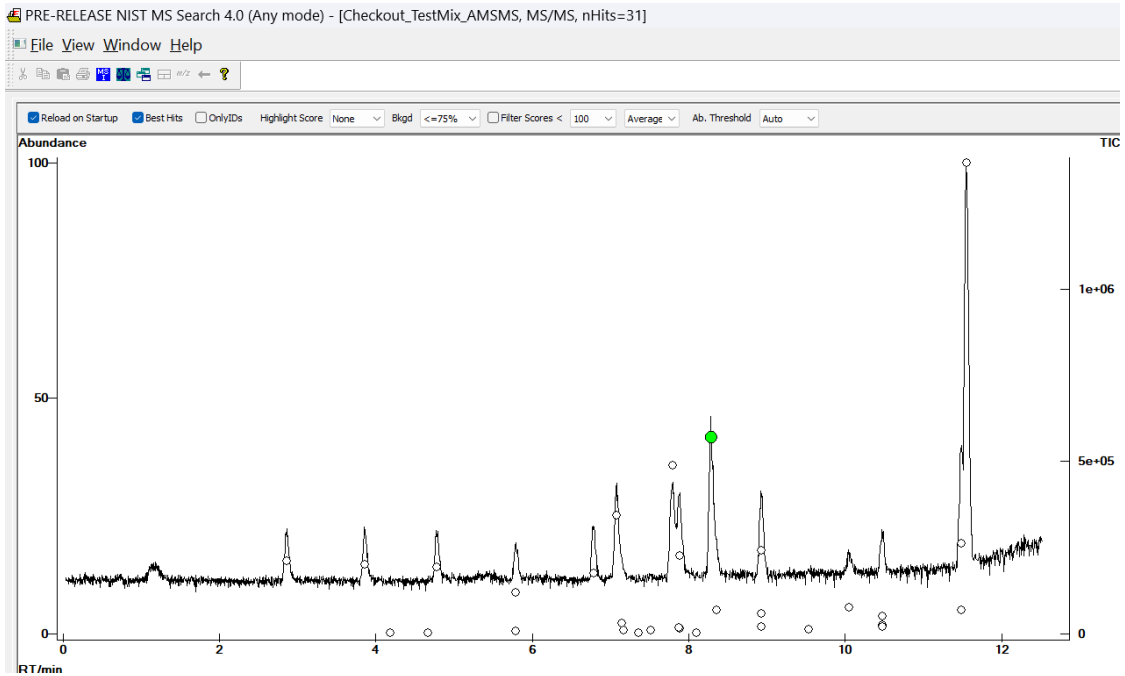
All windows can be resized by letting mouse pause on the *side* or *bottom* of window to see “doubled sided” arrow, left click and drag

