

MS Interpreter for Accurate Mass Data: Correlating Structure to m/z

Video/Handout

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Mass Spec Interpretation Services

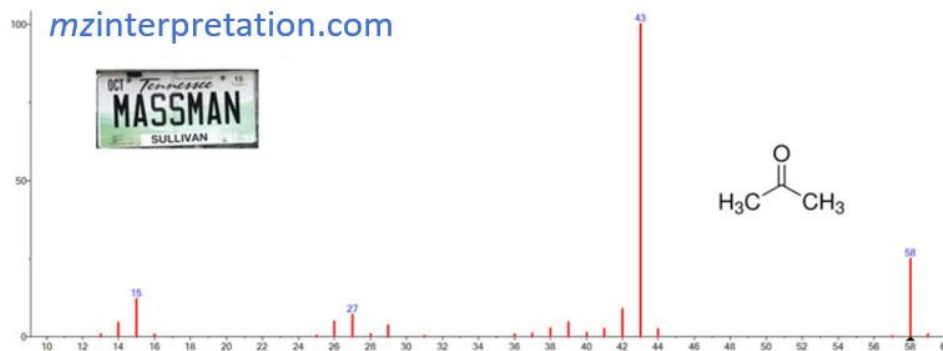
April 24, 2026

mzinterpretation.com

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

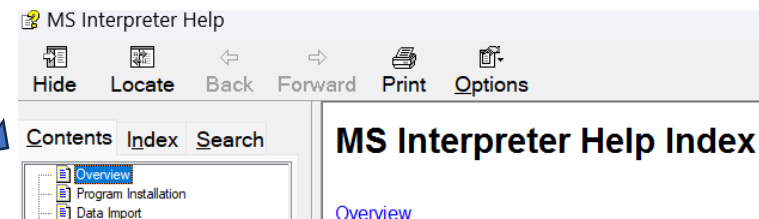
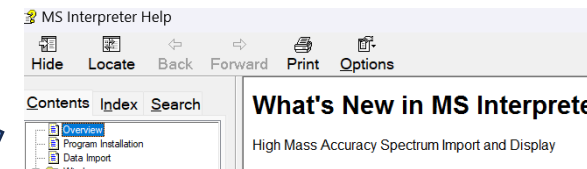
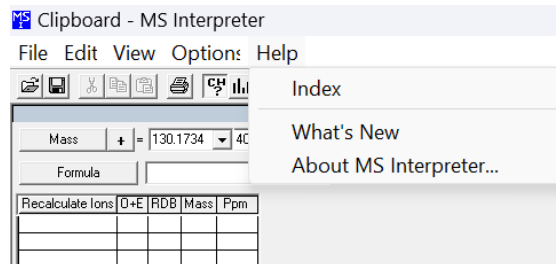
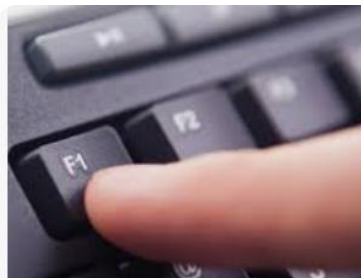
Mass Spec (m/z) Interpretation Services

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



MS Interpreter Help

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)

