LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052924\
Data File : VN082374.D
Acq On : 29 May 2024 16:40
Operator : JC\MD
Sample : P2609-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
426

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: VN082374.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.665	114	121	127	rBV	16795	31812	2.68%	0.409%
2	4.430	410	421	436	rBV	82095	241963	20.36%	3.113%
3	4.724	463	471	479	rVB4	5322	15998	1.35%	0.206%
4	5.524	598	607	613	rBV3	4666	13481	1.13%	0.173%
5	7.230	888	897	906	rBV4	11911	32303	2.72%	0.416%
6	7.488	935	941	949	rBV2	6746	15798	1.33%	0.203%
7	8.171	1047	1057	1061	rBV	155872	368611	31.01%	4.743%
8	8.224	1061	1066	1080	rVB	277120	606833	51.06%	7.807%
9	8.582	1113	1127	1136	rBV	182004	421099	35.43%	5.418%
10	9.100	1207	1215	1225	rBV	404272	839406	70.62%	10.800%
11	9.271	1237	1244	1252	rBV2	9052	19416	1.63%	0.250%
12	10.571	1456	1465	1471	rBV	631070	1188570	100.00%	15.292%
13	10.629	1471	1475	1486	rVB	126806	235579	19.82%	3.031%
14	11.865	1674	1685	1696	rBV	586381	1053435	88.63%	13.553%
15	11.970	1698	1703	1710	rVV4	15419	28262	2.38%	0.364%
16	12.070	1714	1720	1727	rVV2	37343	73446	6.18%	0.945%
17	12.406	1766	1777	1782	rBV6	17220	47098	3.96%	0.606%
18	12.853	1844	1853	1861	rBV	457104	802324	67.50%	10.323%
19	13.259	1915	1922	1930	rBV	267921	423749	35.65%	5.452%
20	13.506	1956	1964	1976	rBV2	66679	118828	10.00%	1.529%
21	13.612	1976	1982	1991	rVB6	9042	25286	2.13%	0.325%
22	13.794	2006	2013	2020	rBV	570378	941945	79.25%	12.119%
23	13.876	2020	2027	2032	rVB2	24362	50311	4.23%	0.647%
24	14.247	2083	2090	2103	rBV	59025	118286	9.95%	1.522%
25	15.400	2278	2286	2294	rBV3	16778	32332	2.72%	0.416%
26	16.017	2385	2391	2400	rBV5	12732	26276	2.21%	0.338%

Sum of corrected areas: 7772447

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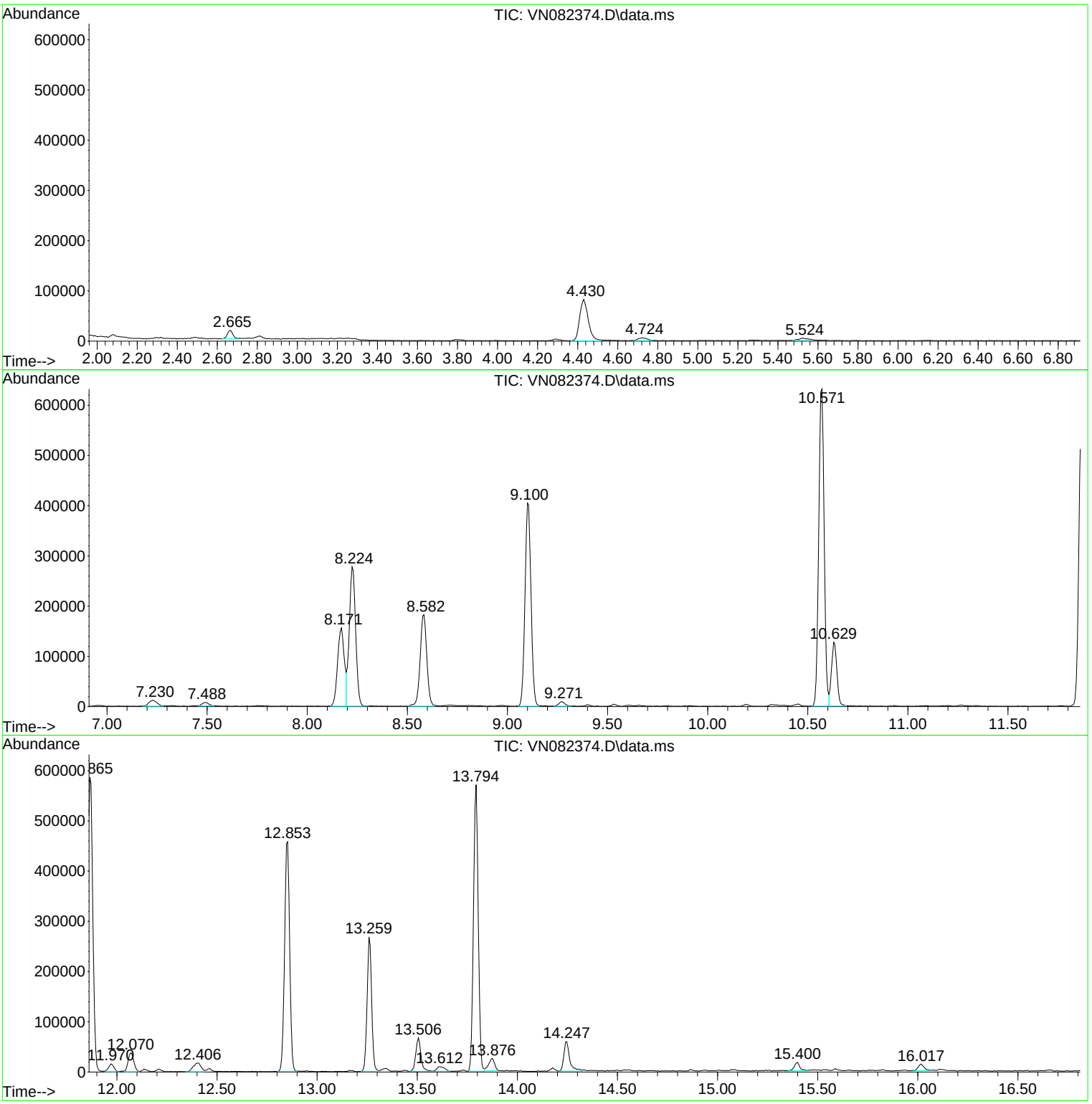
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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



