LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052024\
Data File : VN082211.D
Acq On : 20 May 2024 15:46
Operator : JC\MD
Sample : P2511-06 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
510-B

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Title : SW846 8260

Signal : TIC: VN082211.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.812	138	146	154	rVB4	8726	19778	1.83%	0.306%
2	4.430	409	421	431	rBV	6987	21074	1.95%	0.326%
3	7.430	923	931	939	rBV2	5783	14965	1.38%	0.232%
4	8.171	1044	1057	1061	rBV	137330	333958	30.90%	5.166%
5	8.224	1061	1066	1077	rVB	243607	538923	49.86%	8.337%
6	8.577	1118	1126	1137	rBV	168271	383039	35.44%	5.926%
7	9.100	1206	1215	1228	rBV	375977	768834	71.13%	11.894%
8	10.571	1456	1465	1474	rBV	579624	1080830	100.00%	16.721%
9	11.865	1677	1685	1695	rBV	534639	941867	87.14%	14.571%
10	12.853	1845	1853	1862	rVB	392027	677482	62.68%	10.481%
11	12.953	1862	1870	1883	rBV2	61607	116468	10.78%	1.802%
12	13.794	2005	2013	2019	rBV	473051	793574	73.42%	12.277%
13	13.859	2019	2024	2035	rVB3	57915	107432	9.94%	1.662%
14	14.453	2123	2125	2131	rVV3	6807	13042	1.21%	0.202%
15	14.529	2133	2138	2147	rVV3	19549	39258	3.63%	0.607%
16	14.629	2151	2155	2160	rBV3	10298	16322	1.51%	0.253%
17	14.735	2169	2173	2175	rBV3	12277	17379	1.61%	0.269%
18	14.776	2175	2180	2193	rVV6	35845	117080	10.83%	1.811%
19	14.888	2193	2199	2208	rVB2	30282	56366	5.22%	0.872%
20	15.106	2230	2236	2253	rBV2	68470	146538	13.56%	2.267%
21	15.329	2268	2274	2281	rVB8	11975	24772	2.29%	0.383%
22	15.465	2289	2297	2304	rBV2	57193	109419	10.12%	1.693%
23	15.635	2322	2326	2336	rVB4	14043	33147	3.07%	0.513%
24	16.017	2382	2391	2407	rBV3	38854	92546	8.56%	1.432%