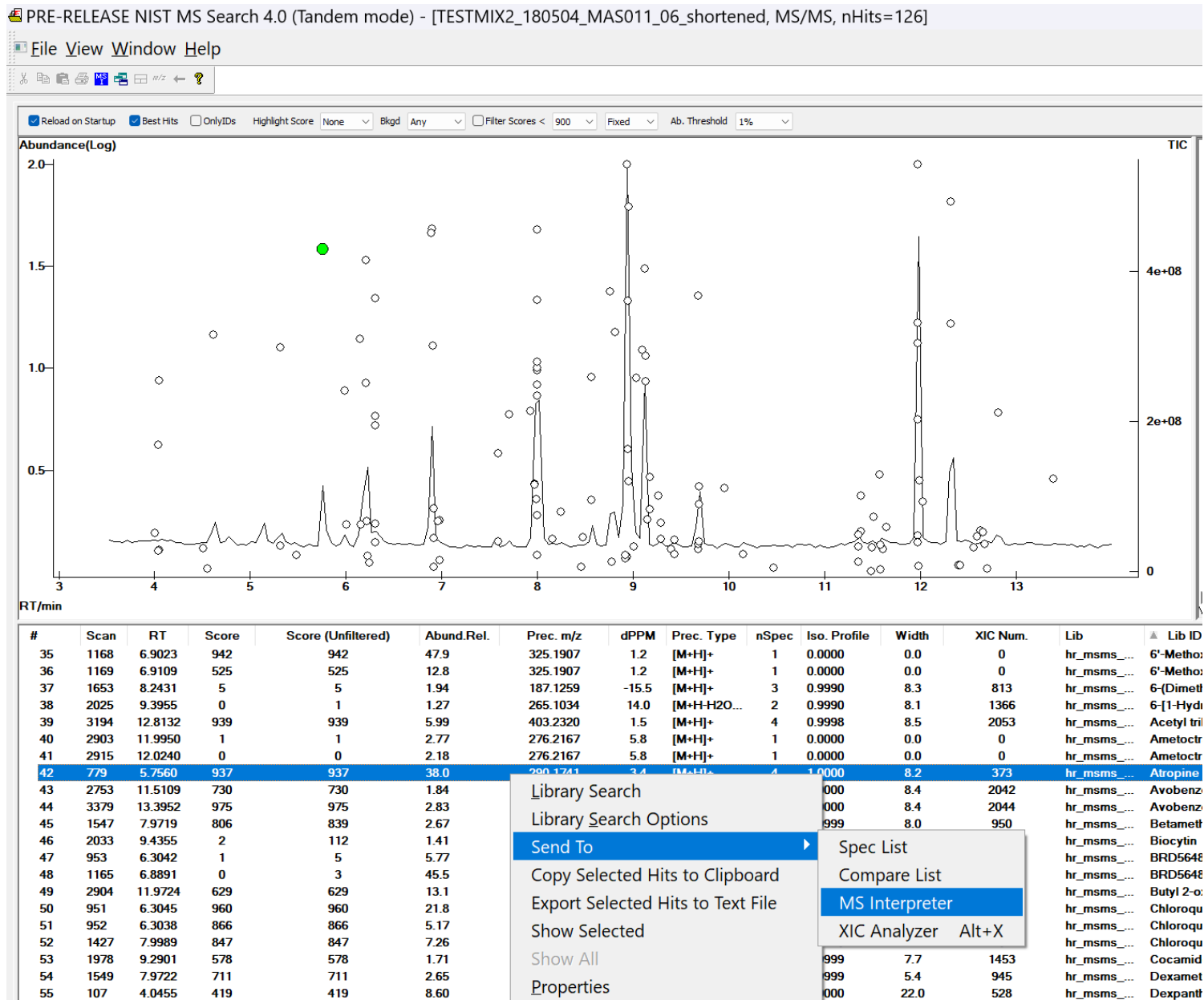
18 Ions	O+E	RDB	Mass	mDa	C	H	N	O
C ₇ H ₂₀ NO ₄	Even	-0.5	182.13868	138	7	20	1	4
C ₈ H ₈ NO ₄	Even	5.5	182.04478	44	8	8	1	4
C ₉ H ₁₀ O ₄	Odd	5	182.05736	57	9	10	0	4
C ₉ H ₁₂ NO ₃	Even	4.5	182.08117	81	9	12	1	3
C ₁₀ HNO ₃	Even	11.5	181.98727	-12	10	0	1	3
C ₁₀ H ₄ O ₃	Odd	4	182.06375	83	10	14	0	3
C ₁₀ H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