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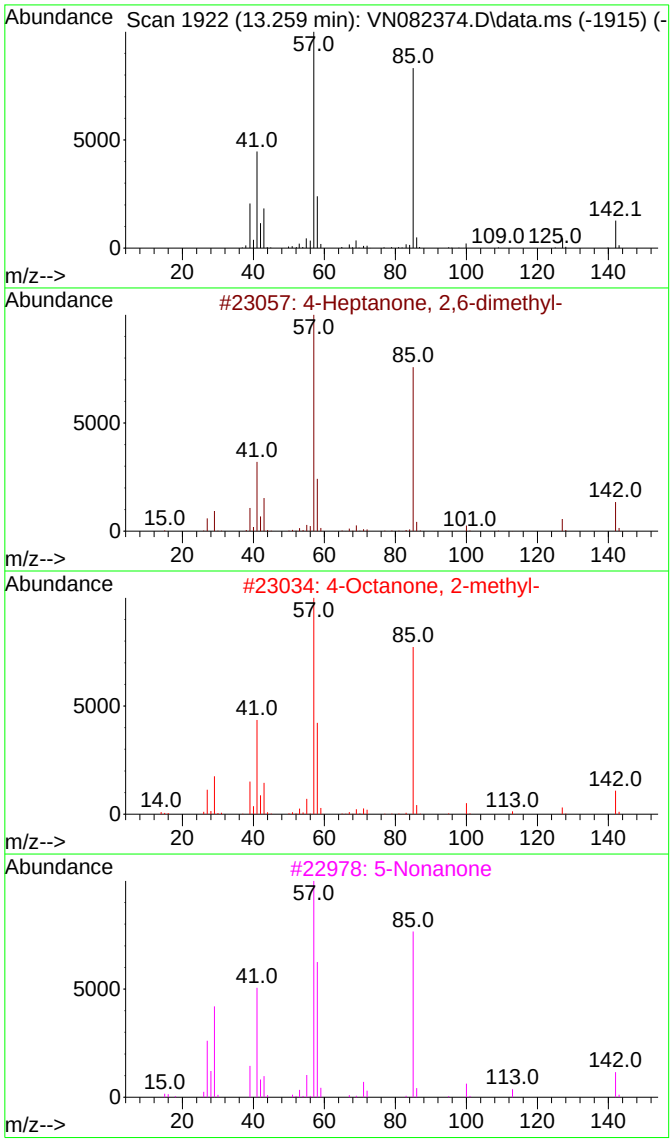
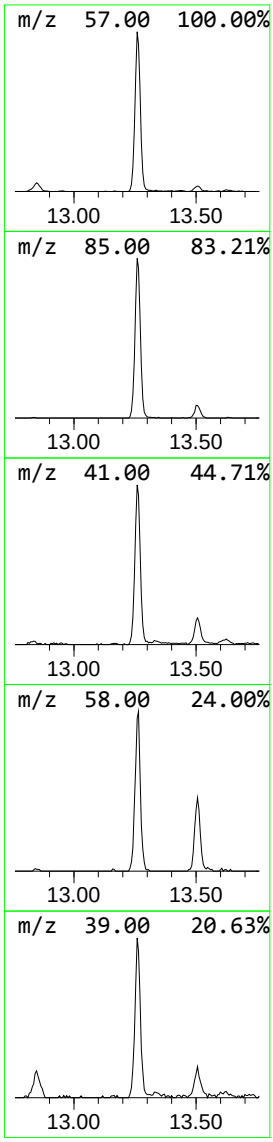
****
Peak Number 1 4-Heptanone, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.259	22.49 ug/l	423749	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	94
2	4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	80
3	5-Nonanone	142	C9H18O	000502-56-7	64
4	t-Butyl isobutyl ketone	142	C9H18O	014705-50-1	59
5	Allyl isovalerate	142	C8H14O2	002835-39-4	50





