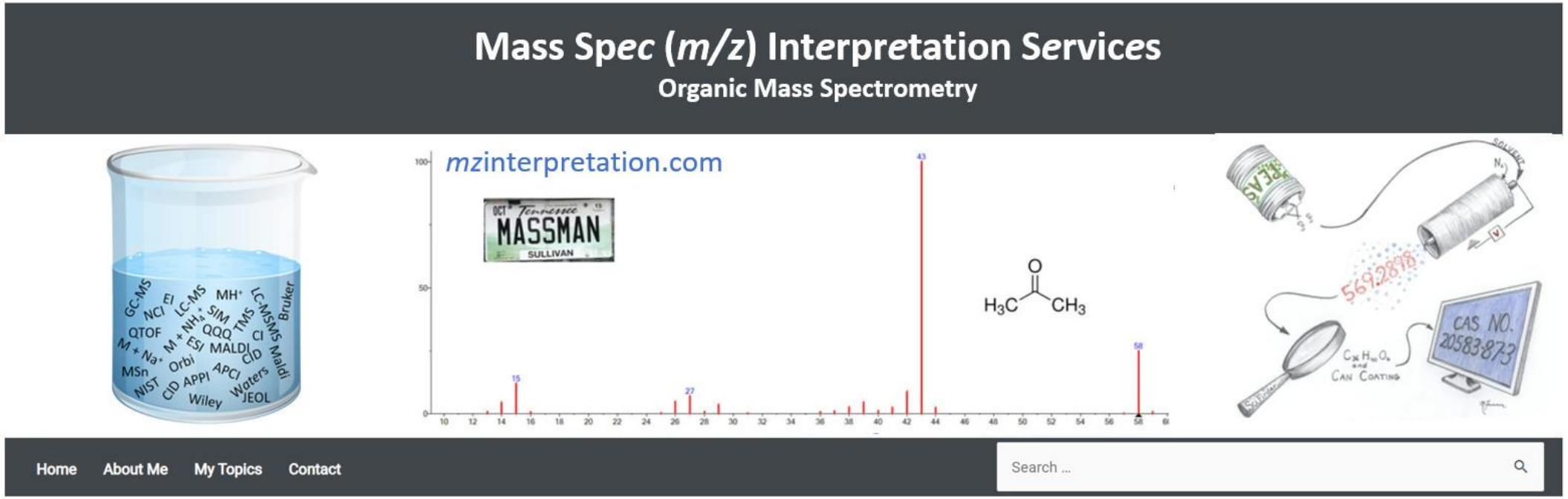
Lib Search: Similarity EI Hybrid Search for Spectra Sent from Chromatogram Window

Video/Handout

James Little
Mass Spec Interpretation Services
April 25, 2026
mzinterpretation.com

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



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*
- However, 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

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
Part III: AMDIS (NIST) for Processing EI Mass Spectral Data Files
Part IV: Advanced NIST Hybrid Search of EI 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

Other Webinar Resources:

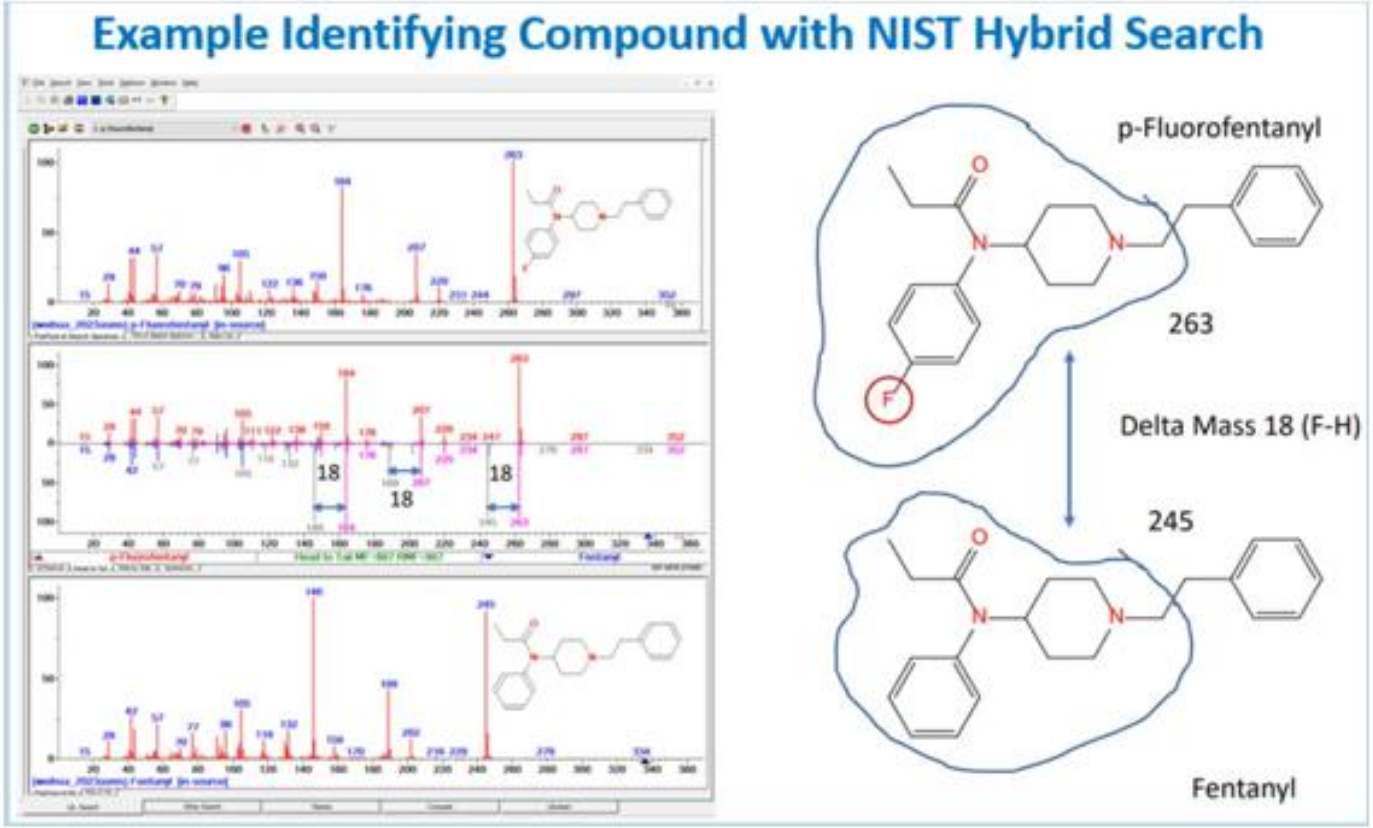
Power of NIST EI Hybrid Search for Unknown Identifications

- NIST EI hybrid search expands the power of traditional EI library matching by enabling detection of structurally related compounds through mass-shifted fragment alignment. This transforms the library from a static reference into a dynamic tool for identifying unknowns, analogs, and emerging compounds not explicitly represented in the database.
- Hybrid search integrates exact and mass-shifted peak matching into a single scoring process, allowing both direct spectral agreement and systematic mass differences to contribute to identification.
- While NIST EI hybrid search does not require a molecular ion, its effectiveness is significantly enhanced when the molecular weight of the unknown is known or constrained. In such cases, the mass difference (Δm) between unknown and library spectra can be interpreted directly, reducing false positives and enabling more confident structural insights.