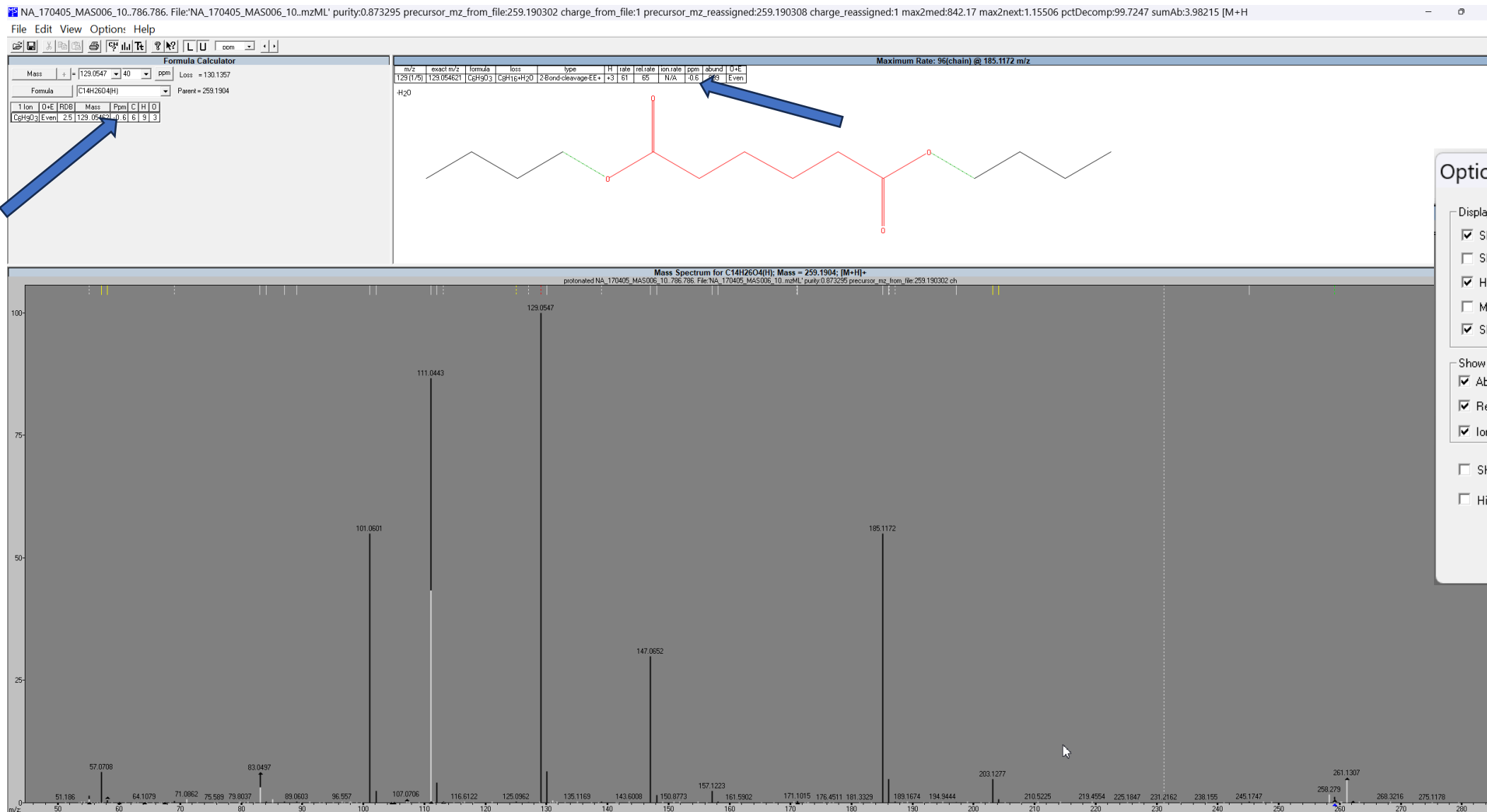
Can Send Any Result in Chromatogram Search Results List to MS Interpreter

When you right click in the list and “Send to MS Interpreter,” your unknown spectrum sent to MS Interpreter and paired with the structure from library identification in list



Left Click on Any Ion in the Spectrum to See Substructure and Associated ppm Accuracy

