Processing of Accurate Mass GC-MS with NIST26 Chromatogram

Video/Handout

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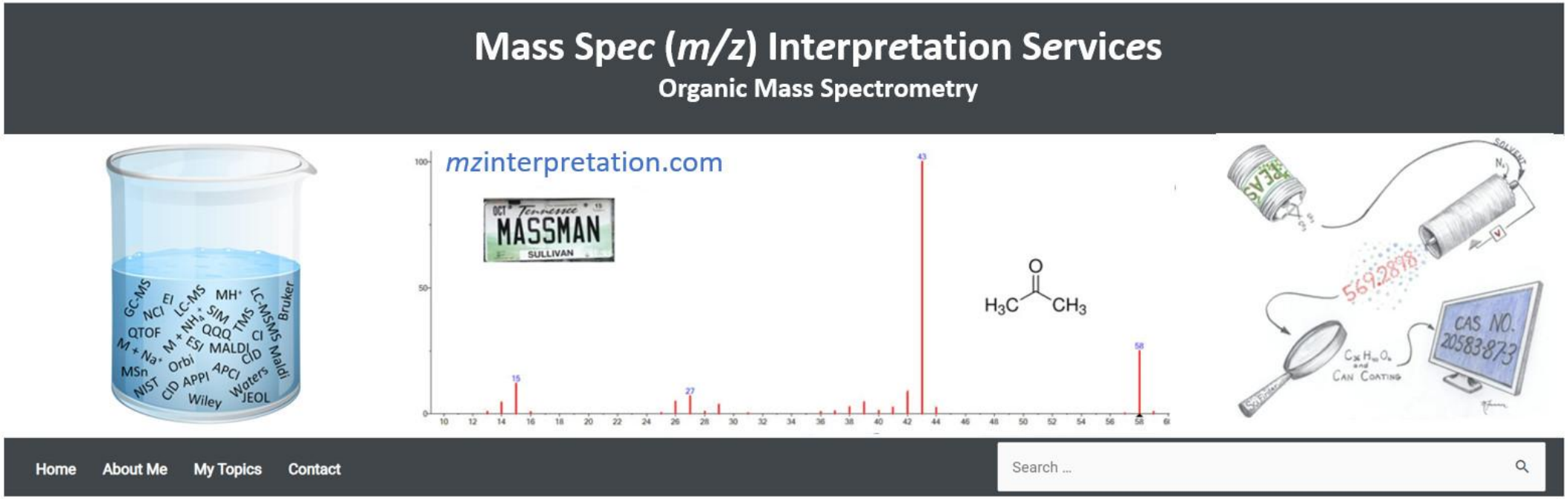
See *Full Course* on NIST26 with new *Integrated* Deconvolution/Library Searching for *EI GC-MS* and *LC-MS/MS*!



AMDIS Integrated within NIST26 Chromatogram Window

- The stand-alone AMDIS does not support accurate mass deconvolution, only integer mass
- NIST used a clever approach to process within the NIST26 Integrated Chromatogram Version
- Workflow as described to me below by Steve Stein

Workflow:

Find XICs (more about XIC's in MSMS Course on my website)

Convert XIC m/z to arbitrary integers (encode)

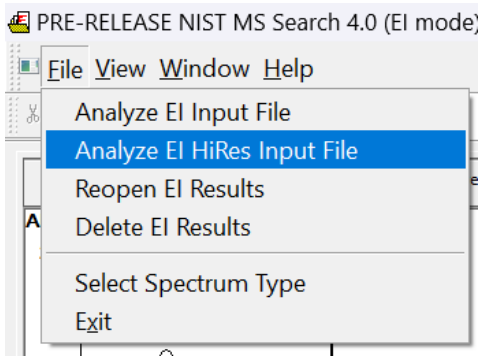
Run AMDIS on these arbitrary integers

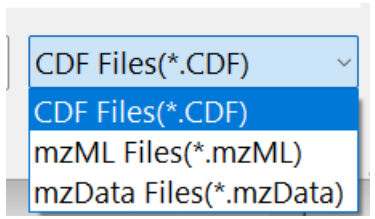
Convert arbitrary integers back to m/z (decode)