More Detailed Information

Novel NIST Hybrid Search for Unknown Identifications

See Link



Excel DeltaMass Table

PDF DeltaMass Table

Videos

YouTube: Advanced NIST Hybrid Search of EI Spectra

YouTube: Advanced NIST Hybrid Search for MS/MS (Tandem) Spectra

YouTube: Application NIST Hybrid in EI in Seized Drug Analyses

Associated Handouts

Handout: Advanced NIST Hybrid Search of EI Spectra

Handout: Advanced NIST Hybrid Search of MS/MS (Tandem) Spectra

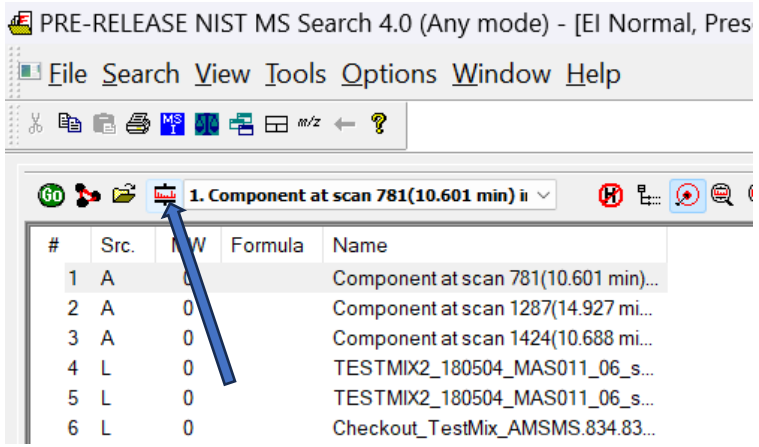
Handout: Application NIST Hybrid in EI in Seized Drug Analyses

Supporting Software Courses for Utilizing Hybrid Search

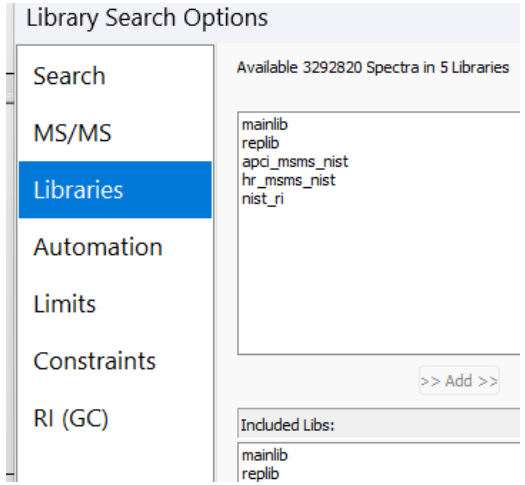
NIST EI Search Software

NIST MSMS Search Software

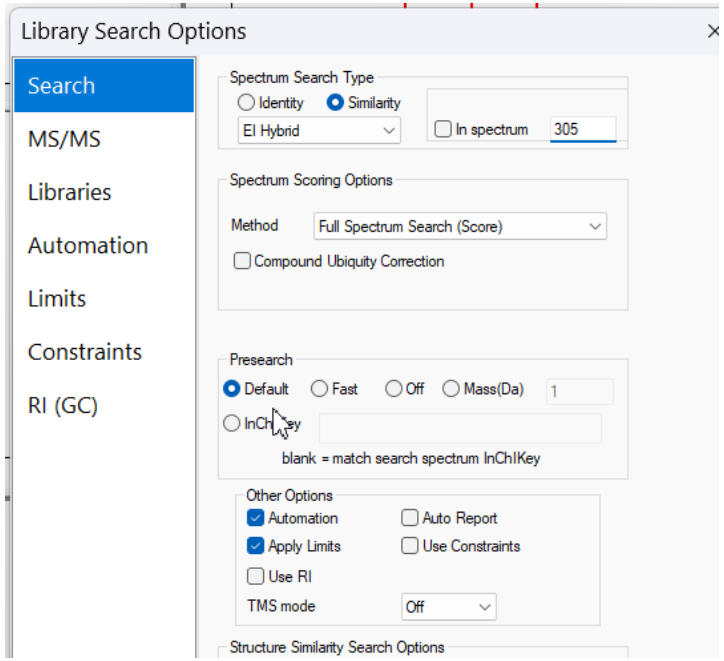
Setup of Hybrid Settings in Lib Search Window



