

MS Interpreter for EI Accurate Mass Data, Correlating Structure to m/z Video/Handout

James Little

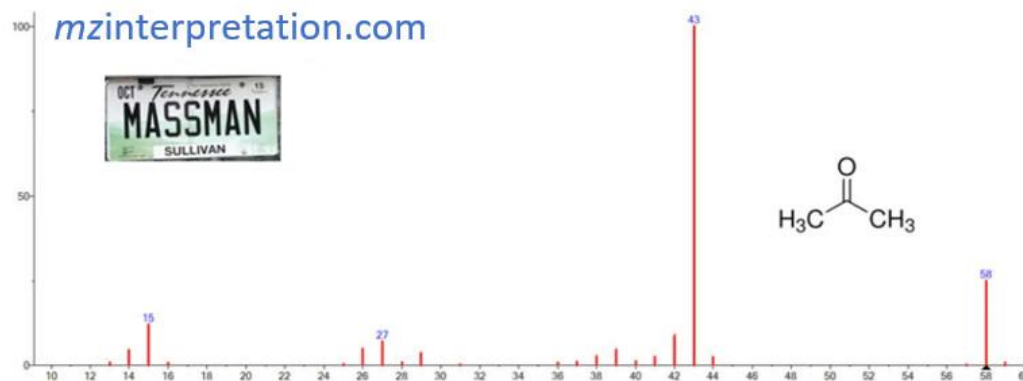
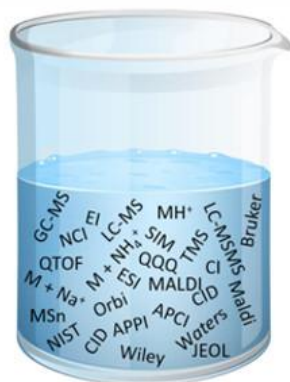
Mass Spec Interpretation Services

April 24, 2026

mzinterpretation.com

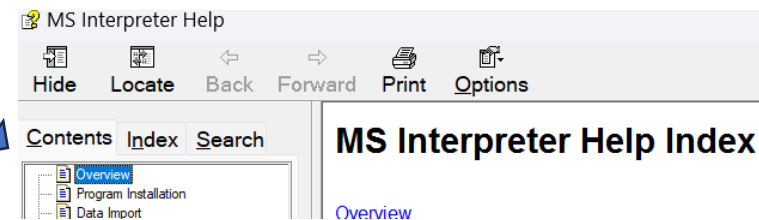
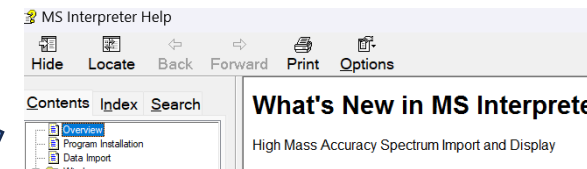
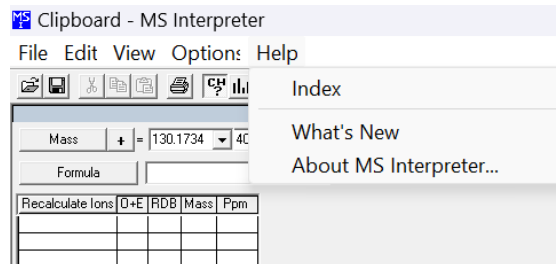
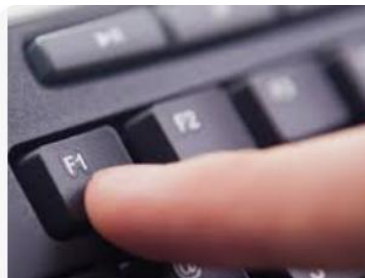
See **Full Course** on NIST26 with new **Integrated** Deconvolution/Library Searching for
EI GC-MS and **LC-MS/MS**!