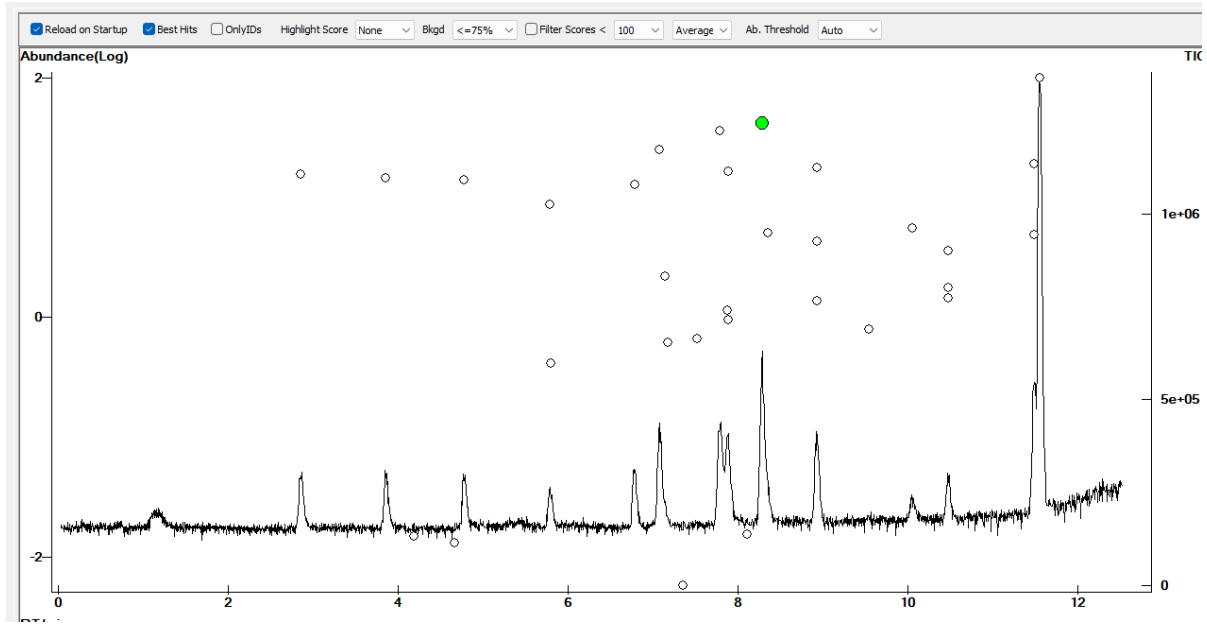


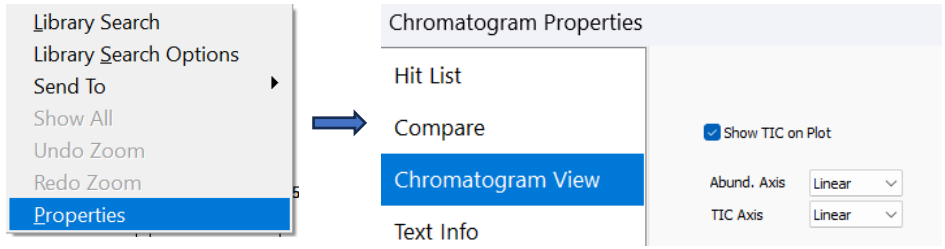


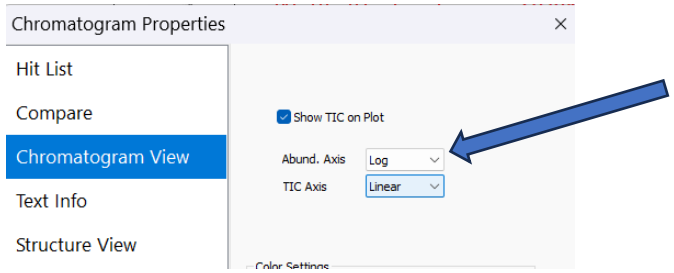
Abundances can be compressed on baseline, often easier to visualize using Abundance Axis *“Log”*

