LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052024\
Data File : VN082210.D
Acq On : 20 May 2024 15:22
Operator : JC\MD
Sample : P2511-05 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
510-A

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: VN082210.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.806	139	145	151	rVB2	6661	13511	1.29%	0.177%
2	4.430	412	421	435	rBV2	11247	34496	3.30%	0.453%
3	7.430	924	931	940	rBV	3872	10916	1.04%	0.143%
4	8.171	1045	1057	1061	rBV	133701	325596	31.10%	4.274%
5	8.224	1061	1066	1075	rVB	231493	520139	49.69%	6.828%
6	8.583	1114	1127	1140	rBV	164015	372170	35.55%	4.885%
7	9.100	1205	1215	1224	rBV	367180	749061	71.56%	9.833%
8	10.571	1456	1465	1473	rBV	566495	1046803	100.00%	13.741%
9	11.865	1677	1685	1695	rBV	517051	917066	87.61%	12.038%
10	12.853	1845	1853	1863	rVB	374243	644212	61.54%	8.457%
11	12.953	1864	1870	1880	rBV	52465	92158	8.80%	1.210%
12	13.794	2005	2013	2019	rBV	459614	756107	72.23%	9.925%
13	13.859	2019	2024	2034	rVB3	51289	92075	8.80%	1.209%
14	14.247	2084	2090	2096	rBV4	6540	11576	1.11%	0.152%
15	14.447	2114	2124	2125	rBV4	6870	13841	1.32%	0.182%
16	14.529	2133	2138	2147	rBV5	23553	51614	4.93%	0.678%
17	14.635	2151	2156	2161	rBV3	10677	17659	1.69%	0.232%
18	14.741	2170	2174	2175	rBV2	11778	14967	1.43%	0.196%
19	14.794	2175	2183	2193	rVV2	171383	403720	38.57%	5.300%
20	14.894	2193	2200	2217	rVB	257537	474205	45.30%	6.225%
21	15.106	2229	2236	2250	rBV	334628	622233	59.44%	8.168%
22	15.329	2268	2274	2281	rVB4	11773	25534	2.44%	0.335%
23	15.464	2288	2297	2305	rBV	61892	113667	10.86%	1.492%
24	15.641	2322	2327	2341	rVB7	24117	64009	6.11%	0.840%
25	16.011	2383	2390	2407	rBV2	86739	213525	20.40%	2.803%
26	16.547	2477	2481	2491	rVB8	7200	17031	1.63%	0.224%