Sum of corrected areas: 6464093

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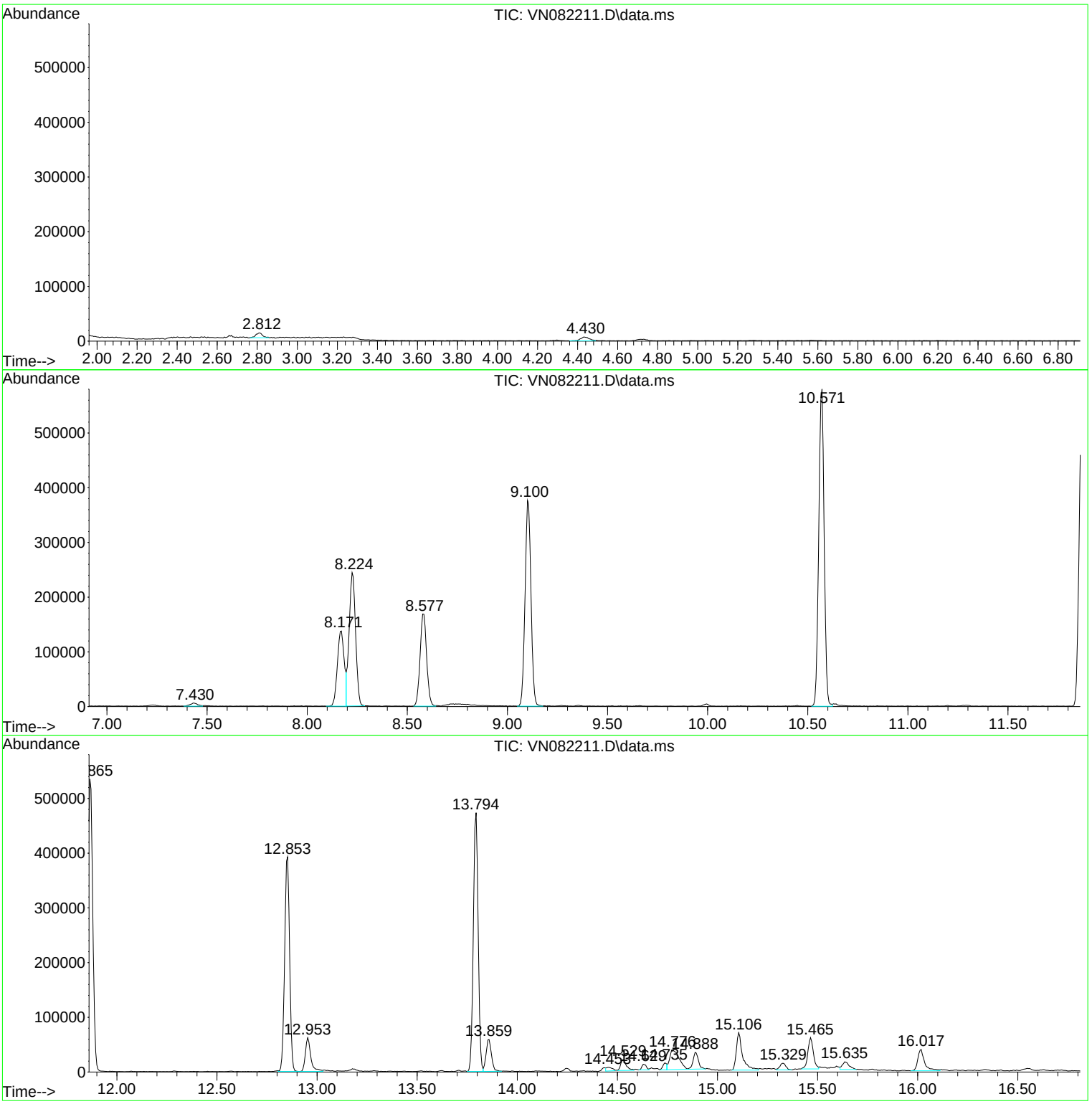
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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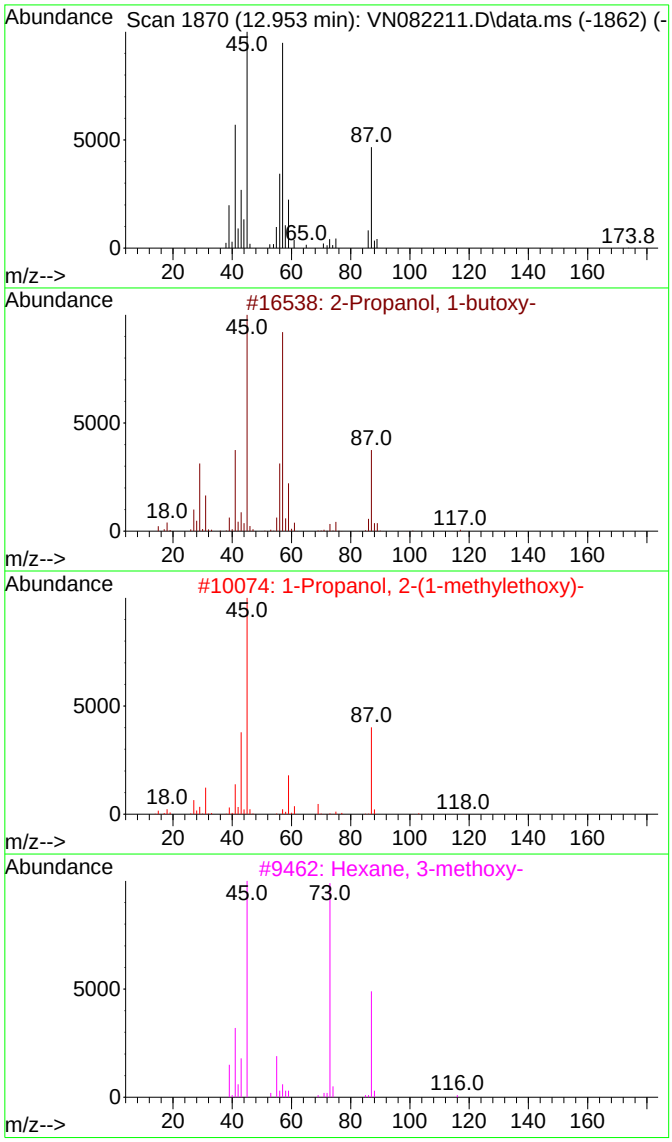
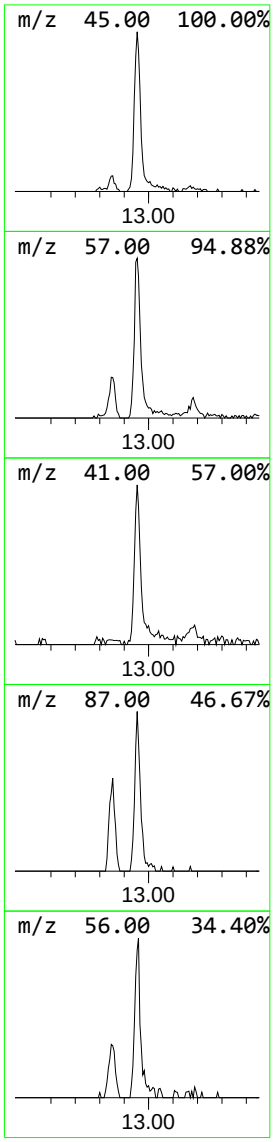
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Propanol, 1-butoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.953	7.34 ug/l	116468	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	90
2	1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	45
3	Hexane, 3-methoxy-	116	C7H16O	054658-01-4	38
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	36
5	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	33