Notice, **Abundance Axis on Left, Total Ion Current, TIC, on right**



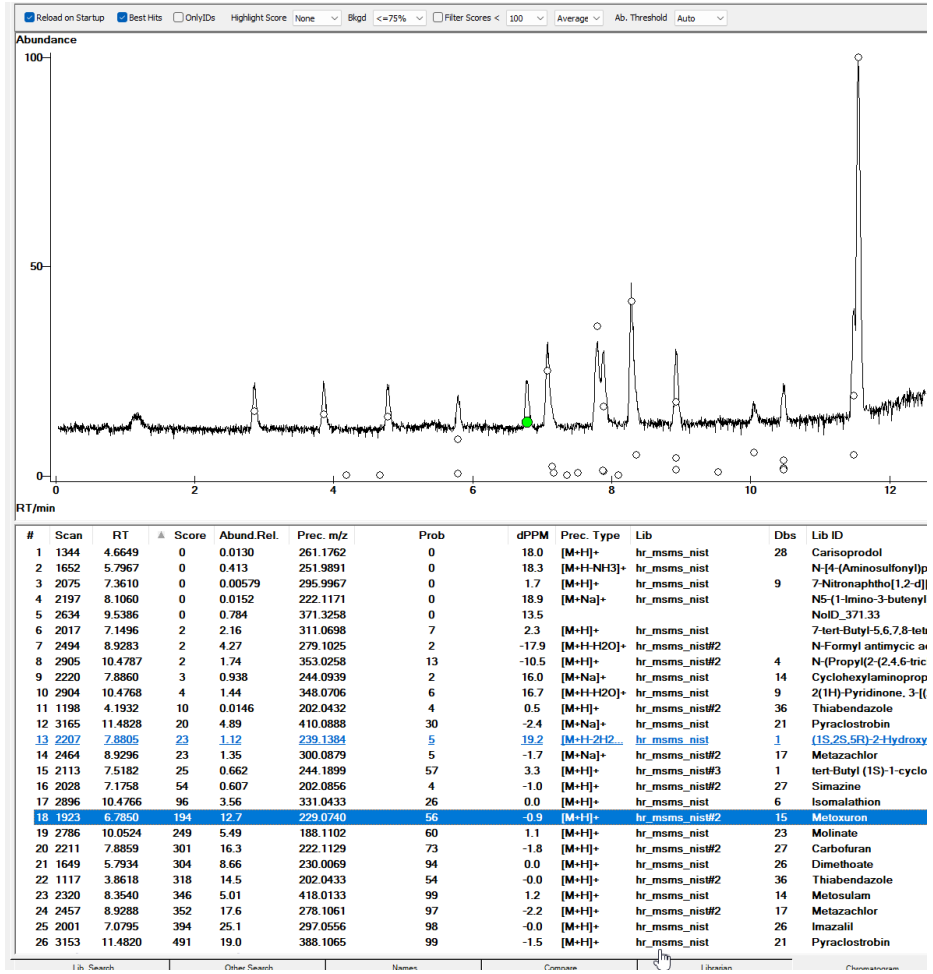






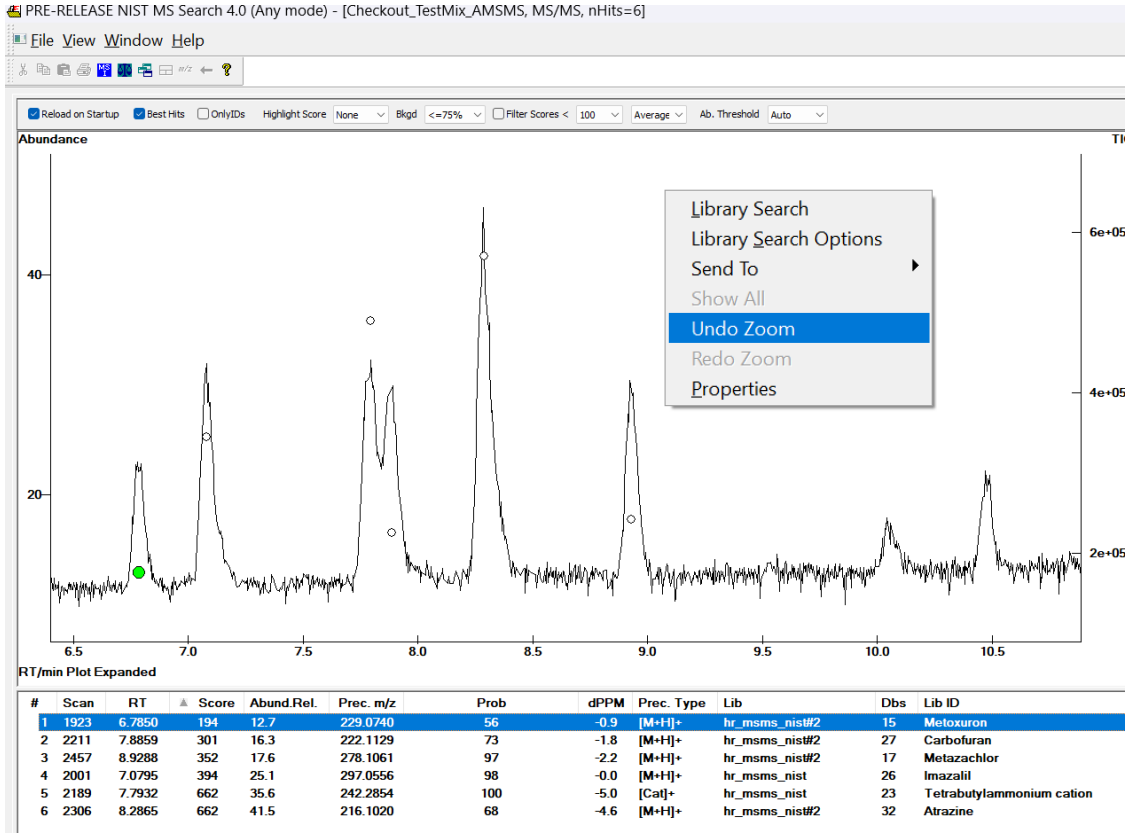
Right click in chromatogram at top and select to get menu

Left Click and Drag in Chromatogram Window *to Expand and Limit* Results in Bottom List



#	Scan	RT	Score	Abund.Rel.	Prec. m/z	Prob	dPPM	Prec. Type	Lib	Dbs	Lib ID
1	1344	4.6649	0	0.0130	261.1762	0	18.0	[M+H]+	hr_msms_nist	28	Carisoprodol
2	1652	5.7967	0	0.413	251.9891	0	18.3	[M+H-NH3]+	hr_msms_nist		N-[4-(Aminosulfonyl)p
3	2075	7.3610	0	0.00579	295.9967	0	1.7	[M+H]+	hr_msms_nist	9	7-Nitronaphtho[1,2-d]
4	2197	8.1060	0	0.0152	222.1171	0	18.9	[M+Na]+	hr_msms_nist		N5-(1-Imino-3-butenyl
5	2634	9.5386	0	0.784	371.3258	0	13.5				NoID_371.33
6	2017	7.1496	2	2.16	311.0698	7	2.3	[M+H]+	hr_msms_nist		7-tert-Butyl-5,6,7,8-tet
7	2494	8.9283	2	4.27	279.1025	2	-17.9	[M+H-H2O]+	hr_msms_nist#2		N-Formyl antimycic a
8	2905	10.4787	2	1.74	353.0258	13	-10.5	[M+H]+	hr_msms_nist#2	4	N-(Propyl(2-(2,4,6-tric
9	2220	7.8860	3	0.938	244.0939	2	16.0	[M+Na]+	hr_msms_nist	14	Cyclohexylaminoprop
10	2904	10.4768	4	1.44	348.0706	6	16.7	[M+H-H2O]+	hr_msms_nist	9	2(1H)-Pyridinone, 3-[(
11	1198	4.1932	10	0.0146	202.0432	4	0.5	[M+H]+	hr_msms_nist#2	36	Thiabendazole
12	3165	11.4828	20	4.89	410.0888	30	-2.4	[M+Na]+	hr_msms_nist	21	Pyraclostrobin
13	2207	7.8805	23	1.12	239.1384	5	19.2	[M+H-2H2...	hr_msms_nist	1	(1S,2S,5R)-2-Hydroxy
14	2464	8.9296	23	1.35	300.0879	5	-1.7	[M+Na]+	hr_msms_nist#2	17	Metazachlor
15	2113	7.5182	25	0.662	244.1899	57	3.3	[M+H]+	hr_msms_nist#3	1	tert-Butyl (1S)-1-cyclo
16	2028	7.1758	54	0.607	202.0856	4	-1.0	[M+H]+	hr_msms_nist#2	27	Simazine
17	2896	10.4766	96	3.56	331.0433	26	0.0	[M+H]+	hr_msms_nist	6	Isomalathion
18	1923	6.7850	194	12.7	229.0740	56	-0.9	[M+H]+	hr_msms_nist#2	15	Metoxuron
19	2786	10.0524	249	5.49	188.1102	60	1.1	[M+H]+	hr_msms_nist	23	Molinate
20	2211	7.8859	301	16.3	222.1129	73	-1.8	[M+H]+	hr_msms_nist#2	27	Carbofuran
21	1649	5.7934	304	8.66	230.0069	94	0.0	[M+H]+	hr_msms_nist	26	Dimethoate
22	1117	3.8618	318	14.5	202.0433	54	-0.0	[M+H]+	hr_msms_nist#2	36	Thiabendazole
23	2320	8.3540	346	5.01	418.0133	99	1.2	[M+H]+	hr_msms_nist	14	Metosulam
24	2457	8.9288	352	17.6	278.1061	97	-2.2	[M+H]+	hr_msms_nist#2	17	Metazachlor
25	2001	7.0795	394	25.1	297.0556	98	-0.0	[M+H]+	hr_msms_nist	26	Imazalil
26	3153	11.4820	491	19.0	388.1065	99	-1.5	[M+H]+	hr_msms_nist	21	Pyraclostrobin