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Quant Title : SW846 8260

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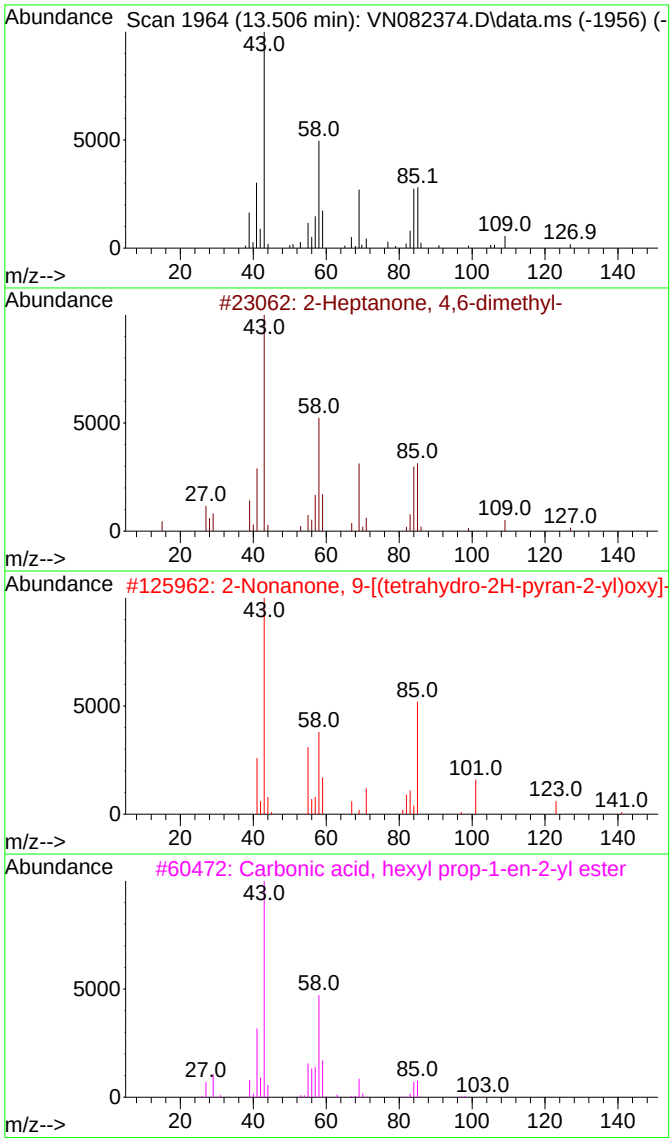
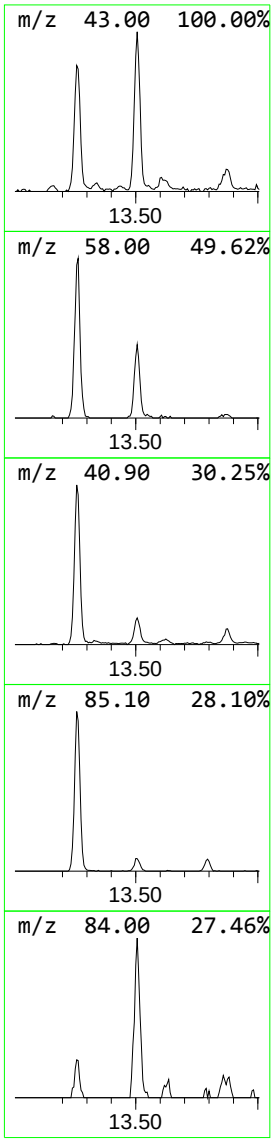
****
Peak Number 2 2-Heptanone, 4,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.506	6.31 ug/l	118828	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone, 4,6-dimethyl-	142	C9H18O	019549-80-5	90
2	2-Nonanone, 9-[(tetrahydro-2H-py...	242	C14H26O3	054699-41-1	59
3	Carbonic acid, hexyl prop-1-en-2...	186	C10H18O3	1000382-54-2	50
4	2-Heptanone, 4-methyl-	128	C8H16O	006137-06-0	38
5	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	38