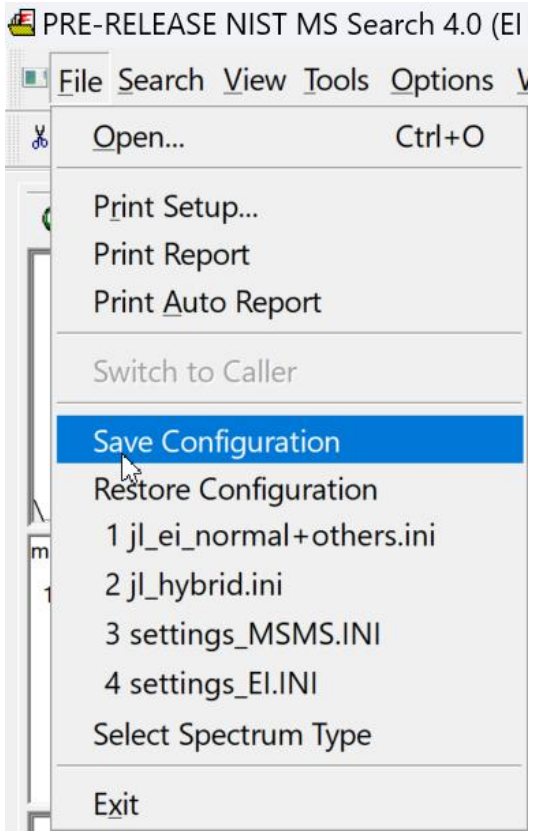
- Select Libraries
- Commercial Libraries *e.g.* Wiley
- User Libraries, *etc.*
- Results combined



- Similarity Radio Button selected
- Hybrid Search
- Normally use “In spectrum” box checked
- Software selects to select MW to limit Hybrid Search
- ***Value*** chosen ***shown*** in bottom right corner after search
- If chosen value not acceptable, ***User can specify*** by unclicking box and entering nominal molecular weight



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



Hybrid Search: Make Sure Library Results Contain Needed Properties

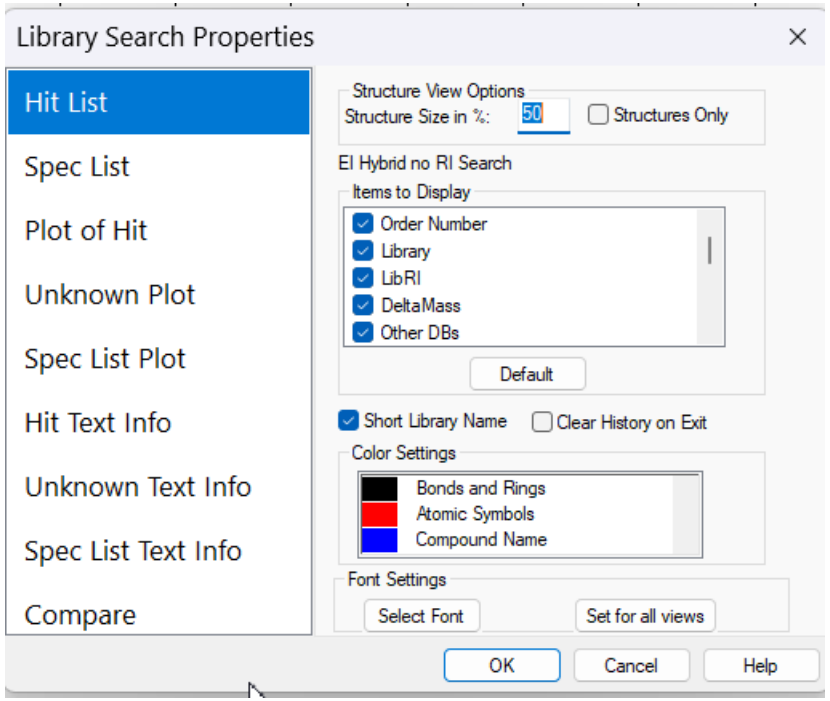
Incorrect Setup

#	Lib.	Match	LibRI	DeltaMass	DBs	Name
1	M	981	3086	-56	5	5-Nonadecylresorcinol, O,O-bis-TMS
2	M	976	3278	-84	5	5-Henicosylresorcinol, O,O-bis-TMS
3	M	976	2306	56	2	5-Undecylbenzene-1,3-diol, 2TMS deriv...
4	M	973	2877	-26	2	5-(8Z-Heptadecenyl)resorcinol, 2TMS
5	M	962	3084	-54	1	1,3-Benzenediol, 5-(10-nonadecenyl)-, (Z...
6	M	946	2676	2	6	Bilobol C15:1 (2TMS)
7	M	941	2502	28	3	1,3-Benzenediol, 5-tridecyl-, 2TMS
8	M	941	2889	-26	3	Bilobol C17:1 (2TMS)
9	M	914	1748	140	13	Olivetol, 2TMS derivative
10	M	901	3703	-236	1	5,5'-(4(Z)-Tetradecene-1,14-diyl)bisresor...