Undo by Right Clicking in Chromatogram and Undo zoom

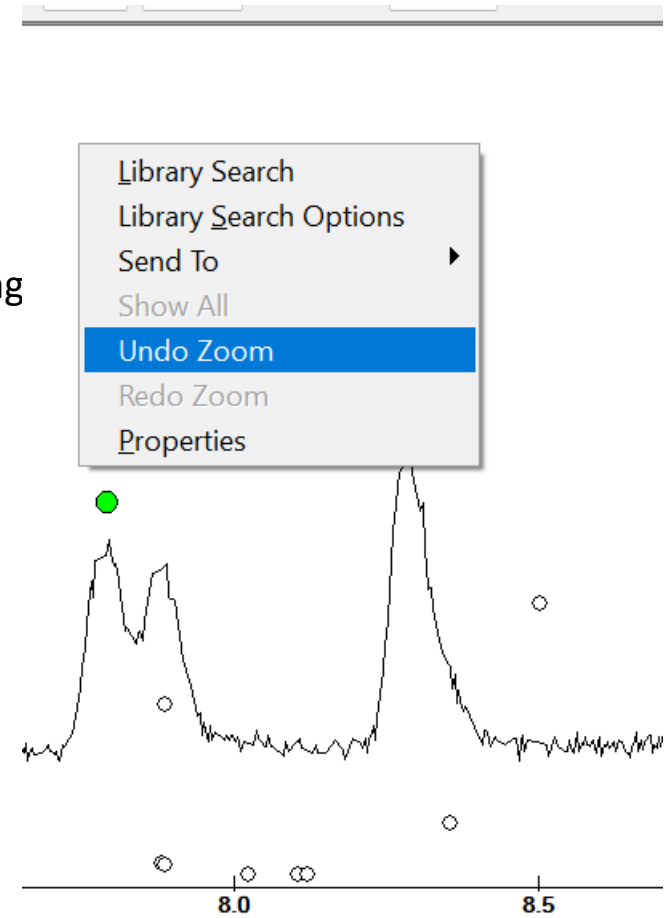


#	Scan	RT	Score	Abund.Rel.	Prec. m/z	Prob	dPPM	Prec. Type	Lib	Dbs	Lib ID
1	1923	6.7850	194	12.7	229.0740	56	-0.9	[M+H]+	hr_msms_nist#2	15	Metoxuron
2	2211	7.8859	301	16.3	222.1129	73	-1.8	[M+H]+	hr_msms_nist#2	27	Carbofuran
3	2457	8.9288	352	17.6	278.1061	97	-2.2	[M+H]+	hr_msms_nist#2	17	Metazachlor
4	2001	7.0795	394	25.1	297.0556	98	-0.0	[M+H]+	hr_msms_nist	26	Imazalil
5	2189	7.7932	662	35.6	242.2854	100	-5.0	[Cat]+	hr_msms_nist	23	Tetrabutylammonium cation
6	2306	8.2865	662	41.5	216.1020	68	-4.6	[M+H]+	hr_msms_nist#2	32	Atrazine