Sum of corrected areas: 7617891

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Instrument :
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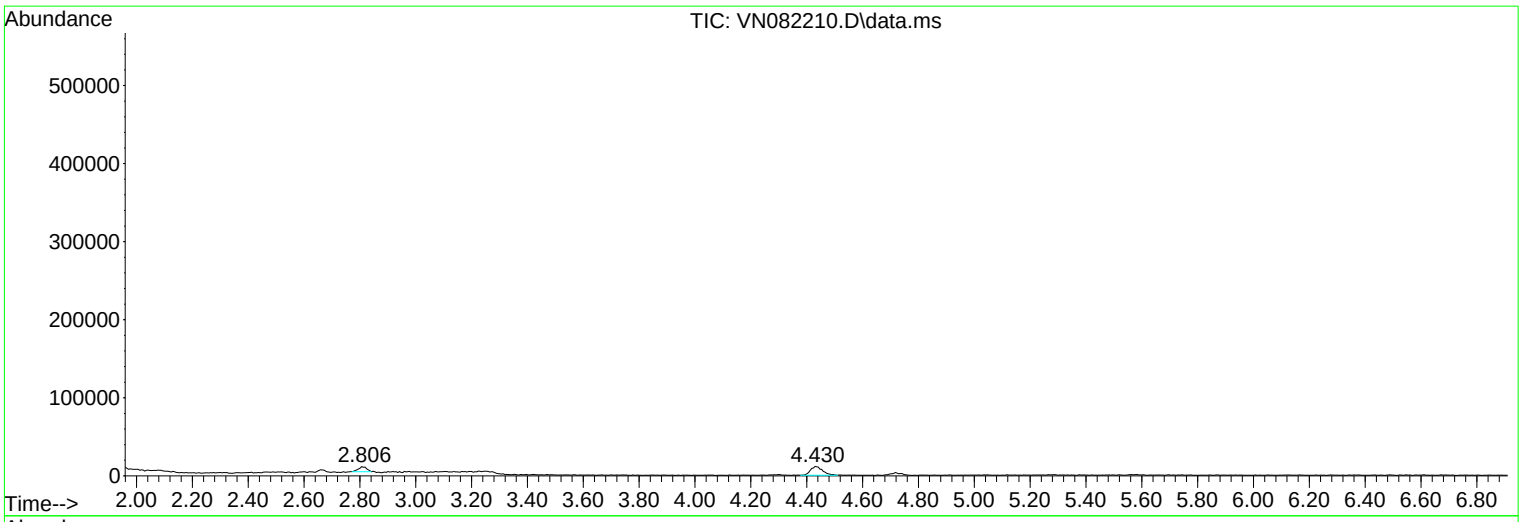
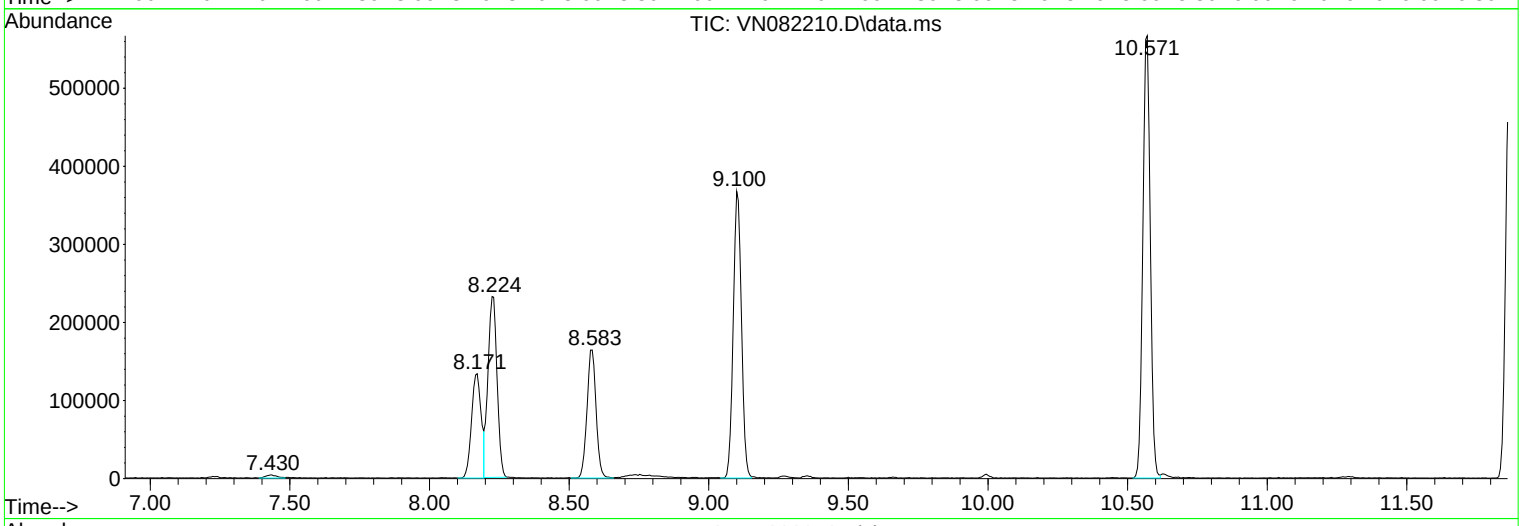
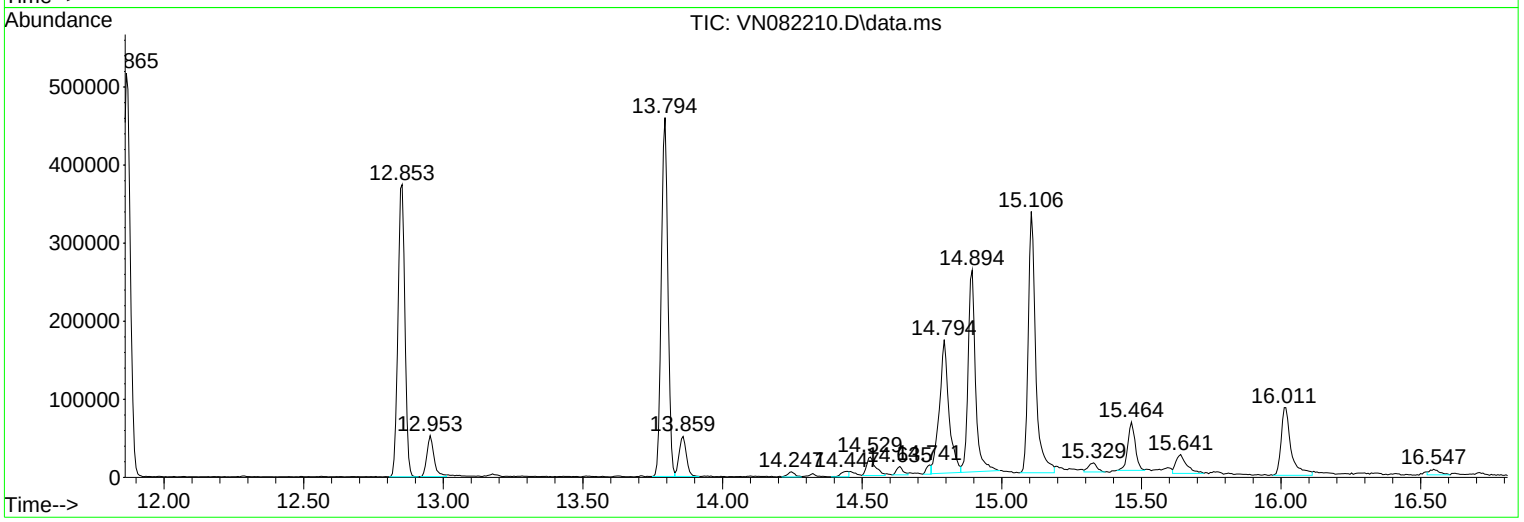
ClientSampleId :
510-A