Search library with deconvoluted spectra

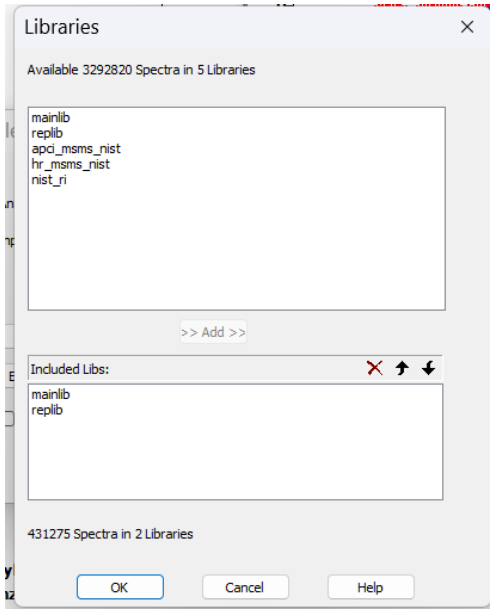
An unexpected effect was and improvement in spectral quality, in particular, better spectra for smaller concentration components

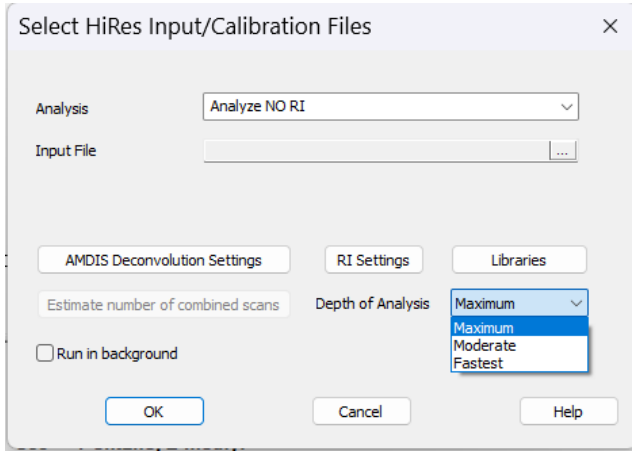
Opening File in NIST26 Chromatogram Program





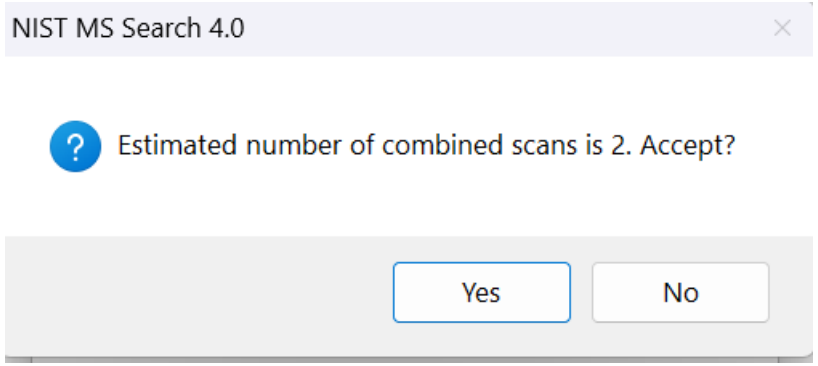
File formats supplied from Vendors' Software or converted with ProteoWizard/msconvert