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



Help in Using MS Interpreter

- Use the Help on Menu Bar and see **Whats New** and **Index**
- **ALSO**, F1 on keyboard when **ANY** of the windows give addition information



Hide Locate Back Forward Print Options

Contents Index Search

Structure window

The structure is displayed at an upper

m/z	exact m/z	formula	loss	typ
182 (1/3)	182.117556	C ₁₀ H ₁₁ N ₂ O ₂	C ₇ H ₅ O ₂	dissoci

The red portion of the structure corresponds to the structure. The first box shows the nominal number of different substructures, and two views of the various possible configurations. A single click of the Right Mouse button will also appear in there is only one possible explanation.

MS Interpreter Help

Hide Locate Back Forward Print Options

Contents Index Search

Mass Spectrum window

There are two primary-views of the **Mass Spectrum** window dependent on the mouse pointer in the **Mass Spectrum** window: 1. the **Show Fragments** view. Selecting one, deselects the other.

Options:

- Show unfiltered peaks
- Show Mouse Position
 - On Cursor
 - On Top
- Show Fragments
 - On Top
 - Off
- m/z Diff. (Select Anchor)
- Log Scale for Spectra
- Cancel

In addition, there is a **Show unfiltered peaks** view, which can be used via the **(RMB)** menu or by use of the **[E]** button on the **Toolbar**. There is also a **Show Fragments** and **m/z Diff. (Select Anchor)** views available.

View 1: Compute Formula Spectrum window (Low mass accuracy)

MS Interpreter Help

Hide Locate Back Forward Print Options

Contents Index Search

Formula Calculator

Displays formulas of ions or neutral losses corresponding to a given accuracy (500 mDa = 1/2 Da)

18 Ions	O+E	RDB	Mass	mDa	C	H	N	O
C ₇ H ₂₀ NO ₄	Even	-0.5	182.13868	138	7	20	1	4
C ₈ H ₈ NO ₄	Even	5.5	182.04478	44	8	8	1	4
C ₉ H ₁₀ O ₄	Odd	5	182.05736	57	9	10	0	4
C ₉ H ₁₂ NO ₃	Even	4.5	182.08117	81	9	12	1	3
C ₁₀ NO ₃	Even	11.5	181.98727	-12	10	0	1	3
C ₁₀ H ₄ O ₃	Odd	4	182.06375	83	10	14	0	3
C ₁₀ H ₁₈ NO ₂	Even	3.5	182.11756	117	10	16	1	2
C ₁₁ H ₂ O ₃	Odd	11	181.99985	-0.2	11	2	0	3