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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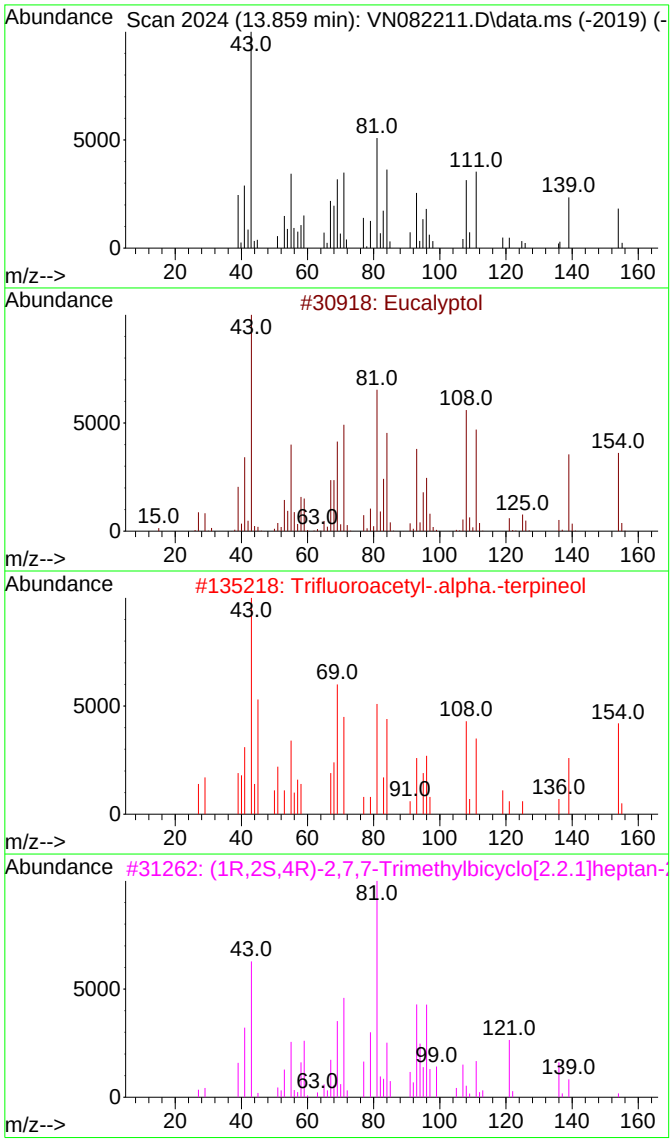
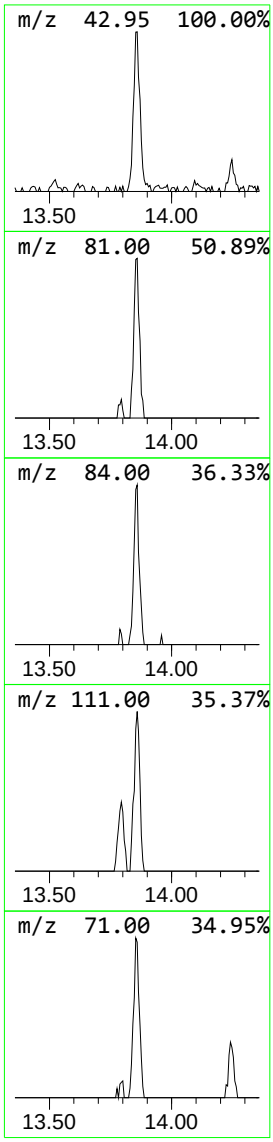
****