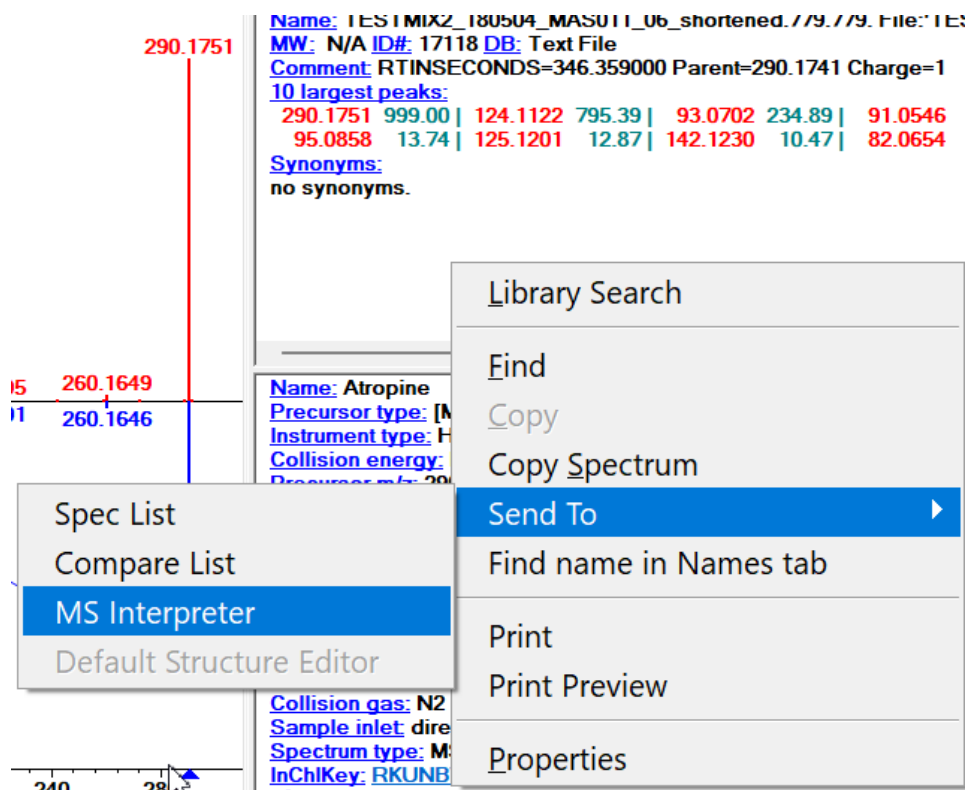
Note in Options, "Protonated" is Selected Automatically



Spectra sent from Text Box of Your “Head to Tail Plot” to MS Interpreter

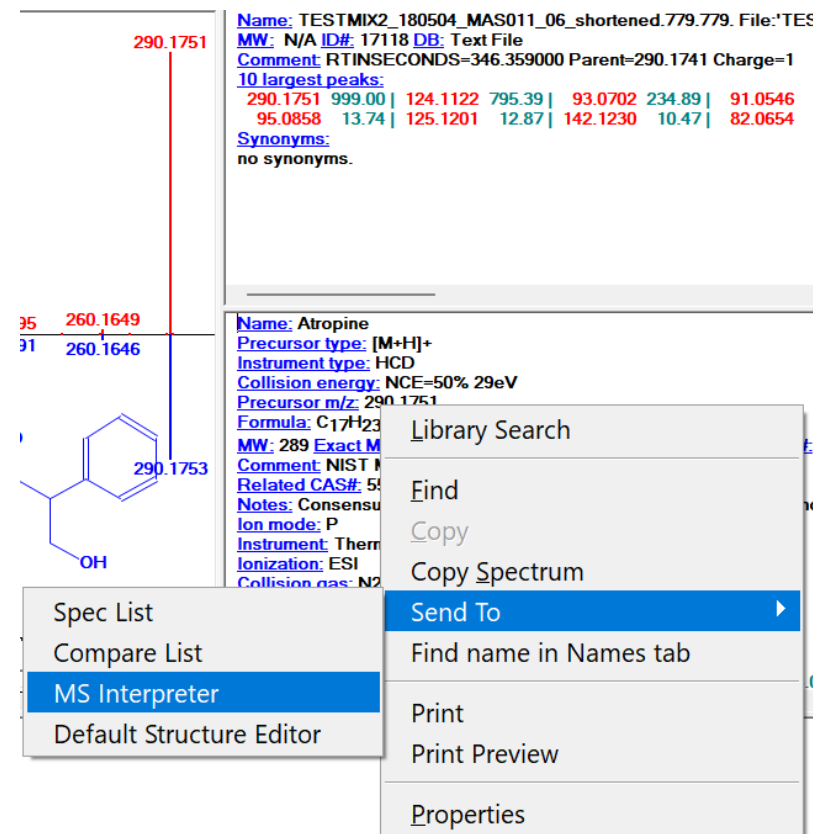
Sent from Text of Unknown with Right Click,
Spectrum of Unknown Sent to MS Interpreter
with **No** structure