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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Quant Title : SW846 8260

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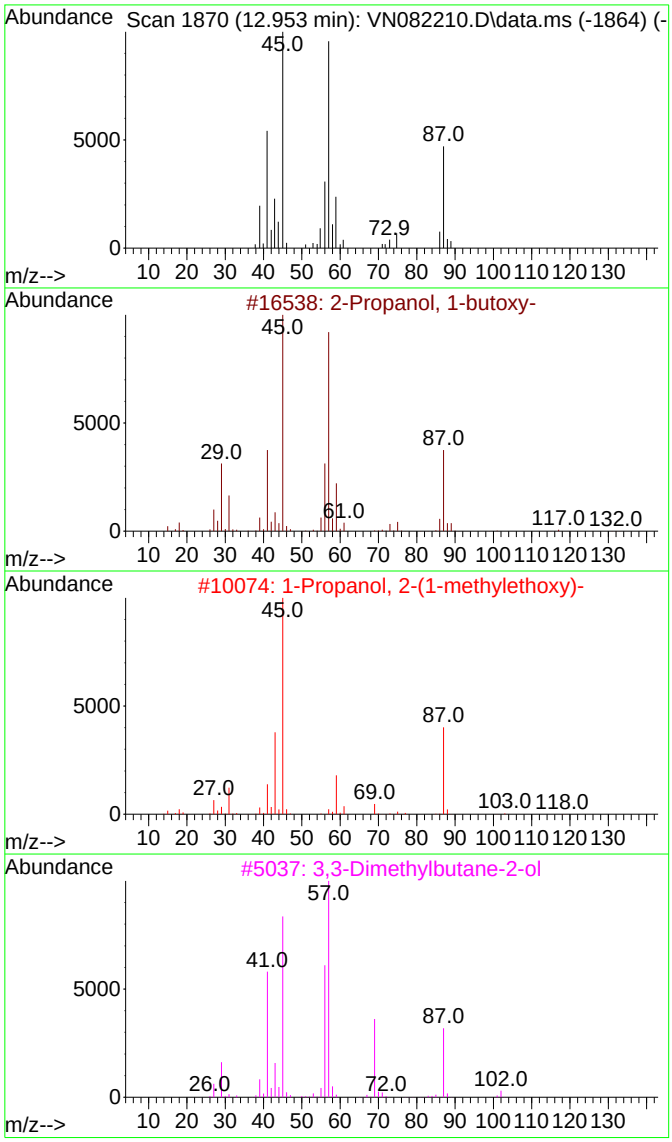
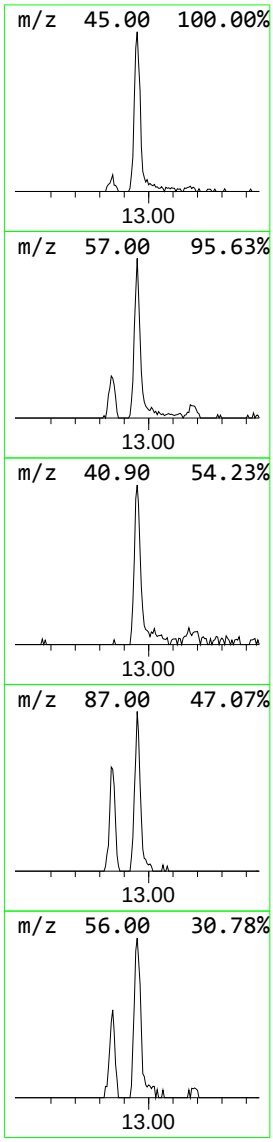
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Propanol, 1-butoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.953	6.09 ug/l	92158	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	42
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	42
4	Hexane, 3-methoxy-	116	C7H16O	054658-01-4	40
5	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	36





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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
510-A