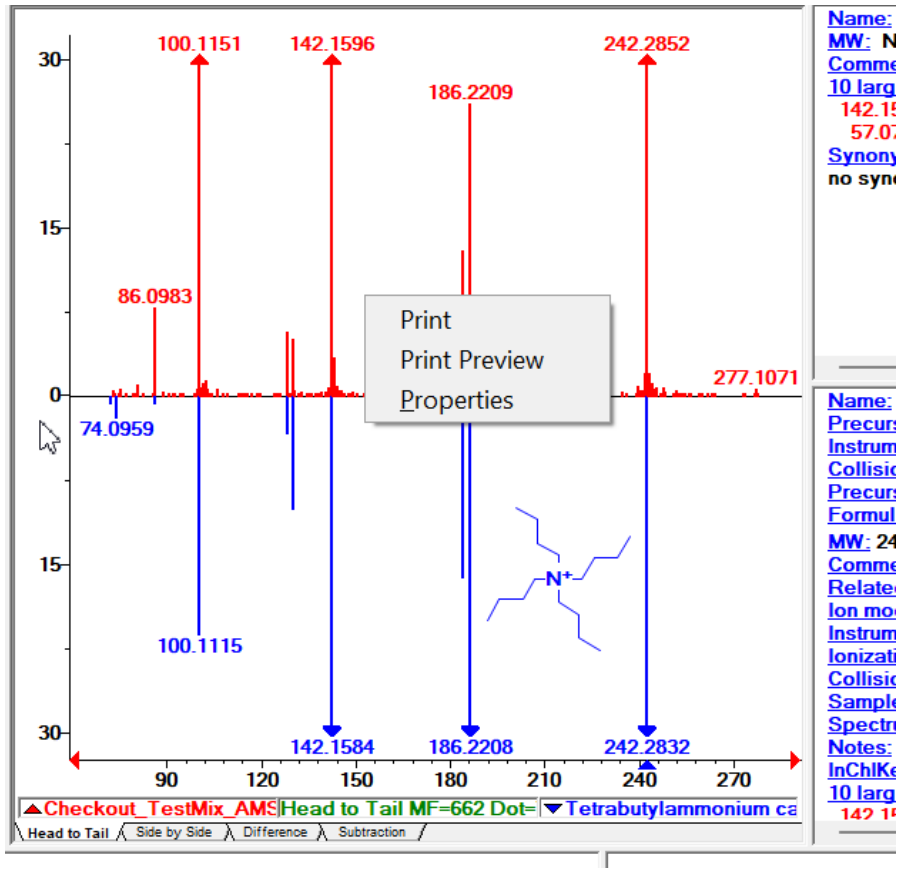
Zooming and "Unzooming" Windows

- ***All*** spectral windows in the NIST Program can be ***zoomed*** by "left click and drag" and forming a box
- ***Almost all*** windows can be ***"Unzoomed"*** by "right clicking and select ***Undo Zoom***
- ***All windows*** can be ***"Unzoomed"*** by "double left clicking" in the window
- The spectral display can ***only*** be "unzoomed" by "double left clicking"

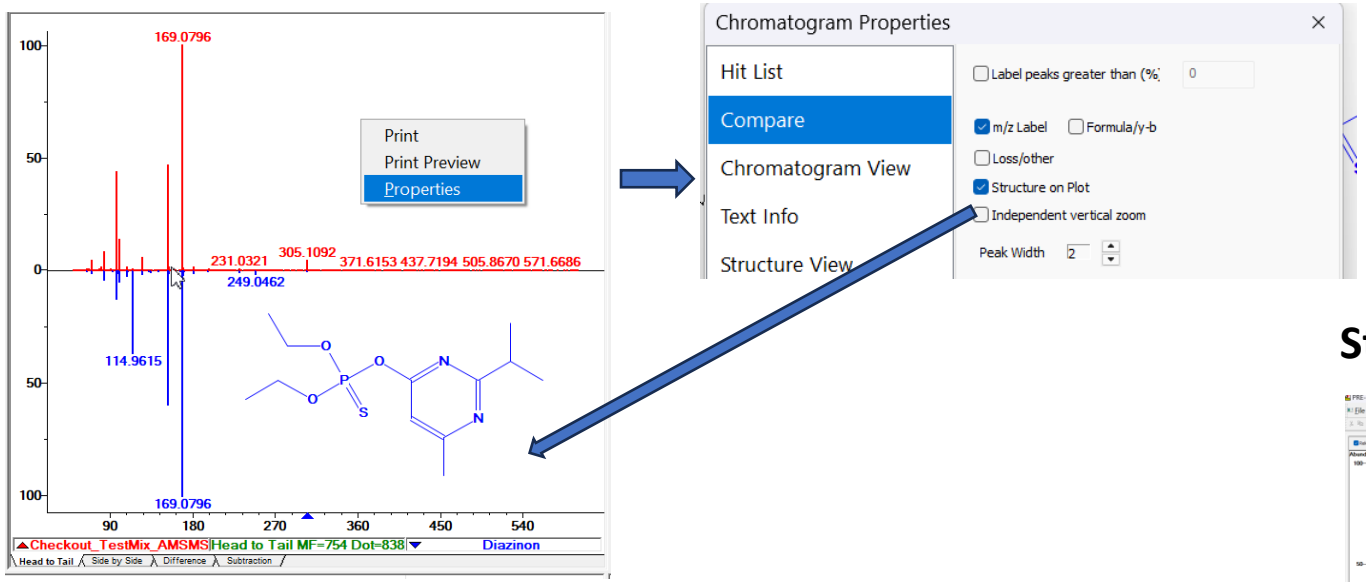
Or "double left clicking in window



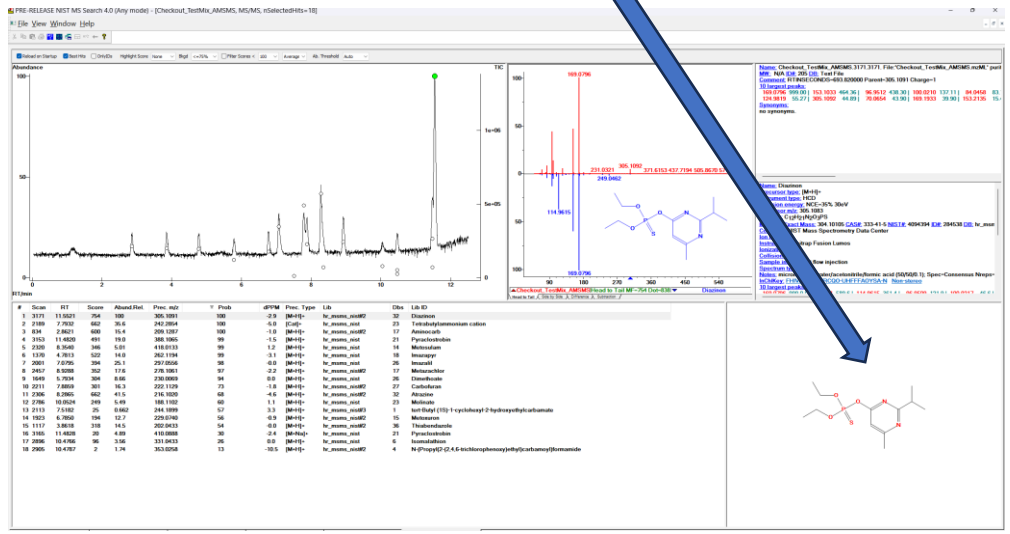
Only "double left clicking" in window in Chromatogram Window to ***"Unzoom"***