Correct Setup, dForm and pctRelForm Added

#	Lib.	Match	DeltaMass	dForm	pctRelForm	DBs	o.Match	Name
1	M	980	18	H-1F	8.8	28	46	Ethanone, 1-(4-methylphenyl)-
2	R	977	18	H-1F	8.8	11	51	Ethanone, 1-(3-methylphenyl)-
3	M	973	18	H-1F	8.8	12	60	Ethanone, 1-(2-methylphenyl)-
4	M	968	-16	O-1	1.6		752	3-Fluoro-4-methylbenzoic acid,
5	M	967	14	CH2	100	1	772	2-Fluoro-5-methylbenzaldehyd
6	M	964	-16	O-1	1.6		756	4-Fluoro-3-methylbenzoic acid,
7	M	963	14	CH2	100	1	775	4-Fluoro-3-methylbenzaldehyd
8	M	963	14	CH2	100	1	767	3-Fluoro-4-methylbenzaldehyd
9	M	961	14	CH2	100	1	776	4-Fluoro-2-methylbenzaldehyd
10	M	961	-16	O-1	1.6	1	756	2-Fluoro-5-methylbenzoic acid

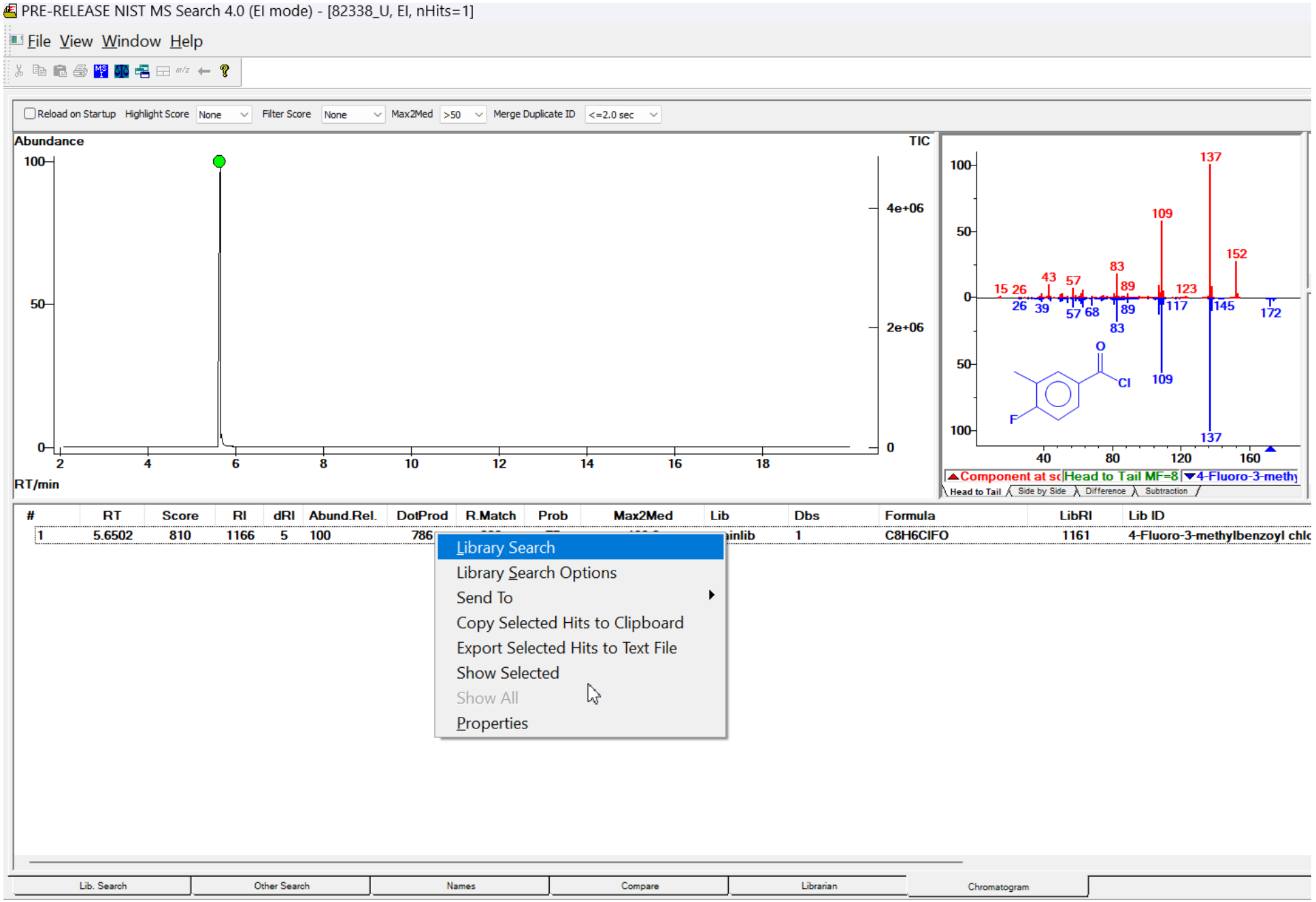
Right Click and Select Properties to add