Peak Number 2 Eucalyptol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.859	6.77 ug/l	107432	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eucalyptol	154	C10H18O	000470-82-6	97
2	Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	83
3	(1R,2S,4R)-2,7,7-Trimethylbicycl...	154	C10H18O	003247-40-3	16
4	Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	15
5	2-Acetonylcyclohexanone	154	C9H14O2	006126-53-0	14





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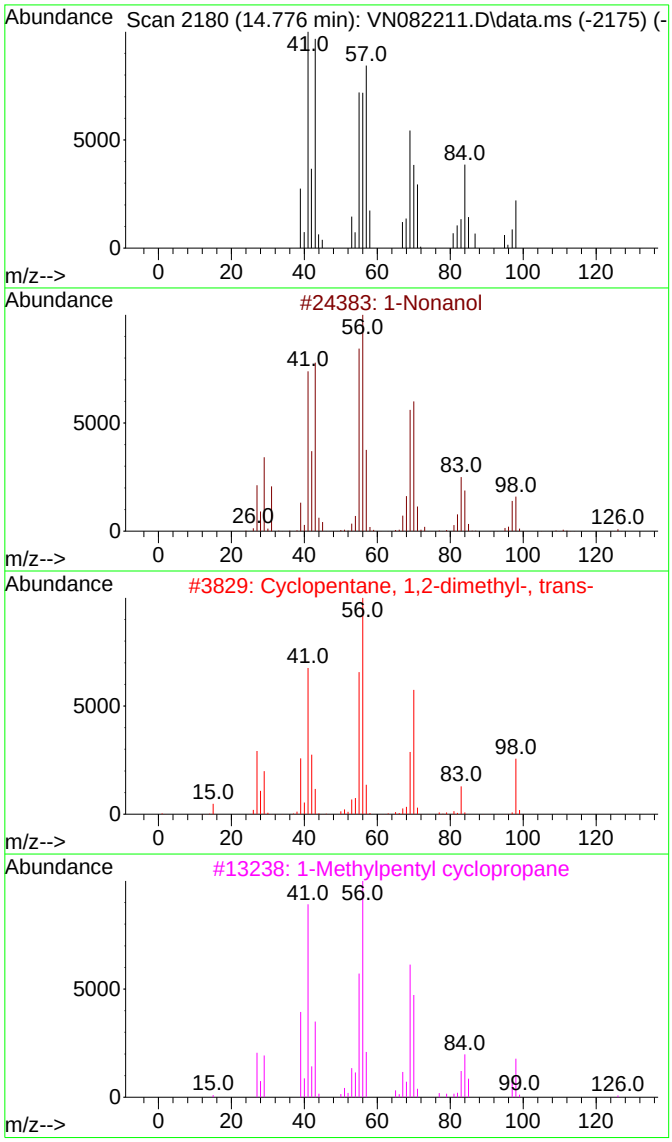
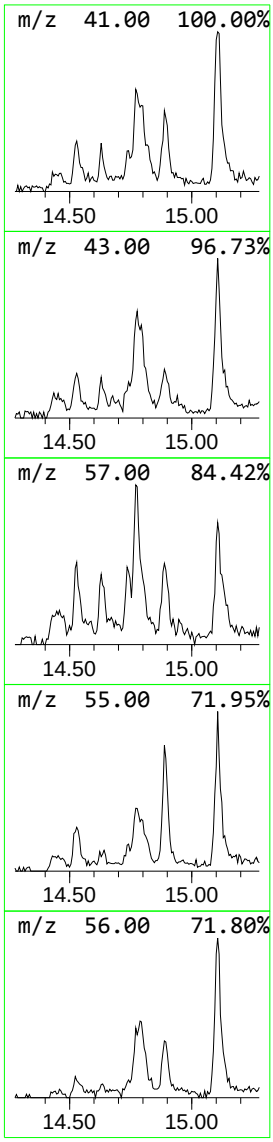
****
Peak Number 3 unknown14.476 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.776	7.38 ug/l	117080	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonanol	144	C9H20O	000143-08-8	43
2	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	43
3	1-Methylpentyl cyclopropane	126	C9H18	006976-28-9	38
4	Cyclopropane, 1,1-diethyl-	98	C7H14	001003-19-6	30
5	1-Octene, 3,7-dimethyl-	140	C10H20	004984-01-4	27