*Note Ionized Selected Automatically, Change to
Protonated in MS Interpreter Options!*



Sent from Text of Library Results with Right Click,
Library Spectrum and Associated Structure Sent
to MS Interpreter

*Note Protonated Selected Automatically in MS
Interpreter Options*



You can add your own spectrum in MS Interpreter, Get a Structure from Results List or Drawing Program

PRE-RELEASE NIST MS Search 4.0 (Tandem mode) - [precursor = 290.1741, Presearch Default - 17 spectra]

File Search View Tools Options Window Help

1. TESTMIX2_180504_MAS011_06_short

#	Src.	MW	For...	Name
1	A	0		TESTMIX2_180504_MAS011_06_s...
2	A	0		TESTMIX2_180504_MAS011_06_s...
4	A	0		TESTMIX2_180504_MAS011_06_s...

Names Structures Spec List

apci_msms_nist_hr_msms_nist_hr_msms_nist#2; 2645452 total spectra

(Text File) TESTMIX2_180504_MAS011_06_shortened.779.779; File: TESTMIX2_180504_MAS011_06_shortened.mzML

TESTMIX2_180504_MAS011_06_shortened.779.779; File: TESTMIX2_180504_MAS011_06_

#	Lib.	Score	DotProd	Prob. (%)	Prec. Type	Instr. Type	Energy	DBs	PSS-Dot
1	hr	937	983	100.0	(M+H) ⁺	HCD	50%	27	988
2	hr	191	348						520
3	hr	61	224						371
4	hr	60	154						218
5	hr	53	184						205
6	hr	41	168						372
7	hr	33	133						227
8	hr	32	183						360
9	hr	23	89						162
10	hr	21	92						174
11	hr	12	83						194
12	hr	2	42						107
13	hr	2	38						102
14	hr	1	43						176
15	hr	1	32						101
16	hr	0	31						101
17	hr	0	10						38

- 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 HR List

(hr_msms_nist) Atropine [M+H]⁺ HCD 50% P=290.2

Plot/Text of Hit Plot of Hit

Then Send the Spectrum of Your Unknown from Spec List Window

PRE-RELEASE NIST MS Search 4.0 (Tandem mode) - [precursor = 290.1741, Presearch Default - 17 spectra]

File Search View Tools Options Window Help

1. TESTMIX2_180504_MAS011_06_short

#	Src.	MW	For...	Name
1	A	0		TESTMIX2_180504
2	A	0		TESTMIX2_180504
4	A	0		TESTMIX2_180504

Library Search
Structure Similarity Search

Cut
Copy
Paste
Select All

Send To

- 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

Spec List
Compare List
MS Interpreter
Default Structure Editor

Plot of Search Spectrum

4_MAS011_06_shortened.779.779. File:'TESTMIX2_180504_MAS011_06_shortened.mzML' purity:0.985513 precu

Can Either Edit/Paste or Ctrl V (keyboard sequence) to add structure to MS Interpreter Window

Clipboard - MS Interpreter

File Edit View Options Help

Formula Calculator

Mass: 290.1751 40 ppm Loss = 0

Formula: Parent = 290

Recalculate Ions	O-E	RDB	Mass	Ppm

m/z	exact m/z	formula	loss	type	H rate	rel rate	ion rate	ppm	abund	O-E	
290	290.17507	C ₁₇ H ₂₄ NO ₃	-	Parent	+1	N/A	N/A	N/A	-0.1	999	Even

Maximum Rate: 112(ring) @ 84.0808 m/z; 101(chain) @ 124.1121 m/z

Mass Spectrum for : protonated TESTMD2_180504_MAS011_06 shortened m/z purity:0.385513 precur

m/z	Relative Intensity (%)
82.0654	~2
93.0702	~25
103.0545	~2
108.0613	~2
121.0652	~2
124.1122	100
129.0705	~2
142.123	~2
157.1017	~2
178.2247	~2
214.1595	~2
242.1543	~2
260.1649	~2
272.1657	~2
290.1751	~95