Added:

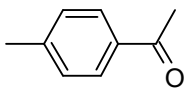
- dForm
- pctRelForm
- o.Match (essentially the standard EI Normal Match)

- **Only** Normal EI Search done in chromatogram
- Send to Lib Search for Novel Hybrid Search

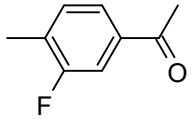


➢ New in NIST26 dForm and pctRelForm, Delta Mass in Previous Versions

#	Lib.	Match	DeltaMass	dForm	pctRelForm	DBs	o.Match	Name
⊞ 1	M	980	18	H-1F	8.8	28	46	Ethanone, 1-(4-methylphenyl)-



Best Hit, 134



Proposed MW 152
Or isomer
Addition of Fluorine Group

DeltaMass Difference in mass of query compound and library compound

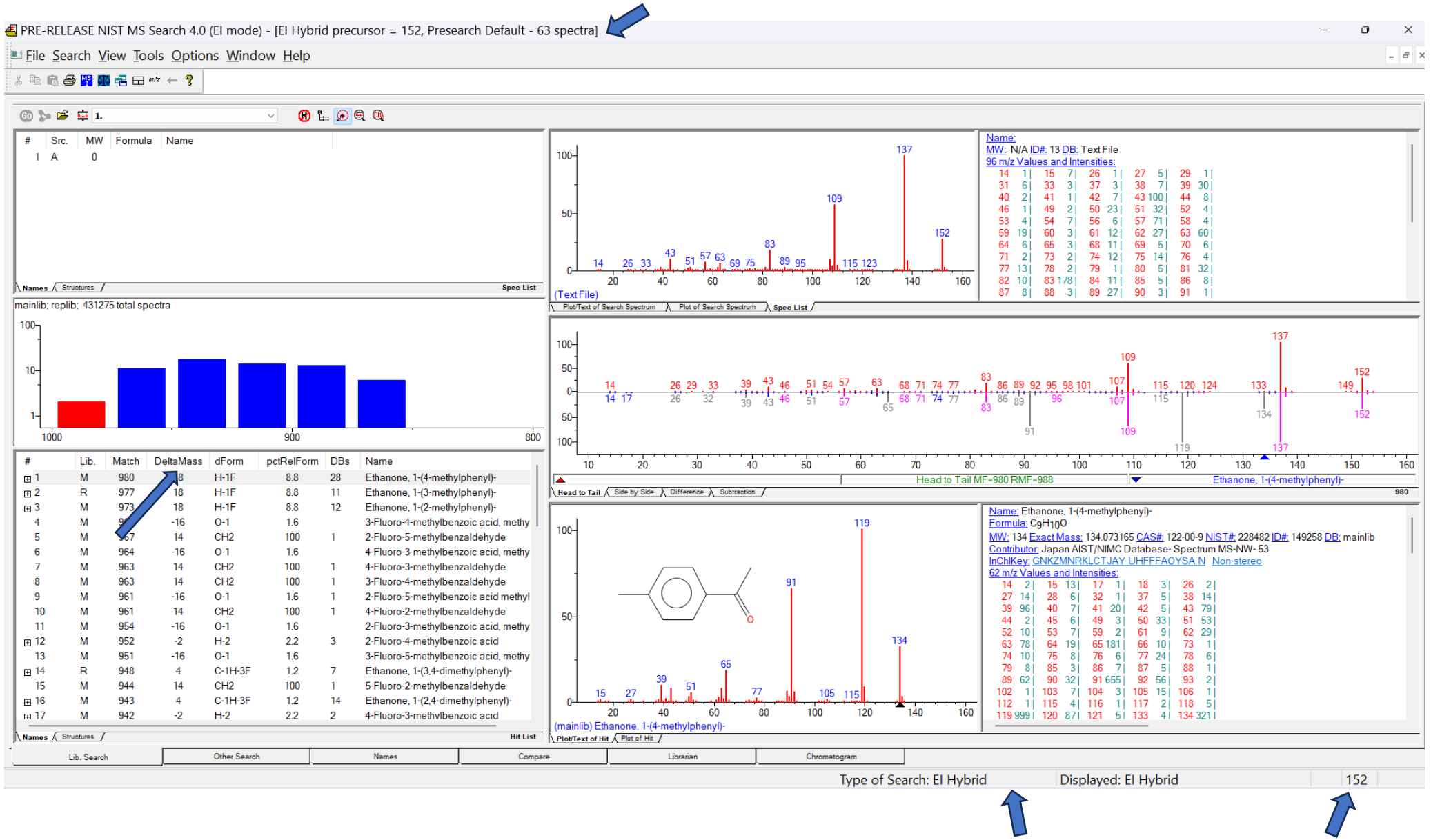
dform highlights mass differences corresponding to plausible structural modifications, guiding interpretation.