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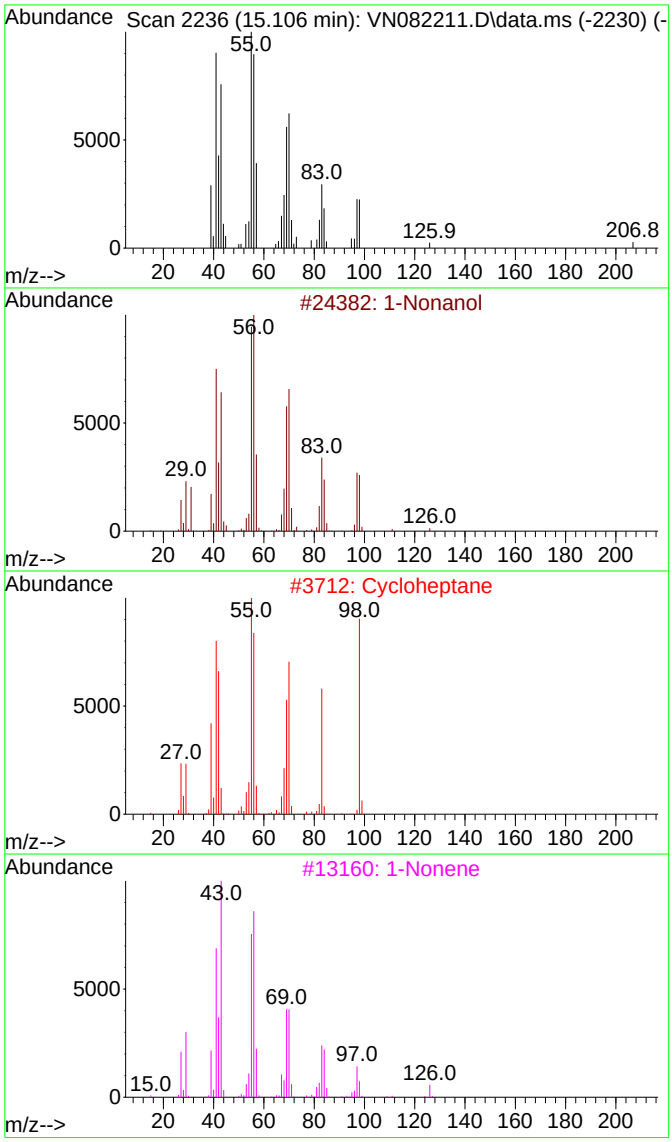
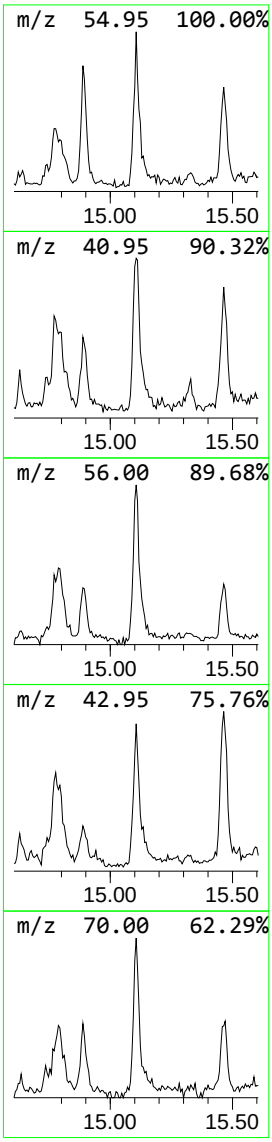
****