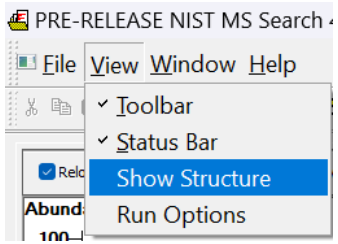
Showing Structures on Butterfly Display, Right Click on window, “add structure on plot”

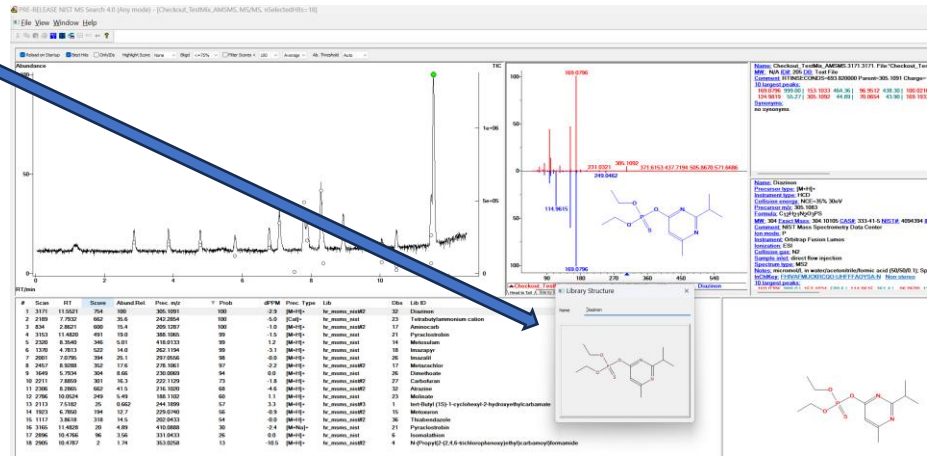


Standard Display on Bottom Right



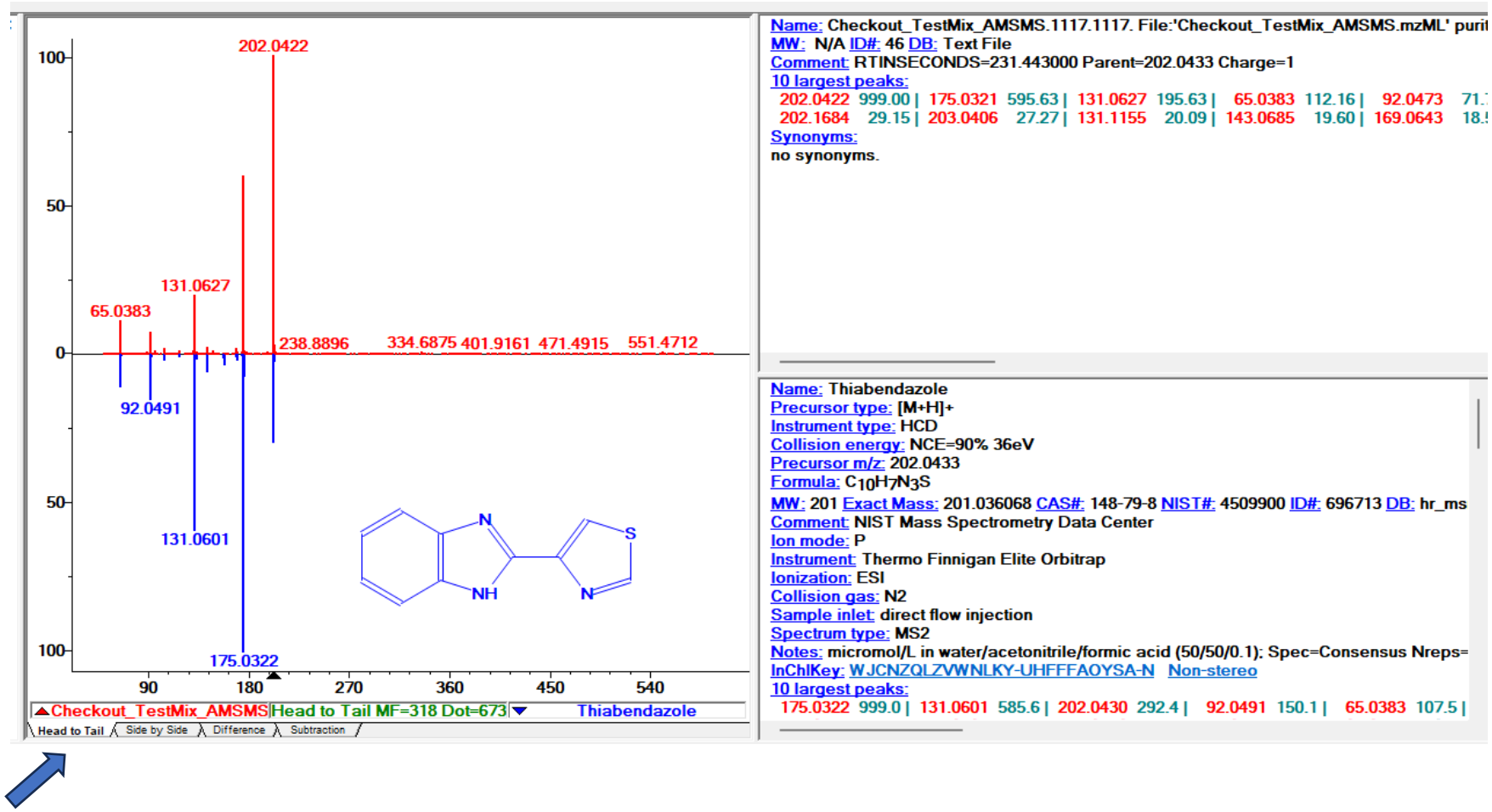
Floating Window



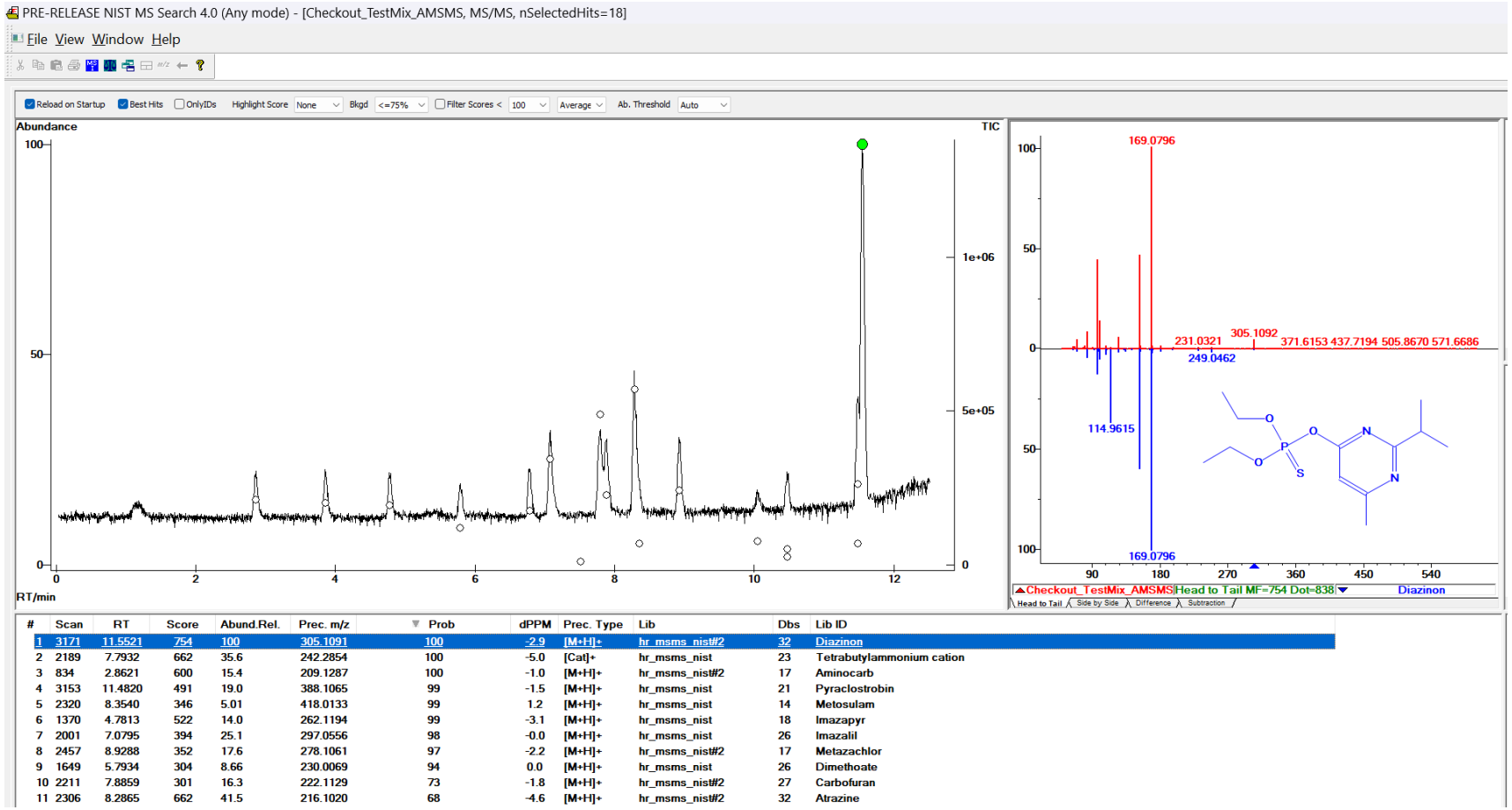


Reviewing Identities Noted in Chromatographic Plot and List in “Butterfly” Head to Tail Plot

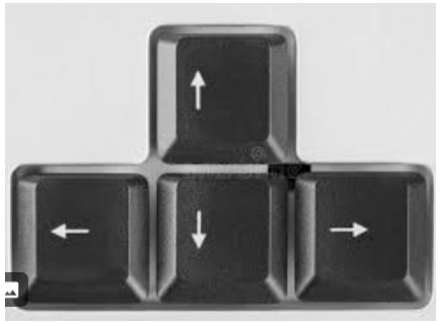
- As circles in either chromatogram or a component in table are clicked, results are previewed in top pane
- MS2 of spectrum is shown in top spectrum of butterfly plot (“Head to tail”)
- Library search results shown in bottom
- Spectrum format changed by tabs on bottom of plot, e.g. “Head to tail” my favorite