pctRefForm Percent: Probability that a dForm is correct. Based on statistics of occurrences of each dForm relative to the most common (CH2 which is assigned 100%) – for high scoring hits (>900). The higher, the most likely correct – values like 0.01 are so rare, they are very likely accidental and wrong for example,

NOTE: ***Much*** more ***Detailed*** information on Hybrid Search Found on my Website at:
See Link1 and Link2

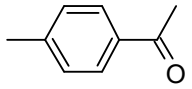
Results Indicate Difference of Fluorine Group

- Note no. of spectra in results top bar
- Type of Search and Displayed results left and middle of bottom bar
- MW determined by computer to limit hybrid search
- Important Hybrid parameters DeltaMass, dform, pctRefForm in search results window

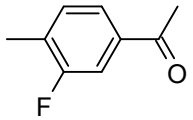


Proposed Structure Consistent with 3 Hits

#	Lib.	Match	DeltaMass	dForm	pctRelForm	DBs	o.Match	Name
⊞ 1	M	980	18	H-1F	8.8	28	46	Ethanone, 1-(4-methylphenyl)-

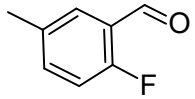


Hit #1
MW 134

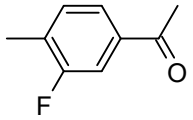


Proposed MW 152
Or isomer
Addition of Fluorine Group

#	Lib.	Match	DeltaMass	dForm	pctRelForm	DBs	o.Match	Name
5	M	967	14	CH2	100	1	772	2-Fluoro-5-methylbenzaldehyde

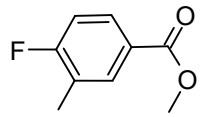


Hit #5
MW 138

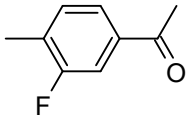


Proposed MW 152
Or isomer
Addition of Fluorine Group

#	Lib.	Match	DeltaMass	dForm	pctRelForm	DBs	o.Match	Name
6	M	964	-16	O-1	1.6		756	4-Fluoro-3-methylbenzoic acid, methyl (