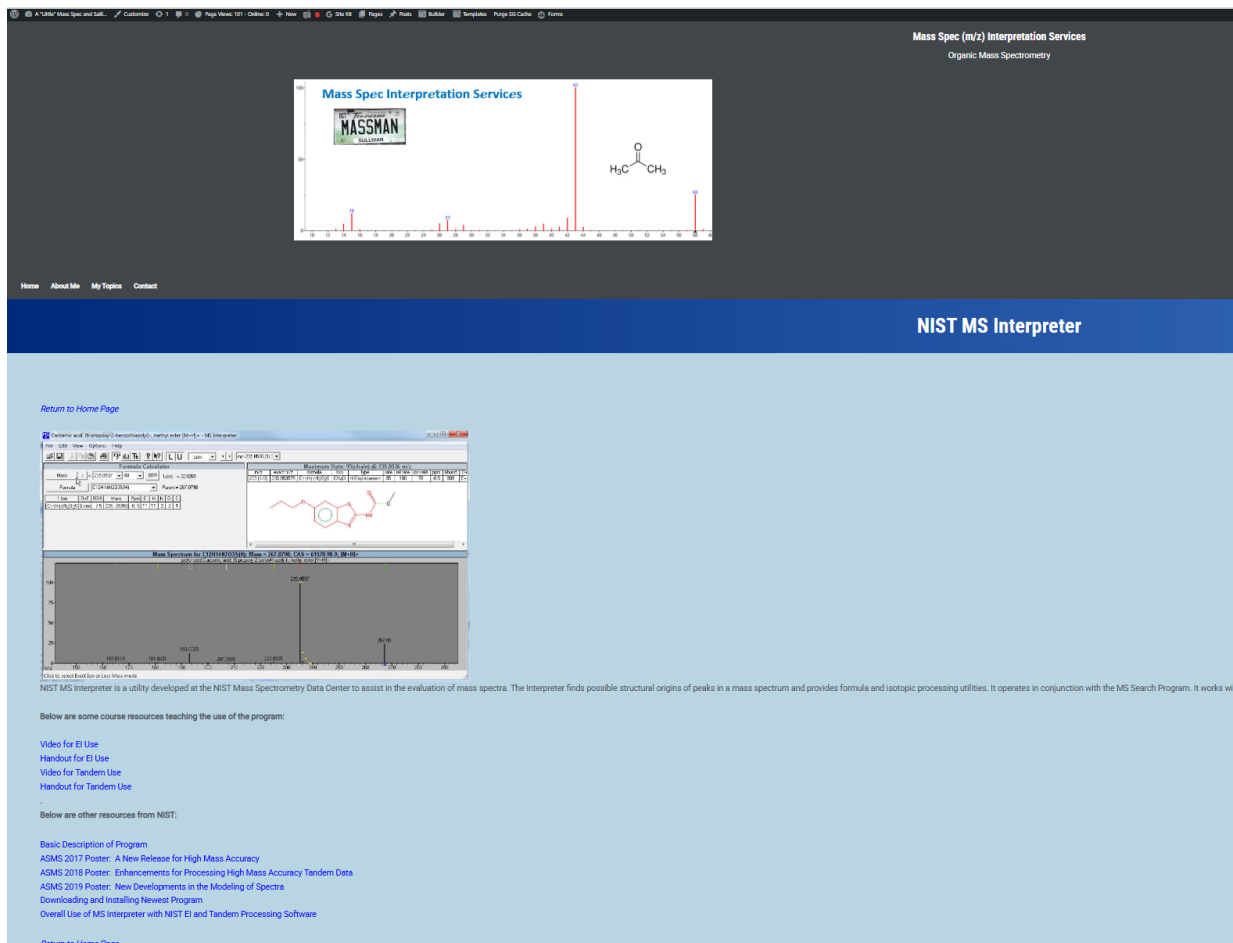
Formula Calculator window when Mass Spectrum window is active

All formulas listed in the table are a subset of the elements in the formula. The first box shows the nominal number of different substructures, and two views of the various possible configurations. A single click of the Right Mouse button will also appear in there is only one possible explanation.

Other Training Videos and Handouts on MS Interpreter

- Many other resources from previous versions
- Very **useful still**, especially for the **new user!**
- **See Links below**

See [link](#)



The screenshot displays the NIST MS Interpreter website. At the top, it says "Mass Spec (m/z) Interpretation Services" and "Organic Mass Spectrometry". Below this is a mass spectrum plot with a chemical structure of acetone (CC(=O)C) shown. The plot has a peak at m/z 43. Below the plot, there is a navigation bar with "Home", "About Me", "My Topics", and "Contact". A blue banner below the navigation bar reads "NIST MS Interpreter".

Below the banner, there is a "Return to Home Page" link. A screenshot of the software interface is shown, displaying a mass spectrum and a chemical structure. The software interface includes a "Mass Spectrum for 1,1-DIBROMOETHANE" and a "Mass Spectrum for 1,1-DIBROMOETHANE" plot. The plot shows a base peak at m/z 200. The chemical structure is 1,1-dibromoethane (CCBr2).