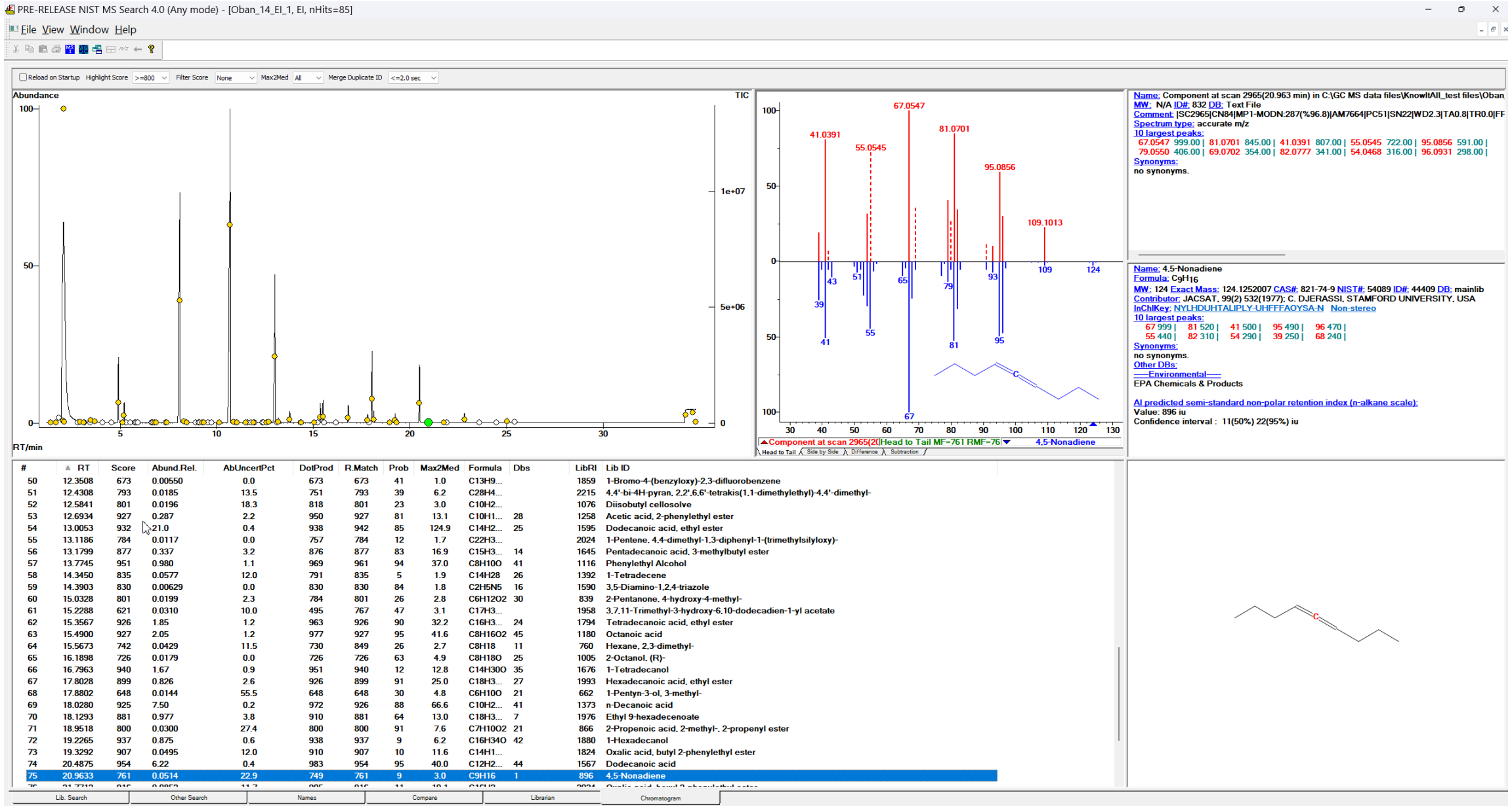
3 levels of sensitivity (depth of analysis), can be changed to if analyses are taking too long, can also run in background if that option chosen

Use combined searches with Wiley, User Libraries, *etc.*



- Often users acquire too many samplings across a peak which incurs increasing process, NIST calculates an optimal number of scans to be combined