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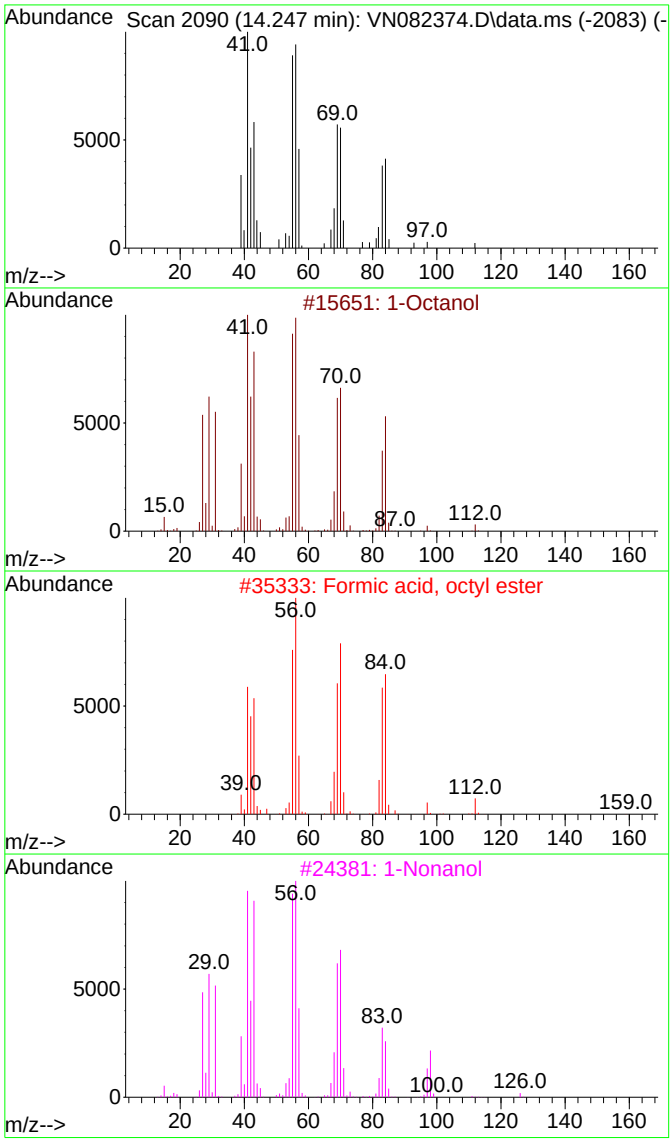
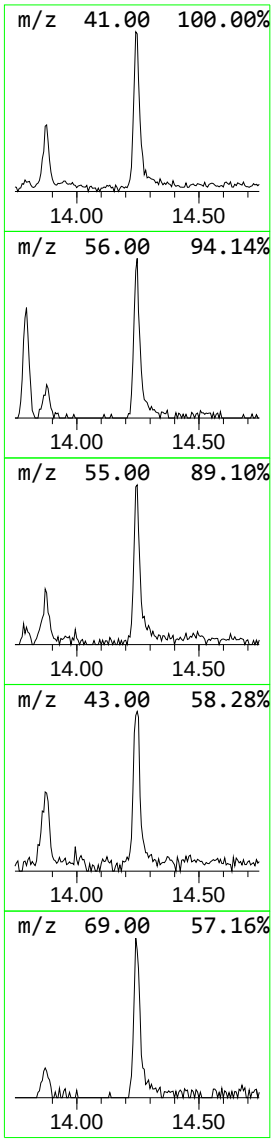
****
Peak Number 3 1-Octanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.247	6.28 ug/l	118286	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol	130	C8H18O	000111-87-5	91
2	Formic acid, octyl ester	158	C9H18O2	000112-32-3	90
3	1-Nonanol	144	C9H20O	000143-08-8	78
4	Cyclobutane, 1,2-diethyl-, trans-	112	C8H16	019341-98-1	52
5	cis-1-Butyl-2-methylcyclopropane	112	C8H16	038851-69-3	50





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
4-Heptanone, 2,...	13.259	22.5	ug/l	423749	4	13.794	941945	50.0
2-Heptanone, 4,...	13.506	6.3	ug/l	118828	4	13.794	941945	50.0
1-Octanol	14.247	6.3	ug/l	118286	4	13.794	941945	50.0