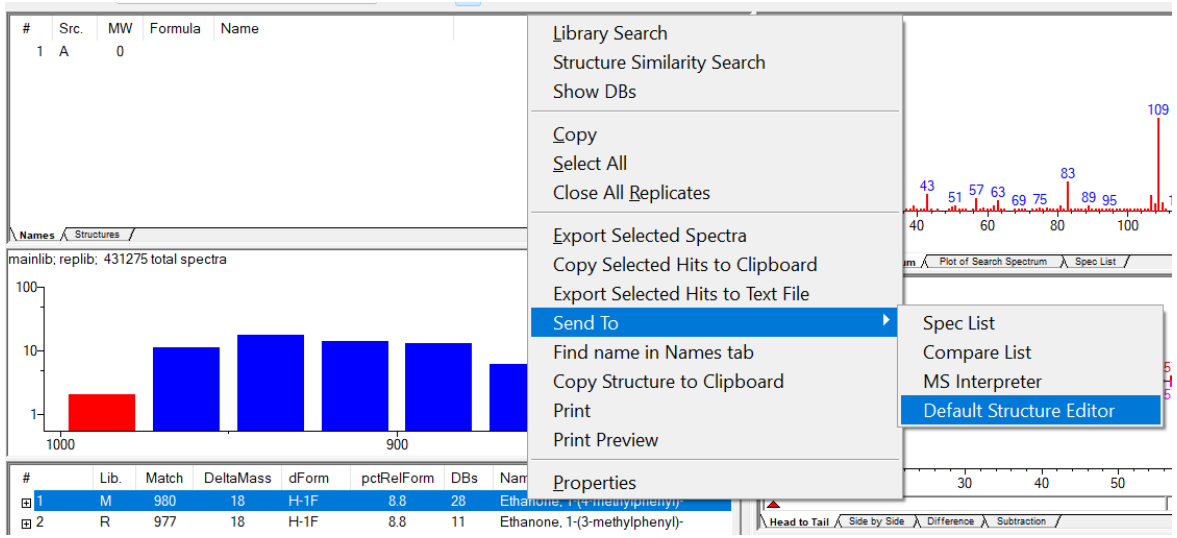
Hit #5
MW 168



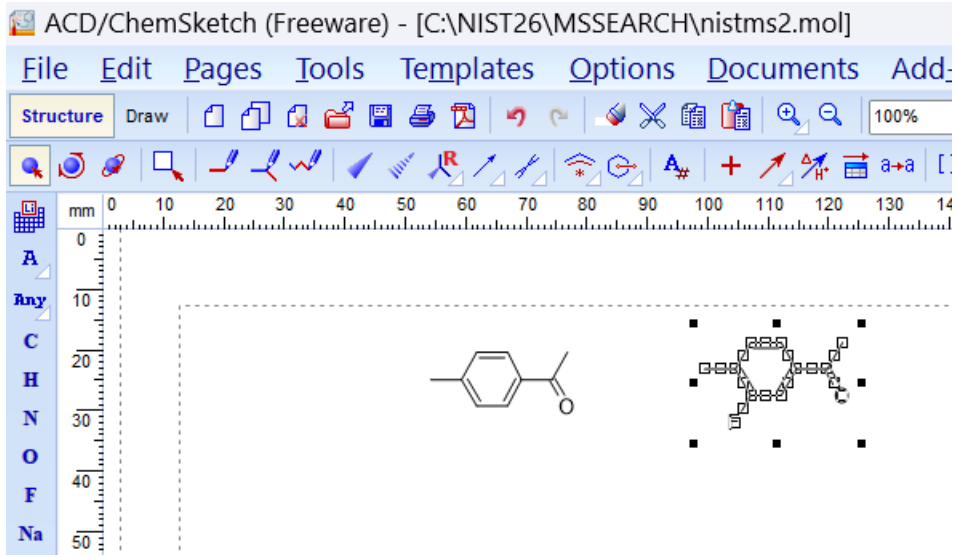
Proposed MW 152
Or isomer
Addition of Fluorine Group

Getting Structure for Proposed Unknown for MS Interpreter

Send Library Structure to Drawing Program



Edit Library Best Hit, and select and copy proposed structure to clipboard with copy command



Structure Drawn in Drawing Program, Unknown Spectrum sent to MS Interpreter and Proposed Structure Inserted

- Detailed MS Interpreter Help
- ***See link***
- Paste in structure copied in Drawing Program
- Use either Paste/Edit or
- Or click on structure box and Keyboard Ctrl V
- Very good fit to proposed structure
- Isotope ratios very consistent
- Position of methyl and fluorine on aromatic ring uncertain