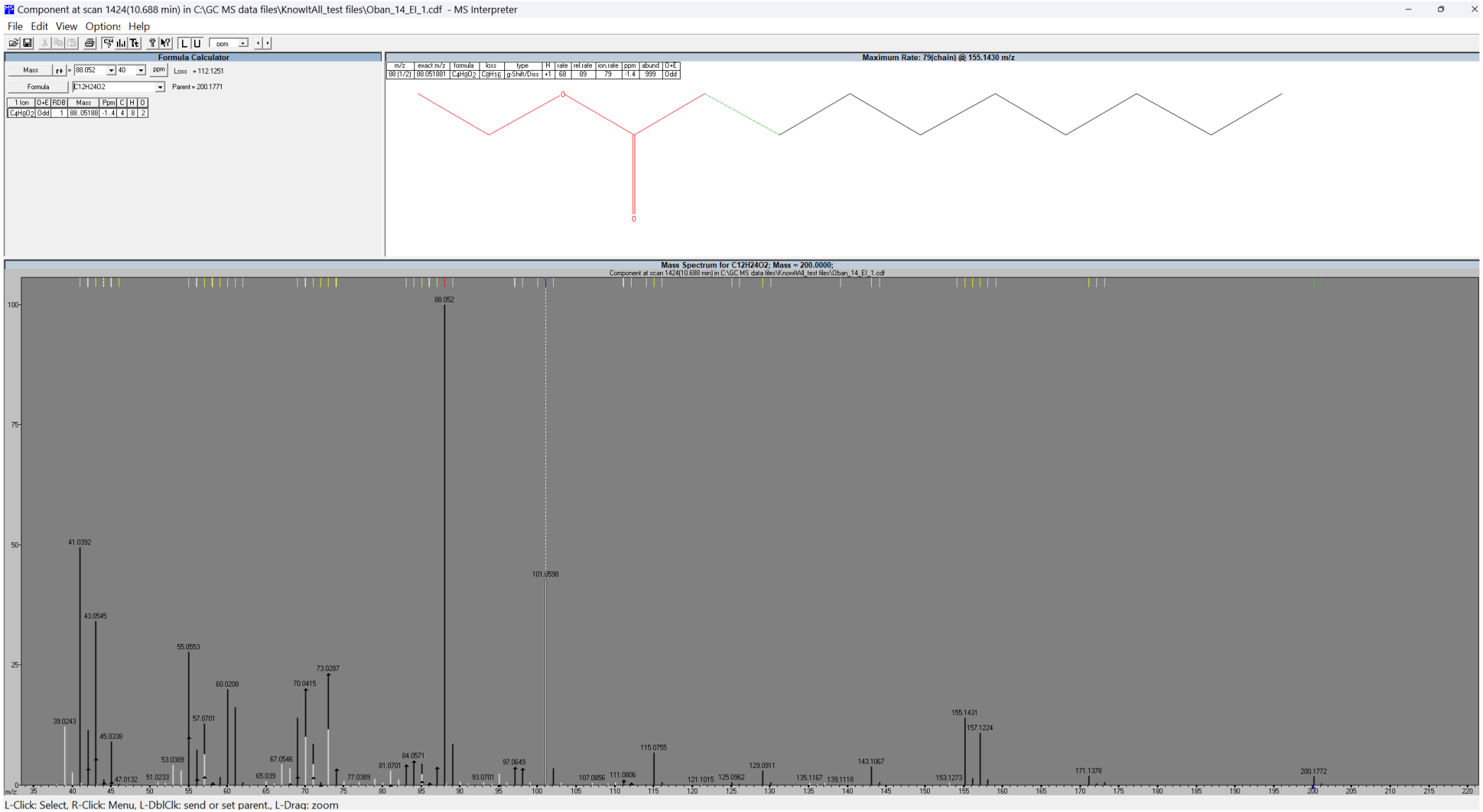
- **User Spectrum shown with accurate mass values in Butterfly Plot, netCDF File from JEOL (C. Cody)**
- **Library Score >800 shown with yellow dot**