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

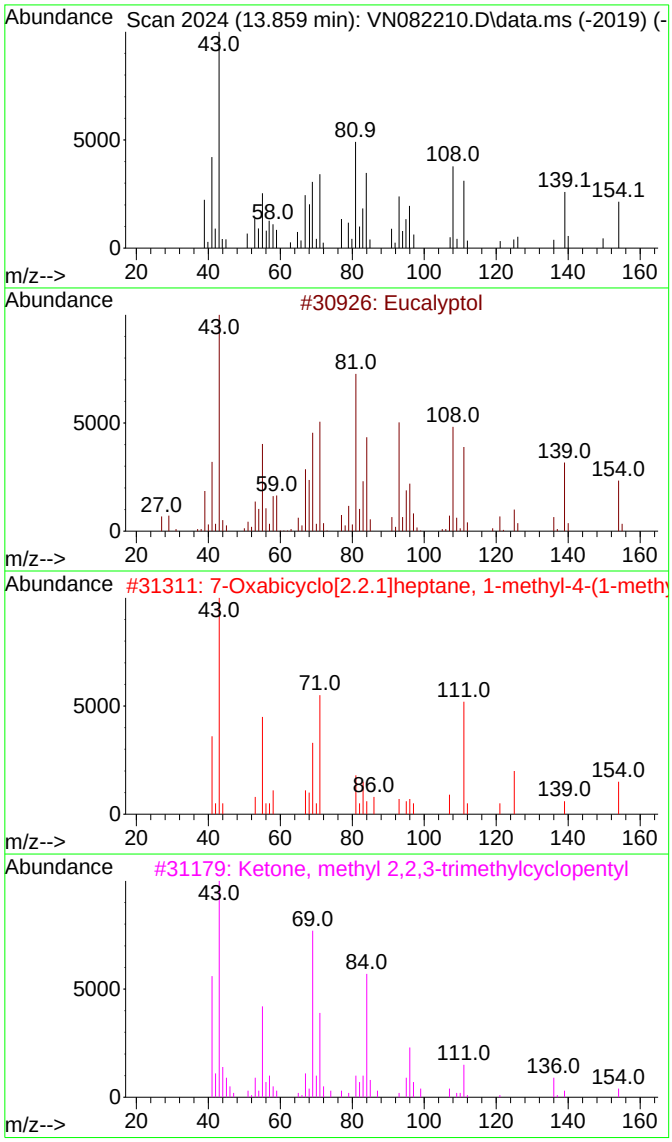
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

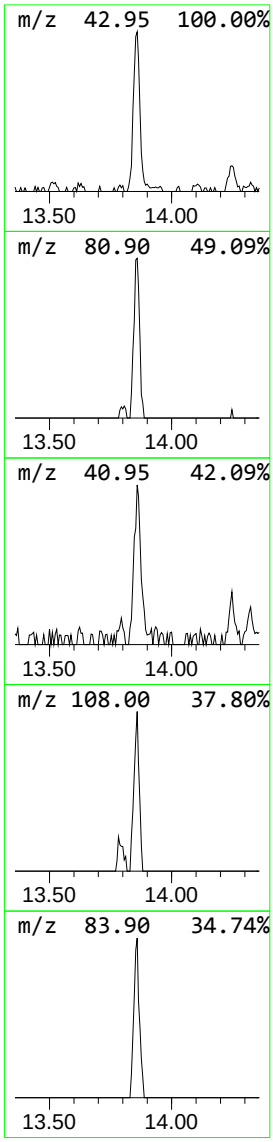
****

Peak Number 2 Eucalyptol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.859	6.09 ug/l	92075	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eucalyptol	154	C10H18O	000470-82-6	93
2	7-Oxabicyclo[2.2.1]heptane, 1-me...	154	C10H18O	000470-67-7	27
3	Ketone, methyl 2,2,3-trimethylcy...	154	C10H18O	017983-22-1	27
4	4-Isopropyl-1-methylcyclohex-2-enol	154	C10H18O	000619-62-5	25
5	2-Isopropyl-5-methylhex-2-enal	154	C10H18O	035158-25-9	22





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Operator : JC\MD
Sample : P2511-05 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
510-A