Peak Number 4 1-Nonanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.106	9.23 ug/l	146538	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonanol	144	C9H20O	000143-08-8	91
2	Cycloheptane	98	C7H14	000291-64-5	81
3	1-Nonene	126	C9H18	000124-11-8	76
4	1-Heptene	98	C7H14	000592-76-7	76
5	1-Decene	140	C10H20	000872-05-9	72





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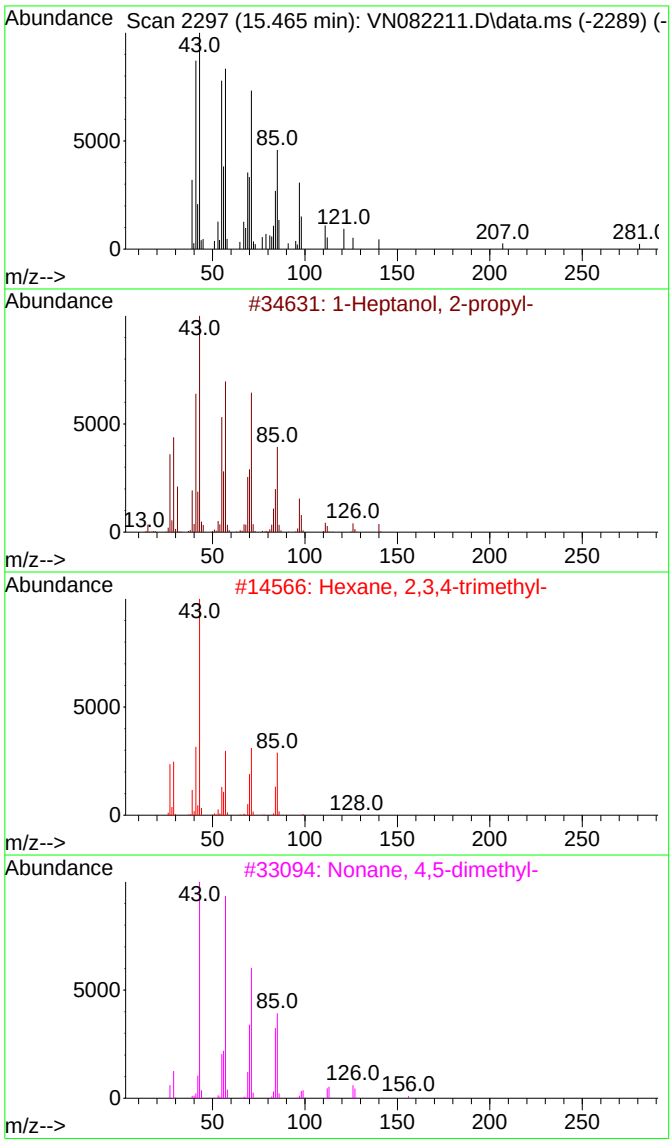
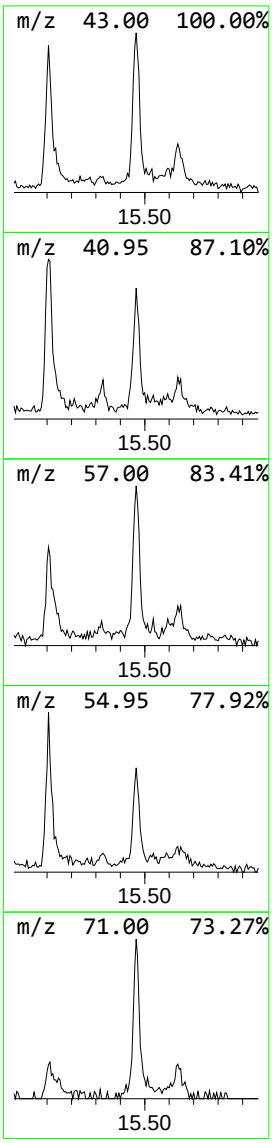
****
Peak Number 5 1-Heptanol, 2-propyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.464	6.89 ug/l	109419	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol, 2-propyl-	158	C10H22O	010042-59-8	80
2	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	53
3	Nonane, 4,5-dimethyl-	156	C11H24	017302-23-7	50
4	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	50
5	Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	47