Below the screenshot, there is a description of the NIST MS Interpreter utility. It states: "NIST MS Interpreter is a utility developed at the NIST Mass Spectrometry Data Center to assist in the evaluation of mass spectra. The Interpreter finds possible structural origins of peaks in a mass spectrum and provides formula and isotopic processing utilities. It operates in conjunction with the MS Search Program. It works with..."

Below the description, there are links to course resources teaching the use of the program:

- Video for EI Use
- Handout for EI Use
- Video for Tandem Use
- Handout for Tandem Use

Below these links, there is a section for "Other resources from NIST":

- Basic Description of Program
- ASMS 2017 Poster: A New Release for High Mass Accuracy
- ASMS 2018 Poster: Enhancements for Processing High Mass Accuracy Tandem Data
- ASMS 2019 Poster: New Developments in the Modeling of Spectra
- Downloading and installing Newest Program
- Overall Use of MS Interpreter with NIST EI and Tandem Processing Software

At the bottom, there is a "Return to Home Page" link.

See [link](#)

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

Videos and Videos Zipped:

NIST26

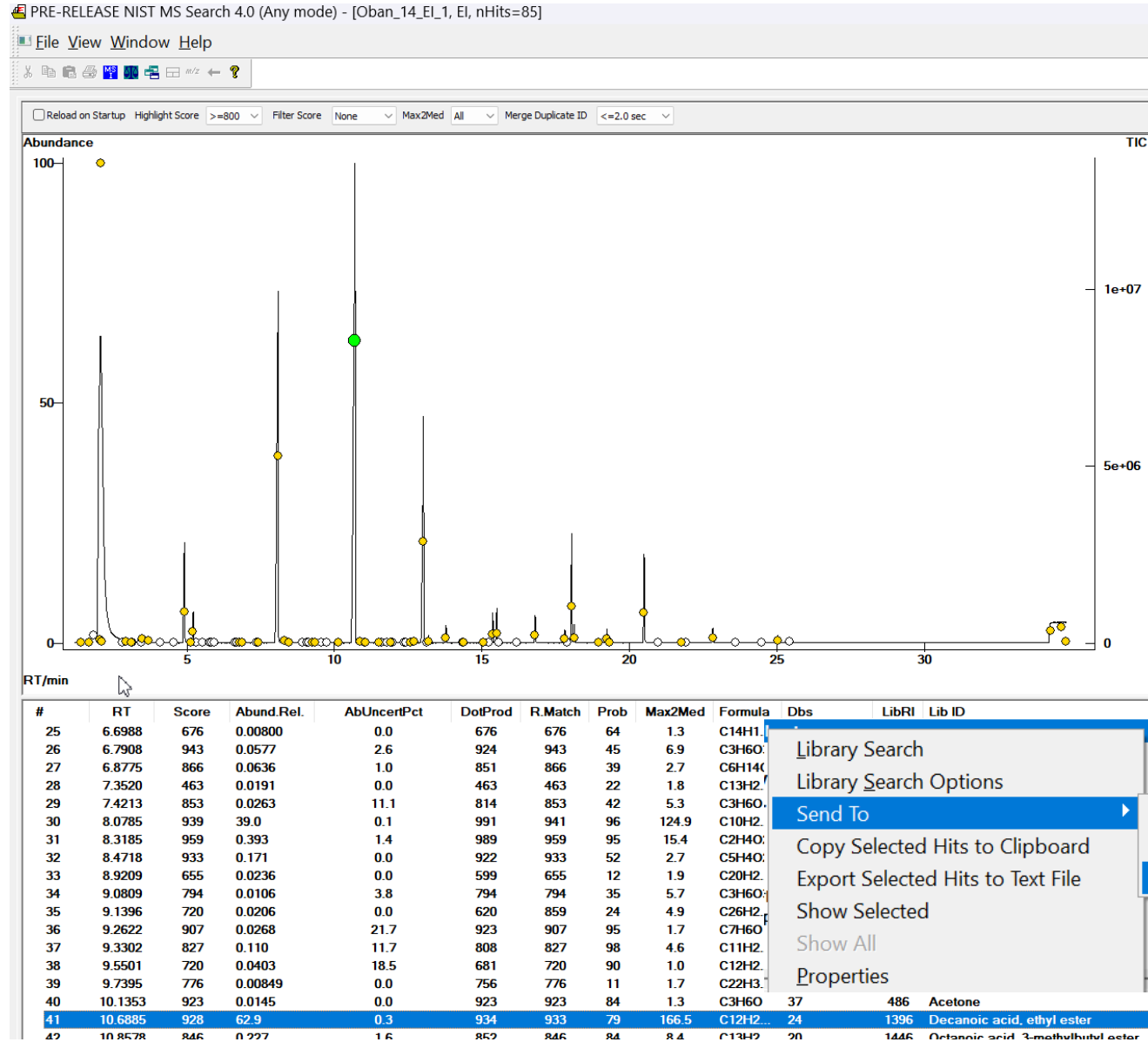
- Part 0: Changes in EI NIST23 Program (V3.0)
- Part I: Spectral Searches with NIST MS Search
- Part II: Structure Searches with MS Search and Using MS Interpreter
- Part III: AMDIS (NIST) for Processing EI Mass Spectral Data Files
- Part IV: Advanced NIST Hybrid Search of EI and MS/MS Spectra
- Part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