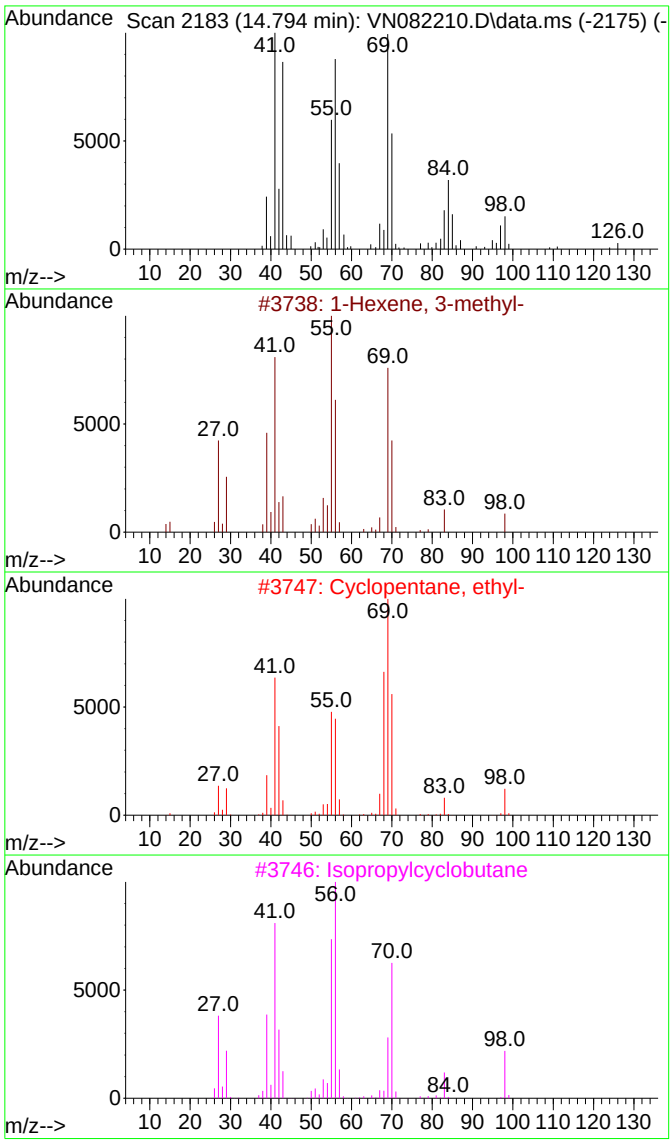
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

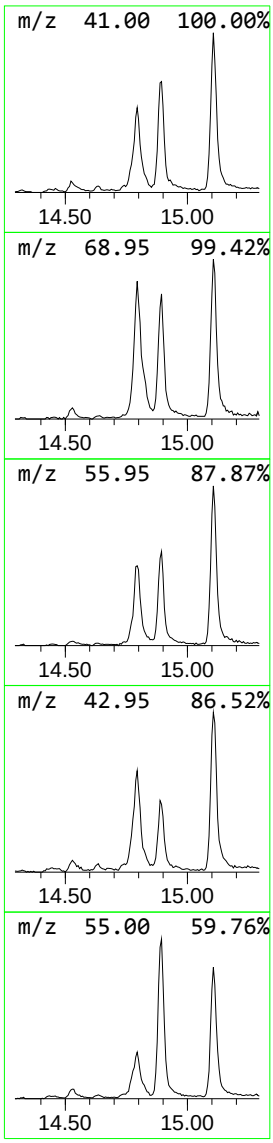
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1-Hexene, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.794	26.70 ug/l	403720	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexene, 3-methyl-	98	C7H14	003404-61-3	64
2	Cyclopentane, ethyl-	98	C7H14	001640-89-7	49
3	Isopropylcyclobutane	98	C7H14	000872-56-0	46
4	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	46
5	1-Hexene, 3,3,5-trimethyl-	126	C9H18	013427-43-5	43





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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
510-A

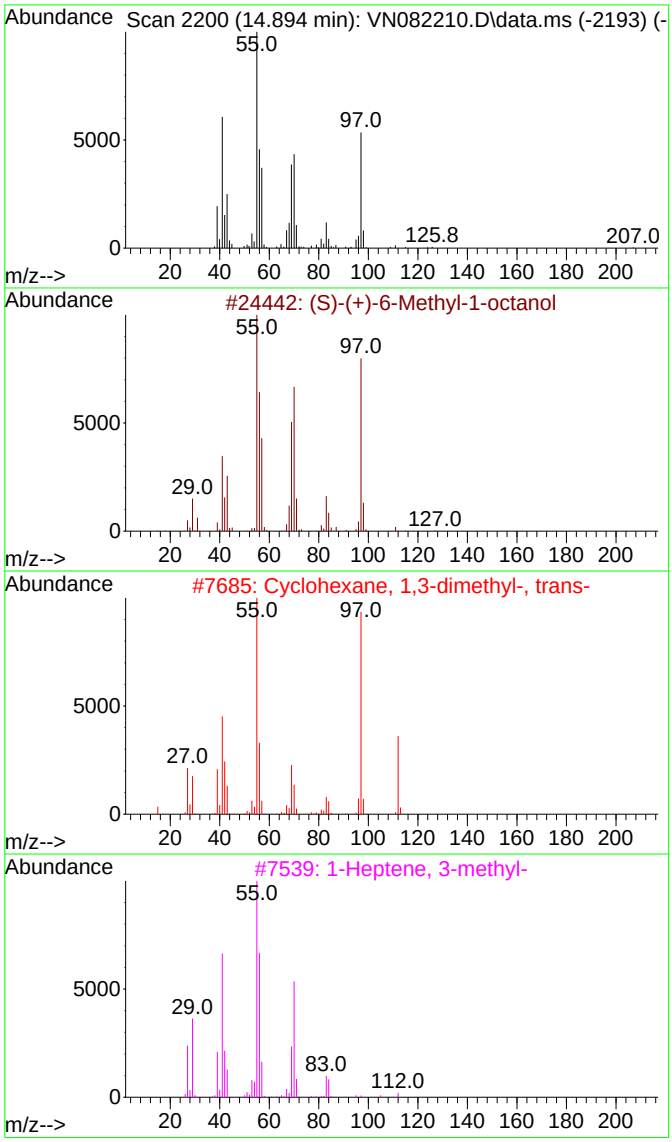
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