#	RT	Score	Abund.Rel.	AbUncertPct	DotProd	R.Match	Prob	Max2Med	Formula	Dbs	LibRI	Lib ID
50	12.3508	673	0.00550	0.0	673	673	41	1.0	C13H9...		1859	1-Bromo-4-(benzyloxy)-2,3-difluorobenzene
51	12.4308	793	0.0185	13.5	751	793	39	6.2	C28H4...		2215	4,4'-bi-4H-pyran, 2,2',6,6'-tetrakis(1,1-dimethylethyl)-4,4'-dimethyl-
52	12.5841	801	0.0196	18.3	818	801	23	3.0	C10H2...		1076	Diisobutyl cellosolve
53	12.6934	927	0.287	2.2	950	927	81	13.1	C10H1...	28	1258	Acetic acid, 2-phenylethyl ester
54	13.0053	932	21.0	0.4	938	942	85	124.9	C14H2...	25	1595	Dodecanoic acid, ethyl ester
55	13.1186	784	0.0117	0.0	757	784	12	1.7	C22H3...		2024	1-Pentene, 4,4-dimethyl-1,3-diphenyl-1-(trimethylsilyloxy)-
56	13.1799	877	0.337	3.2	876	877	83	16.9	C15H3...	14	1645	Pentadecanoic acid, 3-methylbutyl ester
57	13.7745	951	0.980	1.1	969	961	94	37.0	C8H10O	41	1116	Phenylethyl Alcohol
58	14.3450	835	0.0577	12.0	791	835	5	1.9	C14H28	26	1392	1-Tetradecene
59	14.3903	830	0.00629	0.0	830	830	84	1.8	C2H5N5	16	1590	3,5-Diamino-1,2,4-triazole
60	15.0328	801	0.0199	2.3	784	801	26	2.8	C6H12O2	30	839	2-Pentanone, 4-hydroxy-4-methyl-
61	15.2288	621	0.0310	10.0	495	767	47	3.1	C17H3...		1958	3,7,11-Trimethyl-3-hydroxy-6,10-dodecadien-1-yl acetate
62	15.3567	926	1.85	1.2	963	926	90	32.2	C16H3...	24	1794	Tetradecanoic acid, ethyl ester
63	15.4900	927	2.05	1.2	977	927	95	41.6	C8H16O2	45	1180	Octanoic acid
64	15.5673	742	0.0429	11.5	730	849	26	2.7	C8H18	11	760	Hexane, 2,3-dimethyl-
65	16.1898	726	0.0179	0.0	726	726	63	4.9	C8H18O	25	1005	2-Octanol, (R)-
66	16.7963	940	1.67	0.9	951	940	12	12.8	C14H30O	35	1676	1-Tetradecanol
67	17.8028	899	0.826	2.6	926	899	91	25.0	C18H3...	27	1993	Hexadecanoic acid, ethyl ester
68	17.8802	648	0.0144	55.5	648	648	30	4.8	C6H10O	21	662	1-Pentyn-3-ol, 3-methyl-
69	18.0280	925	7.50	0.2	972	926	88	66.6	C10H2...	41	1373	n-Decanoic acid
70	18.1293	881	0.977	3.8	910	881	64	13.0	C18H3...	7	1976	Ethyl 9-hexadecenoate
71	18.9518	800	0.0300	27.4	800	800	91	7.6	C7H10O2	21	866	2-Propenoic acid, 2-methyl-, 2-propenyl ester
72	19.2265	937	0.875	0.6	938	937	9	6.2	C16H34O	42	1880	1-Hexadecanol
73	19.3292	907	0.0495	12.0	910	907	10	11.6	C14H1...		1824	Oxalic acid, butyl 2-phenylethyl ester
74	20.4875	954	6.22	0.4	983	954	95	40.0	C12H2...	44	1567	Dodecanoic acid
75	20.9633	761	0.0514	22.9	749	761	9	3.0	C9H16	1	896	4,5-Nonadiene

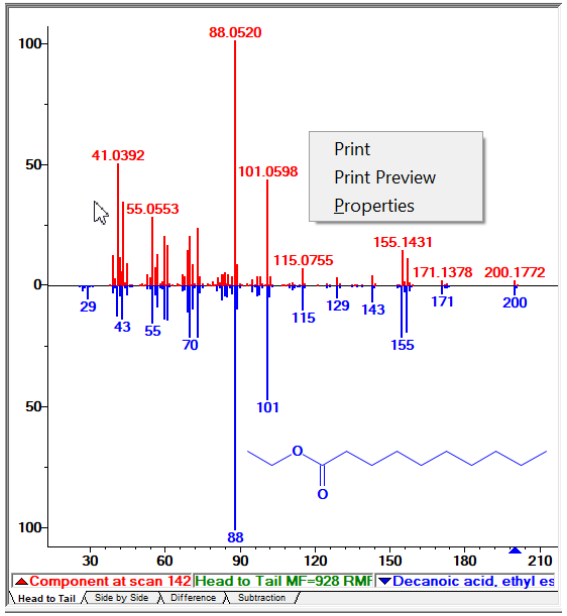
Send Any Structure in Results List to MS Interpreter