Options

Display

- Show fragments
- Show fragments with no peak
- Highlight unfiltered peaks
- Mark Isotope Peaks
- Show Ion for Nearest Annotated Peak

Show Rates

- Absolute
- Relative
- Ion

Import

- Ionized
- Protonated
- Deprotonated

Show up to 39 assignments

Highlight if relative rate < 50

Cancel OK

L-Click: Select, R-Click: Menu, L-DbClick: send or set parent., L-Drag: zoom

Adding Your Own Structure from Drawing Program and Pairing with Unknown Spectrum

Example with Hybrid Search Result in Lib Search Window

PRE-RELEASE NIST MS Search 4.0 (Tandem mode) - [precursor = 468.3887, Presearch Default - 21 spectra]

File Search View Tools Options Window Help

1. TESTMIX2_180504_MAS011_06_short

#	Src.	MW	For...	Name
1	A	0		TESTMIX2_180504_MAS011_06_s...
2	A	0		TESTMIX2_180504_MAS011_06_s...
4	A	0		TESTMIX2_180504_MAS011_06_s...

Names Structures Spec List

apci_msms_nist_hr_msms_nist_hr_msms_nist#2; 2645452 total spectra

(Text File) TESTMIX2_180504_MAS011_06_shortened.2801.2801. File: TESTMIX2_180504_MAS011_06_shortened.mzML purity 0.980377 prec

Plot of Search Spectrum Plot of Search Spectrum Spec List

#	Lib.	Score	DotProd	DeltaMass	dForm	pctRelForm	Prec. Type	Instr. Type	Ener
1	hr	871	908	-132.079	C-6H-12O-3	0.25	[M+NH4]+	HCD	20%
2	hr	864	896	80.1346	C8H16O-2	0.014	[M+NH4]+	HCD	25%
3	hr	787	867	36.1084	C6H12O-3	0.0072	[M+NH4]+	HCD	14%
4	hr	780	841	156.187	-	-	[M+NH4]+	HCD	35%
5	hr	759	817	186.198	-	-	[M+NH4]+	HCD	25%
6	hr	743	849	-7.9178	C4H8O-4	0.036	[M+NH4]+	HCD	14%
7	hr	732	793	98.1452	-	-	[M+NH4]+	HCD	20%
8	hr	676	799	-139.997	C-2H-4O-7	0.0072	[M+NH4]+	HCD	20%
9	hr	663	784	230.224	C14H30O2	0.043	[M+NH4]+	HCD	20%
10	hr	654	784	100.088	C6H12O	0.44	[M+NH4]+	HCD	14%
11	hr	590	751	-184.023	-	-	[M+NH4]+	HCD	15%
12	hr	558	679	229.240	C14H31NO	0.0072	[M+H]+	IT-FT	35%
13	hr	551	679	229.240	C14H31NO	0.0072	[M+H-C12..	IT-FT	35%
14	hr	520	688	273.266	-	-	[M+H-C6H...	IT-FT	35%
15	hr	520	662	105.151	-	-	[M+H-C6H...	HCD	15%
16	hr	513	682	185.214	-	-	[M+H]+	IT-FT	35%
17	hr	512	769	200.213	-	-	[M+NH4]+	HCD	20%
18	hr	507	675	104.047	C4H8O3	1.1	[M+NH4]+	HCD	20%
19	hr	485	695	273.266	-	-	[M+H]+	HCD	25%
20	hr	465	660	273.266	-	-	[M+H]+>>[...	IT-FT	35%
21	hr	459	676	-18.8052	-	-	[M+Na]+	HCD	9%