Parts 0-VI Zipped

Detailed Handouts:

- Part 0: Changes in EI NIST23 Program (V3.0)
- Part I: Spectral Searches with NIST MS Search
- Part II: Structure Searches with NIST Search and MS Interpreter
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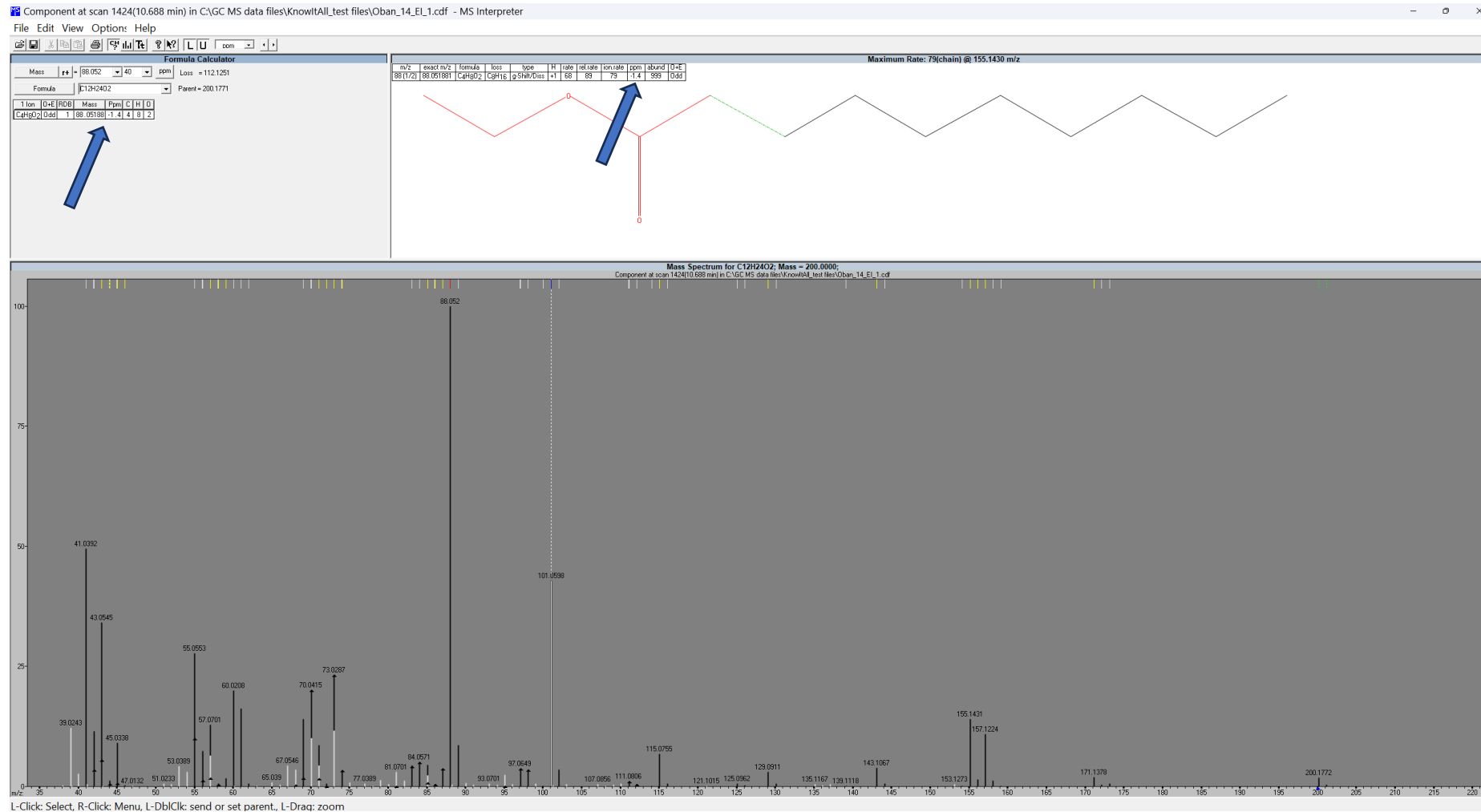
Can Send Any Result in Chromatogram List