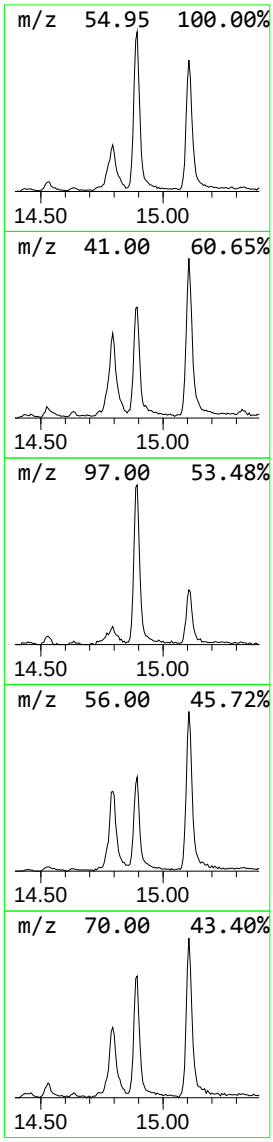
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (S)-(+)-6-Methyl-1-octanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.894	31.36 ug/l	474205	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-6-Methyl-1-octanol	144	C9H20O	110453-78-6	86
2	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	53
3	1-Heptene, 3-methyl-	112	C8H16	004810-09-7	50
4	1-Octene, 3-methyl-	126	C9H18	013151-08-1	47
5	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-77-7	47





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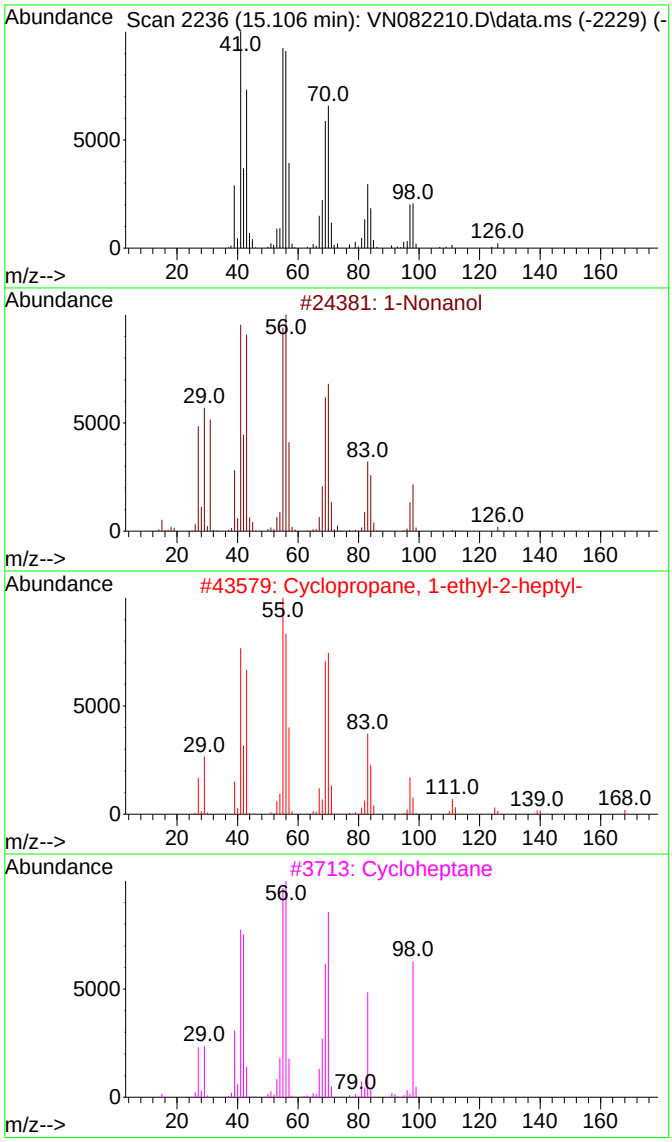
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