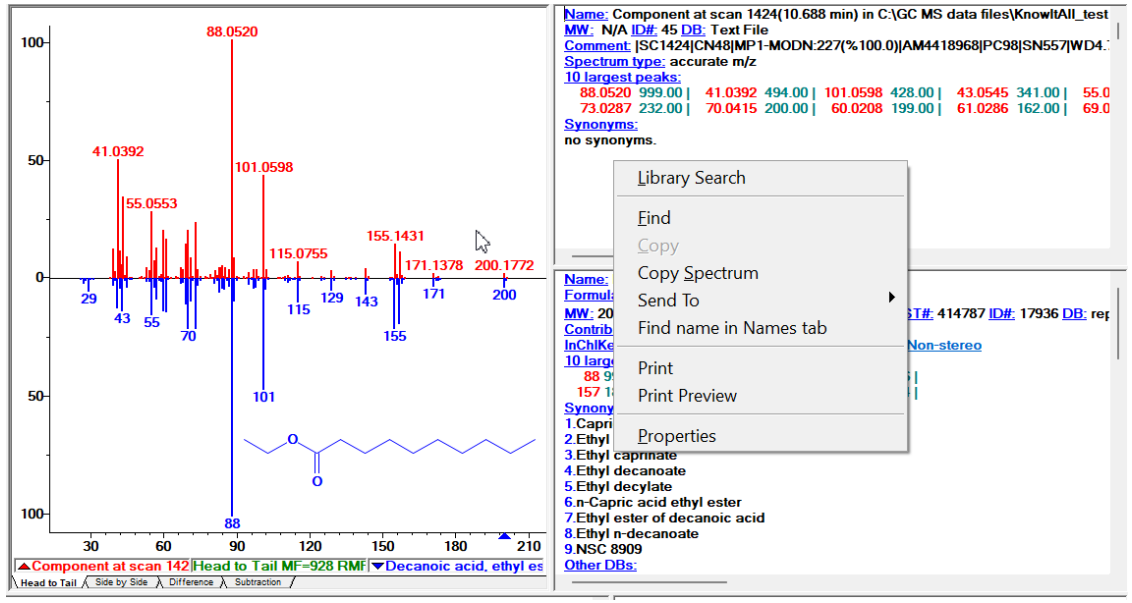
- Spectrum is sent from Chromatogram for the unknown identification to MS Interpreter,
- Structure is paired with the Unknown's EI spectrum in transfer process
- User gets the accurate mass errors in ppm and the proposed substructures assigned to observed fragment ions!

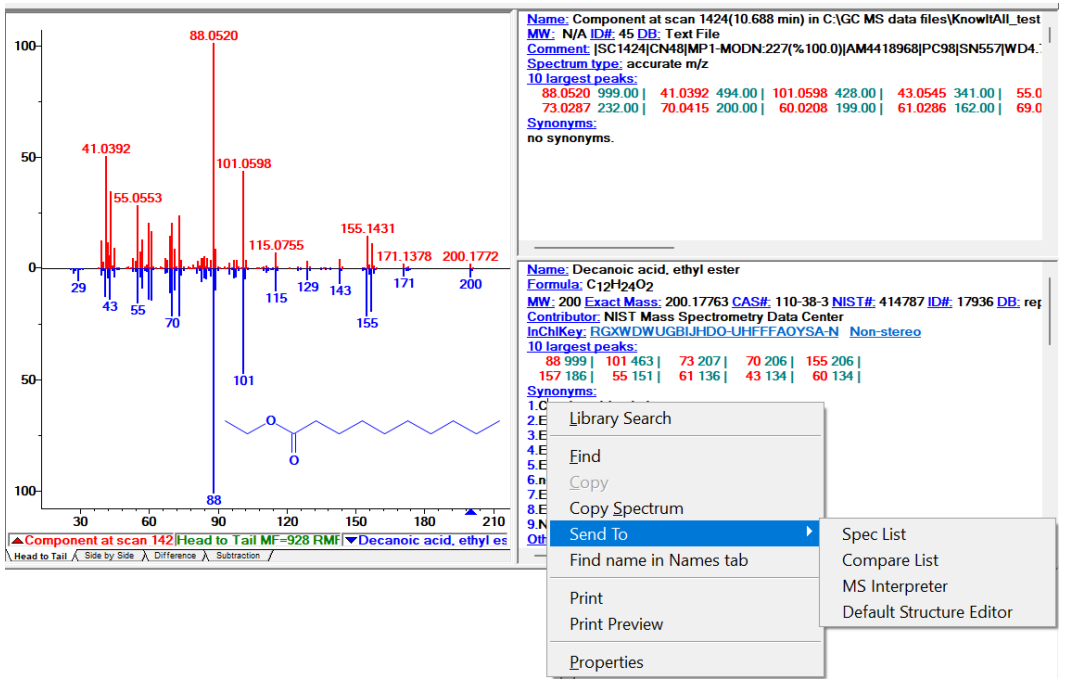


Send to MS Interpreter from “Head to Tail”

- There is no Send to MS Interpreter when right clicking in either the top or bottom spectra in this display
- If you click in the Text part of the top box, it will send the accurate mass spectrum to MS Interpreter, but no structure
- If you click on the Text box of the bottom box, it will send the nominal library spectrum and its structure to MS Interpreter
- ***Thus, much preferable*** in most cases to Send to MS Interpreter with the results in Chromatogram as shown on previous slide







More Information on Accurate Mass Data and Structures for Chromatogram Window and MS Interpreter

See following Video/Associated Handout for additional information

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

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April 24, 2026
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