- Library Search
- Library Search Options
- Send To
 - Spec List
 - Compare List
 - MS Interpreter
- Copy Selected Hits to Clipboard
- Export Selected Hits to Text File
- Show Selected
- Show All
- Properties

Overall Process

- Spectrum is sent from Chromatogram for the unknown identification from bottom list to MS Interpreter,
- Structure for known is **paired** with the Unknown's EI spectrum in transfer process
- User gets the accurate mass errors in ppm and the proposed substructures assigned to observed fragment ions
- Can send spectrum from text section of "Head to tail" display, but for the top one just get the accurate mass spectrum no structure
- For the bottom one, get the library spectrum and its structure



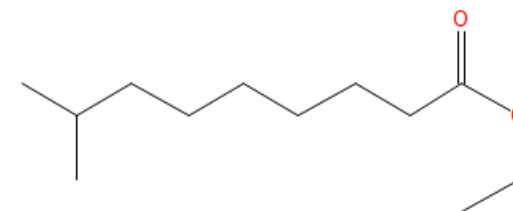
Sending Unknown Accurate Mass Spectrum to MS Interpreter and Adding Structure of Identified Component from Lib Search Window (*First Step*)

- Use this approach if the best hit in Chromatogram is *not* the best candidate
- Compare a hit with lower Match Factor
- Copy the structure of second-best match in Lib Search Window to clipboard