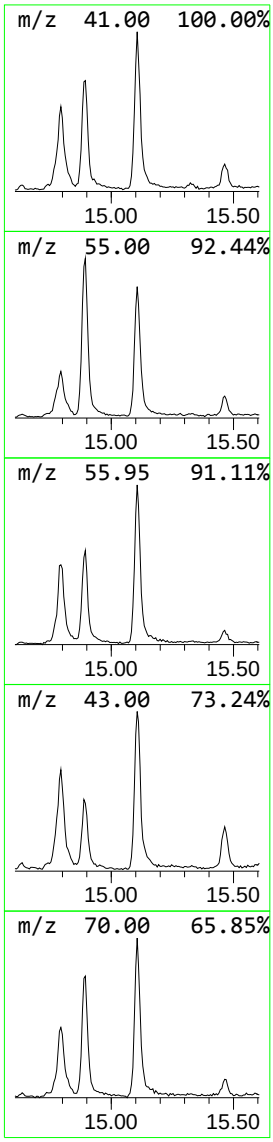
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Nonanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.106	41.15 ug/l	622233	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	Cyclopropane, 1-ethyl-2-heptyl-	168	C12H24	074663-86-8	80
3	Cycloheptane	98	C7H14	000291-64-5	74
4	Isopropylcyclobutane	98	C7H14	000872-56-0	68
5	Cyclopropane, 1-methyl-2-pentyl-	126	C9H18	041977-37-1	58





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TIC Library : C:\Database\NIST20.L
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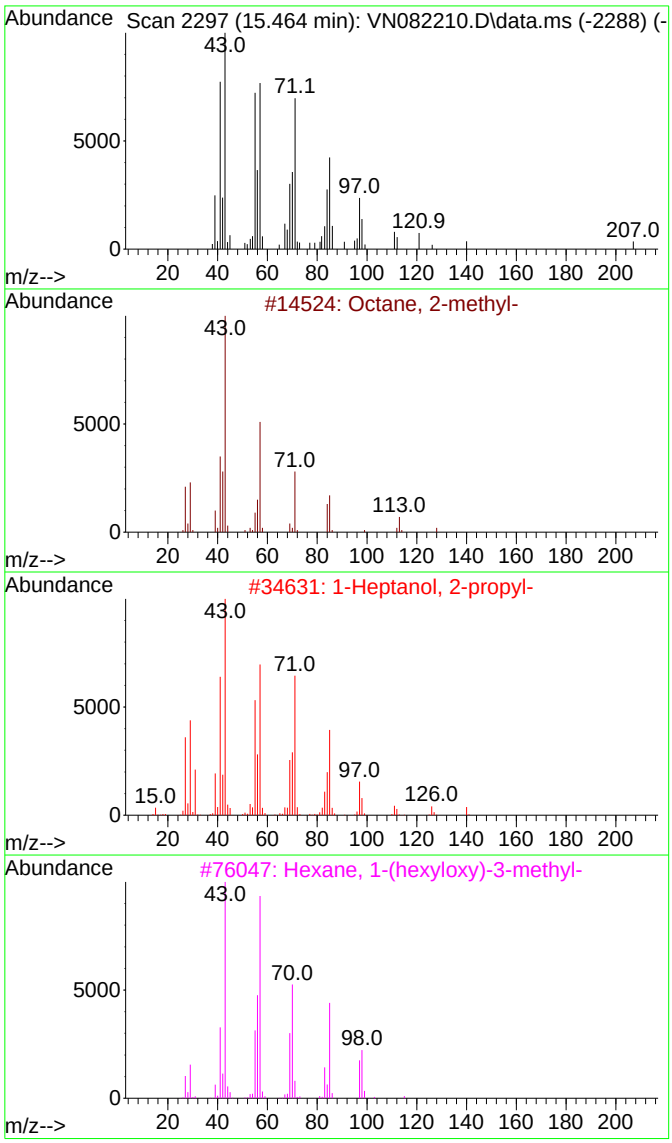
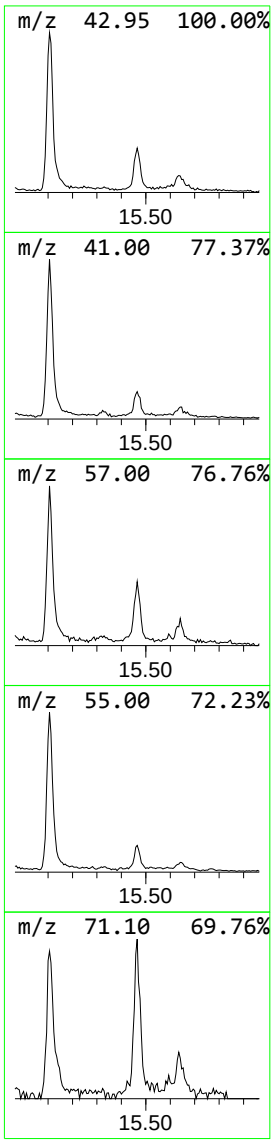
****
Peak Number 6 Octane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.464	7.52 ug/l	113667	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-methyl-	128	C9H20	003221-61-2	59
2	1-Heptanol, 2-propyl-	158	C10H22O	010042-59-8	58
3	Hexane, 1-(hexyloxy)-3-methyl-	200	C13H28O	074421-18-4	38
4	1-Decene	140	C10H20	000872-05-9	30
5	Oxalic acid, 2-ethylhexyl ethyl ...	230	C12H22O4	1000309-38-4	27