Names Structures Hit List

Head to Tail Side by Side Difference Subtraction

TESTMIX2_180504_MAS011_06_shortened.2801.2801. File: TESTMIX2_180504_MAS011_0

Head to Tail MF=871 Dot=908

Nonaethylene glycol monododecyl ether

871 908R 0.00P

Plot of Hit Plot of Hit

(hr_msms_nist#2) Nonaethylene glycol monododecyl ether [M+NH4]+ HCD 20% P=600.5

Name: Nonaethylene glycol monododecyl ether
Precursor type: [M+NH4]+
Instrument type: HCD
Collision energy: NCE=20% 24eV
Precursor m/z: 600.4681
Formula: C30H62O10
MW: 582 ExactMass: 582.4343 CAS#: 3055-99-0 NIST#: 4801732 ID#: 960430 DB: hr_msms_nist#2
Comment: NIST Mass Spectrometry Data Center
Ion mode: P
Instrument: Thermo Finnigan Elite Orbitrap
Ionization: ESI
Collision gas: N2
Sample inlet: direct flow injection
Spectrum type: MS2
Notes: micromole/L in water/acetonitrile/formic acid (50/50/1). Spec=Consensus Nreps=9/9 Mz_diff=1.0ppm Via_ID=69591 Data_source:M
InChIKey: ONJQDTZCDESESW-UHFFFAQYSA-N Non-steroid
51 m/z Values and Intensities:
57.0697 69.2 C4H9-p-C26H57NO10/-3.2ppm 9/9
71.0853 94.5 C6H11-p-C25H55NO10/-3.2ppm 9/9
73.0646 43.7 C4H9O-p-C26H57NO9/-2.6ppm 9/9
83.0853 7.0 C6H11-p-C24H55NO10/-2.6ppm 5/9
83.6991 3.0 7/9

- Take Advantage of Modifying Structures with NIST Windows
- **Much faster** than drawing from scratch!
- e.g., I had a proposed structure that differed by 3 ethylene oxide groups
- Took best match and sent to structure editor

#	Lib.	Score	DotProd	DeltaMass	dForm	pctRelForm	Prec. Type	Instr. Type	Energy	DBs	Name
1	hr	871	908	-132.079	C-6	0.014	[M+NH4] ⁺	HCD	20%	25	Nonaethylene glycol
2	hr	787	867	36.1084	C6H	-	-	-	-	12	Nonaethylene glycol
3	hr	864	896	80.1346	C8H	-	-	-	-	15	Octaethylene glycol
4	hr	721	842	-132.079	C-6	0.014	[M+NH4] ⁺	HCD	20%	25	Nonaethylene glycol
5	hr	286	650	-33.9851	C-3	-	-	-	-	3	4-Nonylphenol hex
6	hr	743	849	-7.9178	C4H	-	-	-	-	11	Decaethylene glycol
7	hr	336	642	30.0462	C2H	-	-	-	-	3	Glycolic acid tetrae
8	hr	392	687	30.0462	C2H	-	-	-	-	3	Glycolic acid tetrae
9	hr	309	663	-78.0113	C-5	-	-	-	-	8	4-Nonylphenol hep
10	hr	262	647	-210.090	C-1	-	-	-	-	7	4-Nonylphenol dec
11	hr	77	222	140.156	C10	-	-	-	-	4	Hexaethyleneglycol
12	hr	222	624	-254.116	C-1	-	-	-	-	-	4-Nonylphenol und
13	hr	794	851	80.1346	C8H	-	-	-	-	15	Octaethylene glycol
14	hr	780	841	156.187	-	-	-	-	-	3	2-Hydroxymethyl-1
15	hr	685	824	36.1084	C6H	-	-	-	-	-	-
16	hr	654	784	100.088	C6H	-	-	-	-	-	-
17	hr	697	824	156.187	-	-	-	-	-	-	-
18	hr	676	799	-139.997	C-2	-	-	-	-	-	-
19	hr	512	769	200.213	-	-	-	-	-	-	-
20	hr	310	665	-166.064	C-9	-	-	-	-	-	-
21	hr	219	621	-166.064	C-9	-	-	-	-	-	-
22	hr	171	599	-210.090	C-1	-	-	-	-	-	-
23	hr	406	693	-228.049	-	-	-	-	-	-	-
24	hr	170	547	-109.986	C-1	-	-	-	-	-	-
25	hr	782	829	80.1346	C8H16O-2	0.014	[M+NH4] ⁺	HCD	20%	15	Octaethylene glycol
26	hr	337	661	-272.075	-	-	[M+NH4] ⁺	HCD	15%	6	PEG17
27	hr	354	664	-166.064	C-9H-100-3	0.17	[M+NH4] ⁺	HCD	20%	18	26-(Nonylphenoxy)

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

Evaluation of Proposed Structure in MS Interpreter After Editing Similar Structure in Structure Drawing Program

Note: Change from Ionized as Default to Protonated