#	Lib.	Match	Prob. (%)	DBs	PSS.Match	R.Match	Name
1	M	921	76.3	24	921	921	Decanoic acid, ethyl ester
2	M	873	10.5				Decanoic acid, ethyl ester
3	M	846	4.42				Decanoic acid, ethyl ester
4	M	832	2.83	19			Decanoic acid, ethyl ester
5	M	805	1.19	25			Decanoic acid, ethyl ester
6	M	783	0.59	10			Decanoic acid, ethyl ester
7	M	782	0.57	24			Decanoic acid, ethyl ester
8	M	769	0.37	12			Decanoic acid, ethyl ester
9	M	754	0.23	7			Decanoic acid, ethyl ester
10	M	754	0.23	27			Decanoic acid, ethyl ester
11	M	744	0.17	25			Decanoic acid, ethyl ester
12	M	739	0.14				Decanoic acid, ethyl ester
13	M	732	0.11	2			Decanoic acid, ethyl ester
14	M	732	0.11	24			Decanoic acid, ethyl ester
15	M	731	0.11	24			Decanoic acid, ethyl ester
16	M	730	0.10	2			Decanoic acid, ethyl ester
17	M	730	0.10	1			Decanoic acid, ethyl ester
18	M	728	0.10	2			Decanoic acid, ethyl ester
19	M	728	0.10	1			Decanoic acid, ethyl ester
20	M	727	0.09	5			Decanoic acid, ethyl ester
21	M	725	0.09	2			Decanoic acid, ethyl ester
22	M	722	0.08				Decanoic acid, ethyl ester
23	M	720	0.07	2			Decanoic acid, ethyl ester
24	M	718	0.07	5			Decanoic acid, ethyl ester
25	M	711	0.08				Decanoic acid, ethyl ester
26	M	710	0.05				Decanoic acid, ethyl ester
27	M	707	0.05	5			Decanoic acid, ethyl ester

Library Search
Structure Similarity Search
Show DBs
Copy
Select All
Close All Replicates
Export Selected Spectra
Copy Selected Hits to Clipboard
Export Selected Hits to Text File
Send To
Find name in Names tab
Copy Structure to Clipboard
Print
Print Preview
Properties

Names Structures / InLib = 133, Hit List



Sending Unknown Accurate Mass Spectrum to MS Interpreter and Adding Structure an Identified Component (*Second Step*)

- Send the accurate mass spectrum from top window in Lib Search to MS Interpreter

The screenshot displays a software interface with a table at the top and a mass spectrum plot below. The table has columns for '#', 'Src.', 'MW', 'Formula', and 'Name'. The first row contains the value '1' in the '#' column, 'A' in 'Src.', '0' in 'MW', and 'Component of scan 1424(10.688 mi)' in 'Name'. Below the table, there are tabs for 'Names' and 'Structures', and a status bar indicating 'mainlib: 382180 total spectra'. The mass spectrum plot shows relative intensity on the y-axis (log scale from 1 to 100) and m/z on the x-axis (from 1000 to 600). A single prominent peak is visible at approximately m/z 900. A context menu is overlaid on the plot, listing various actions. The 'Send To' option is highlighted in blue, and its sub-menu is open, with 'MS Interpreter' also highlighted in blue. Other options in the main menu include Library Search, Structure Similarity Search, Cut, Copy, Paste, Select All, Find name in Names tab, Import, Export Selected Spectra, Copy Selected Items to Clipboard, Export Selected Items to Text File, Insert Clipboard Structure, Copy Structure to Clipboard, Insert Clipboard Spectra, Print, Print Preview, and Properties. The sub-menu for 'Send To' includes Spec List, Compare List, MS Interpreter, and Default Structure Editor.

#	Src.	MW	Formula	Name
1	A	0		Component of scan 1424(10.688 mi)

Paste Second Best Hit Into Accurate Mass Spectrum Into MS Interpreter

Clipboard - MS Interpreter

File Edit View Options Help

Clipboard icons: Copy, Paste, Print, Undo, Redo, Find, Zoom, etc. ppm mz=87.0804 (2/2)