Left click on first entry in bottom window, then step through with keyboard arrows to ***review results***



#	Scan	RT	Score	Abund.Rel.	Prec. m/z	Prob	dPPM	Prec. Type	Lib	Dbs	Lib ID
1	3171	11.5521	754	100	305.1091	100	-2.9	[M+H]+	hr_msms_nist#2	32	Diazinon
2	2189	7.7932	662	35.6	242.2854	100	-5.0	[Cat]+	hr_msms_nist	23	Tetrabutylammonium cation
3	834	2.8621	600	15.4	209.1287	100	-1.0	[M+H]+	hr_msms_nist#2	17	Aminocarb
4	3153	11.4820	491	19.0	388.1065	99	-1.5	[M+H]+	hr_msms_nist	21	Pyraclostrobin
5	2320	8.3540	346	5.01	418.0133	99	1.2	[M+H]+	hr_msms_nist	14	Metosulam
6	1370	4.7813	522	14.0	262.1194	99	-3.1	[M+H]+	hr_msms_nist	18	Imazapyr
7	2001	7.0795	394	25.1	297.0556	98	-0.0	[M+H]+	hr_msms_nist	26	Imazalil
8	2457	8.9288	352	17.6	278.1061	97	-2.2	[M+H]+	hr_msms_nist#2	17	Metazachlor
9	1649	5.7934	304	8.66	230.0069	94	0.0	[M+H]+	hr_msms_nist	26	Dimethoate
10	2211	7.8859	301	16.3	222.1129	73	-1.8	[M+H]+	hr_msms_nist#2	27	Carbofuran
11	2306	8.2865	662	41.5	216.1020	68	-4.6	[M+H]+	hr_msms_nist#2	32	Atrazine



Use *Ctrl* and *Shift* Keys with *Left Click* to Select Items in the Bottom Window

Use **Shift** to select continuous ranges of cells or rows in a table by clicking the first item, holding Shift, and clicking the last item. Use **Ctrl** to select non-adjacent (separate) items by clicking each item while holding down Ctrl.

#	Scan	RT	Score	Abund.Rel.	Prec. m/z	Prob	dPPM	Prec. Type	Lib	Dbs	Lib ID
1	3171	11.5521	754	100	305.1091	100	-2.9	[M+H]+	hr_msms_nist#2	32	Diazinon
2	2189	7.7932	662	35.6	242.2854	100	-5.0	[Cat]+	hr_msms_nist	23	Tetrabutylamm
3	834	2.8621	600	15.4	209.1287	100	-1.0	[M+H]+	hr_msms_nist#2	17	Aminocarb
4	3153	11.4820	491	19.0	388.1065	99	-1.5	[M+H]+	hr_msms_nist	21	Pyraclostrobin
5	2320	8.3540	346	5.01	418.0133	99	1.2	[M+H]+	hr_msms_nist	14	Metosulam
6	1370	4.7813	522	14.0	262.1194	99	-3.1	[M+H]+	hr_msms_nist	18	Imazapyr

Show Selected to remove unwanted entries, always *undo by Show All*

#	Scan	RT	Score	Abund.Rel.	Prec. m/z	Prob	dPPM
3	2075	7.3610	0	0.00579	295.9967	0	1.7
4	2197	8.1060	0	0.0152	222.1171	0	18.9
5	2634	9.5386	0	0.784	371.3258	0	13.5
6	2017	7.1496	2	2.16	311.0698	7	2.3
7	2494	8.9283	2	4.27	279.1025	2	-17.9
8	2905	10.4787	2	1.74	353.0258	13	-10.5
9	2220	7.8860	3	0.938			
10	2904	10.4768	4	1.44			
11	1198	4.1932	10	0.0146			
12	3165	11.4828	20	4.89			
13	2207	7.8805	23	1.12			
14	2464	8.9296	23	1.35			
15	2113	7.5182	25	0.662			
16	2028	7.1758	54	0.607			
17	2896	10.4766	96	3.56			
18	1923	6.7850	194	12.7			
19	2786	10.0524	249	5.49			

#	Scan	RT	Score	Abund.Rel.	Prec. m/z	Prob	dPPM	Prec. Type	Lib	Dbs
1	2075	7.3610	0	0.00579	295.9967	0	1.7	[M+H]+	hr_msms_nist	9
2	2197	8.1060	0	0.0152	222.1171	0	18.9	[M+Na]+	hr_msms_nist	
3	2634	9.5386	0	0.784	371.3258	0	13.5			
4	2017	7.1496	2	2.16	311.0698	7	2.3	[M+H]+	hr_msms_nist	
5	2494	8.9283	2	4.27	279.1025	2	-17.9	[M+H-H2O]+	hr_msms_nist#2	
6	2905	10.4787	2	1.74	353.0258	13	-10.5	[M+H]+	hr_msms_nist#2	4
7	2220	7.8860	3	0.938	244.0939	2	16.0	[M+Na]+	hr_msms_nist	14
8	2904	10.4768	4	1.44	348.0706	6	16.7	[M+H-H2O]+	hr_msms_nist	9
9	1198	4.1932	10	0.0146	202.0432	4	0.5	[M+H]+	hr_msms_nist#2	36
10	3165	11.4828	20	4.89	410.0888	30	-2.4	[M+Na]+	hr_msms_nist	21
11	2207	7.8805	23	1.12	239.1384	5	19.2	[M+H-2H2...	hr_msms_nist	1