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Quant Title : SW846 8260

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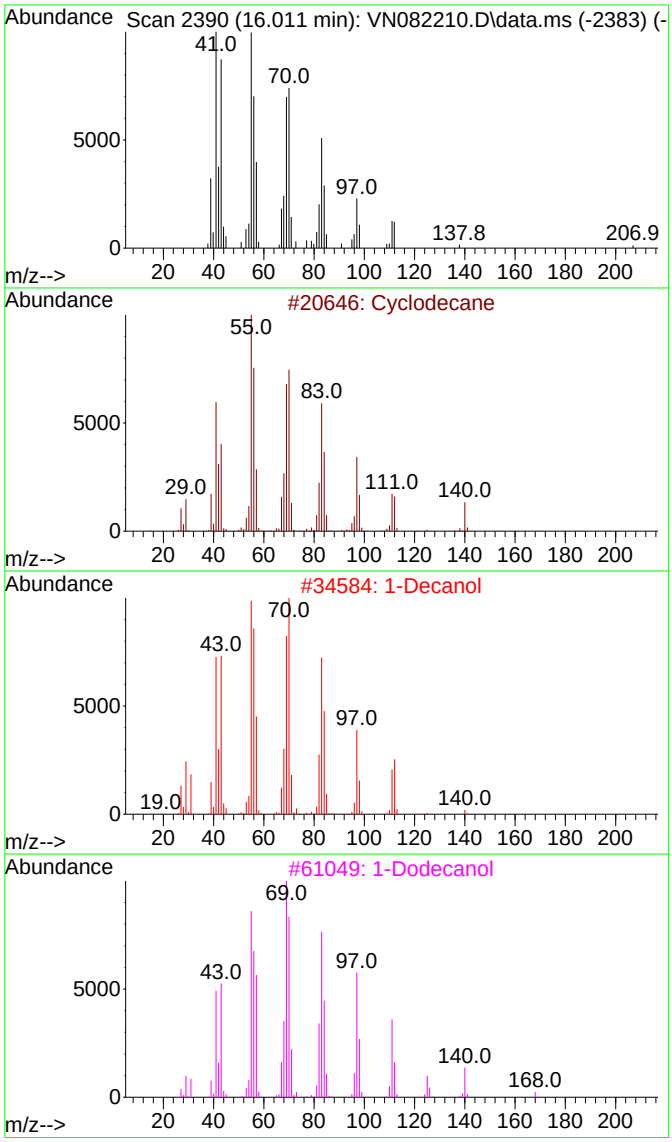
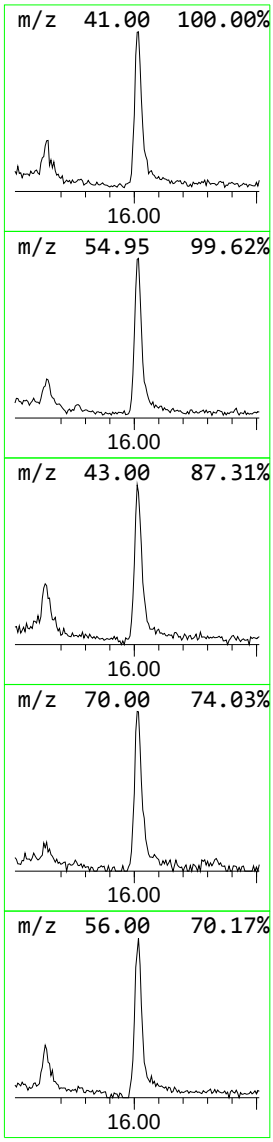
****

Peak Number 7 Cyclodecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.012	14.12 ug/l	213525	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclodecane	140	C10H20	000293-96-9	91
2	1-Decanol	158	C10H22O	000112-30-1	91
3	1-Dodecanol	186	C12H26O	000112-53-8	91
4	1-Undecanol	172	C11H24O	000112-42-5	90
5	Pentafluoropropionic acid, decyl...	304	C13H21F5O2	959000-65-8	90





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	6.1	ug/l	92158	4	13.794	756107	50.0
Eucalyptol	13.859	6.1	ug/l	92075	4	13.794	756107	50.0
1-Hexene, 3-met...	14.794	26.7	ug/l	403720	4	13.794	756107	50.0
(S)-(+)-6-Methy...	14.894	31.4	ug/l	474205	4	13.794	756107	50.0
1-Nonanol	15.106	41.1	ug/l	622233	4	13.794	756107	50.0
Octane, 2-methyl-	15.464	7.5	ug/l	113667	4	13.794	756107	50.0
Cyclodecane	16.012	14.1	ug/l	213525	4	13.794	756107	50.0