Formula Calculator

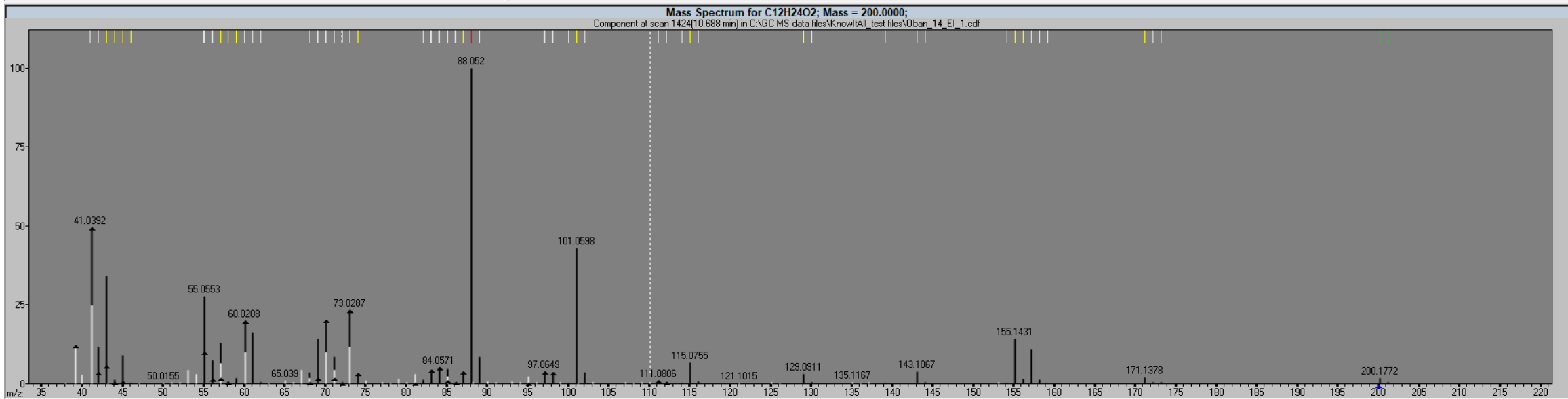
Mass $r+$ = 88.052 40 ppm Loss = 112.1251

Formula C₁₂H₂₄O₂ Parent = 200.1771

1 Ion	D+E	RDB	Mass	Ppm	C	H	O
C ₄ H ₈ O ₂	Odd	1	88.05188	-1.4	4	8	2

Maximum Rate: 79(chain) @ 155.1430 m/z

m/z	exact m/z	formula	loss	type	H	rate	rel.rate	ion.rate	ppm	abund	D+E
88 (1/2)	88.051881	C ₄ H ₈ O ₂	C ₈ H ₁₆	g-Shift/Diss	+1	68	89	79	-1.4	999	Odd



User Proposed Structure for Accurate Mass Spectrum

- First approach, user draws a spectrum in their preferred structural program
- Circle the structure in structural program
- Copy which puts in window clipboard
- Open accurate mass spectrum of interest in MS interpreter (send from Lib Search window)
- Edit/Paste or click on structure box in MS Interpreter then Ctrl V
- Second Approach shown below, *Often easier*, send structure from Lib Search to Structural program and modify it
- Much *more efficient* than drawing from scratch

Library Search
Structure Similarity Search
Show DBs

Copy
Select All
Close All Replicates

Export Selected Spectra
Copy Selected Hits to Clipboard
Export Selected Hits to Text File

Send To
Find name in Names tab
Copy Structure to Clipboard
Print
Print Preview

Properties

Spec List
Compare List
MS Interpreter
Default Structure Editor

29 43 55 60 73

ACD/ChemSketch (Freeware) - [C:\NIST26\MSEARCH\nistms1.mol]

File Edit Pages Tools Templates Options Documents Add-Ons

Structure Draw

mm 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150

Any
C
H
N
O

CCCCCCCCCCCC(=O)OCC

Clipboard - MS Interpreter

File Edit View Options Help

Formula Calculator

Mass: 111.948
Formula: C₁₈H₃₆O₂
Parent: 200

Maximum Ratio: 79.36141 @ 155.1430 m/z

Mass Spectrum for: Component at scan 1424(10.688 min) in C:\GC MS data\lib\500484.txt\lib\Copy_14_E_1.cdf

m/z	Relative Intensity
41.0362	~45
41.0545	~40
43.0338	~35
55.0389	~25
57.0701	~20
60.0208	~15
67.0544	~10
70.0415	~15
73.0287	~15
88.052	100
101.0598	~60
155.1430	~25
157.1224	~20