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Quant Title : SW846 8260

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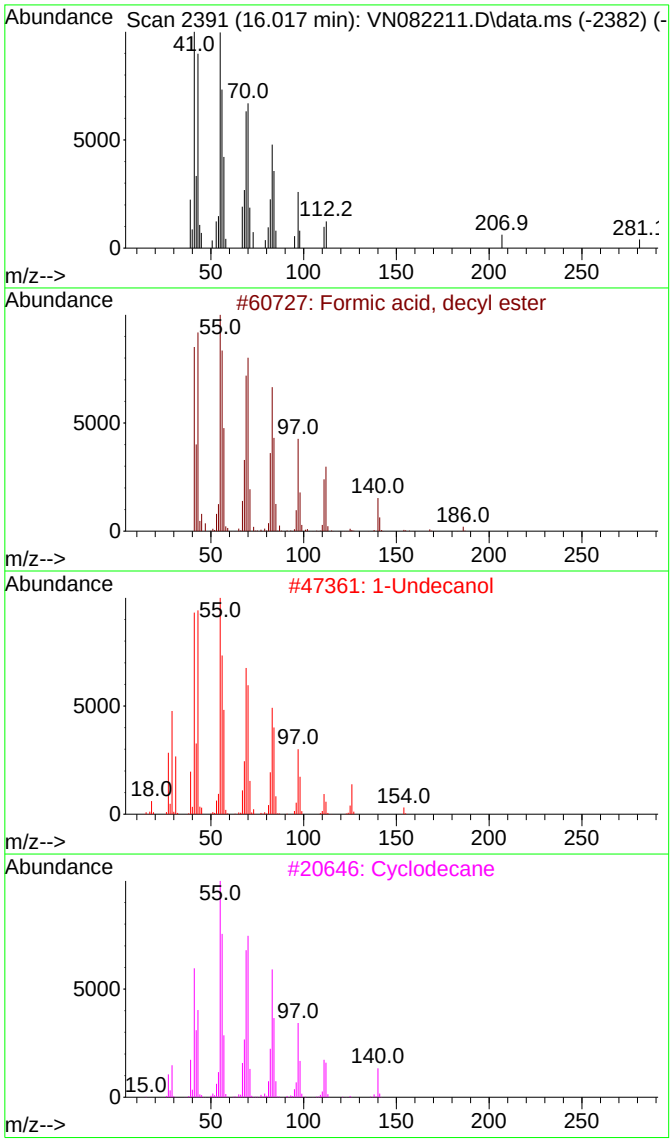
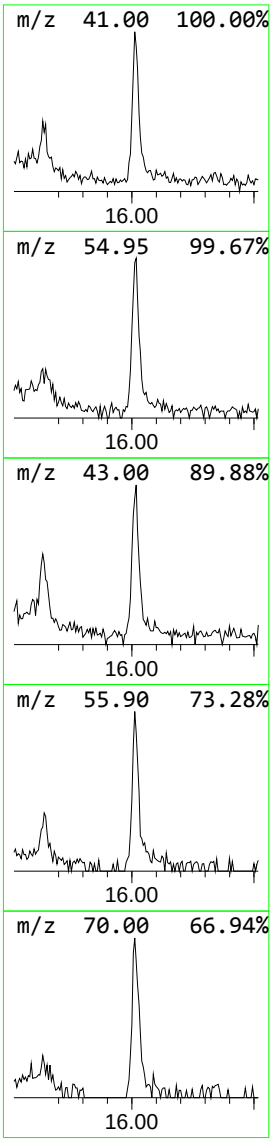
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Formic acid, decyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.017	5.83 ug/l	92546	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Formic acid, decyl ester	186	C11H22O2	005451-52-5	91
2	1-Undecanol	172	C11H24O	000112-42-5	90
3	Cyclodecane	140	C10H20	000293-96-9	90
4	1-Dodecanol	186	C12H26O	000112-53-8	80
5	Cyclopropane, octyl-	154	C11H22	001472-09-9	72





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Propanol, 1-b...	12.953	7.3	ug/l	116468	4	13.794	793574	50.0
Eucalyptol	13.859	6.8	ug/l	107432	4	13.794	793574	50.0
unknown14.476	14.776	7.4	ug/l	117080	4	13.794	793574	50.0
1-Nonanol	15.106	9.2	ug/l	146538	4	13.794	793574	50.0
1-Heptanol, 2-p...	15.464	6.9	ug/l	109419	4	13.794	793574	50.0
Formic acid, de...	16.017	5.8	ug/l	92546	4	13.794	793574	50.0