LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051821\
Data File : VN067131.D
Acq On : 18 May 2021 16:51
Operator : JC/MD
Sample : M2387-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 31055

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\82N051421W.M
Title : SW846 8260

Signal : TIC: VN067131.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.305	203	211	222	rVB	18791	28933	1.07%	0.159%
2	3.241	543	560	601	rVB	287618	798213	29.49%	4.396%
3	3.772	739	758	775	rBV2	80550	214221	7.91%	1.180%
4	4.019	828	850	881	rBV2	57006	178585	6.60%	0.984%
5	6.468	1740	1763	1789	rBV4	58166	186192	6.88%	1.025%
6	6.760	1855	1872	1896	rBV2	27642	87076	3.22%	0.480%
7	7.130	1990	2010	2041	rBV5	21495	73700	2.72%	0.406%
8	7.519	2132	2155	2169	rBV2	355401	904825	33.43%	4.983%
9	7.597	2170	2184	2216	rVB	662777	1613195	59.60%	8.885%
10	7.962	2295	2320	2353	rBV3	378504	957426	35.37%	5.273%
11	8.525	2510	2530	2569	rBV	873899	1879234	69.43%	10.350%
12	8.737	2592	2609	2638	rBV2	192679	472746	17.47%	2.604%
13	10.037	3074	3094	3109	rVV	1440904	2706660	100.00%	14.907%
14	10.102	3109	3118	3147	rVB	136654	274385	10.14%	1.511%
15	10.826	3373	3388	3413	rBV2	117196	225537	8.33%	1.242%
16	11.360	3569	3587	3619	rBV	1077589	2094357	77.38%	11.535%
17	11.574	3656	3667	3689	rBV2	45629	102501	3.79%	0.565%
18	11.711	3705	3718	3741	rBV3	21331	54296	2.01%	0.299%
19	11.931	3779	3800	3835	rVB5	49841	183877	6.79%	1.013%
20	12.357	3942	3959	4008	rBV	728321	1682217	62.15%	9.265%
21	13.301	4297	4311	4345	rBV	800578	1724044	63.70%	9.495%
22	13.427	4349	4358	4385	rVV5	60019	202316	7.47%	1.114%
23	13.685	4443	4454	4484	rVB	97428	219087	8.09%	1.207%
24	14.117	4608	4615	4623	rBV9	36695	56722	2.10%	0.312%
25	14.186	4636	4641	4653	rVB3	49889	62419	2.31%	0.344%
26	14.597	4785	4794	4810	rVB2	237623	377480	13.95%	2.079%
27	15.071	4959	4971	5006	rVB3	273238	796755	29.44%	4.388%

Sum of corrected areas: 18156999

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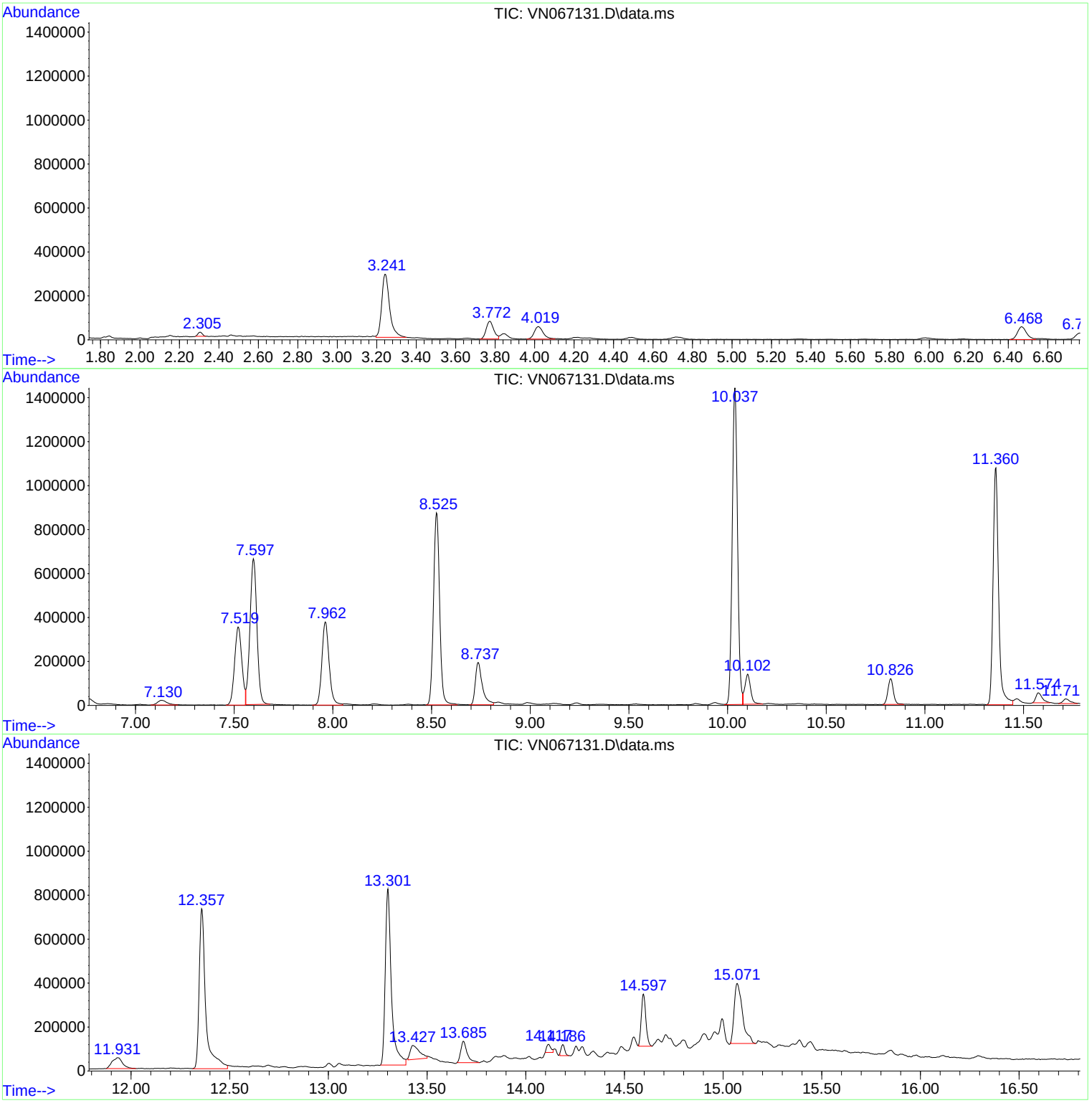
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31055

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Data File : VN067131.D
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ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 31055

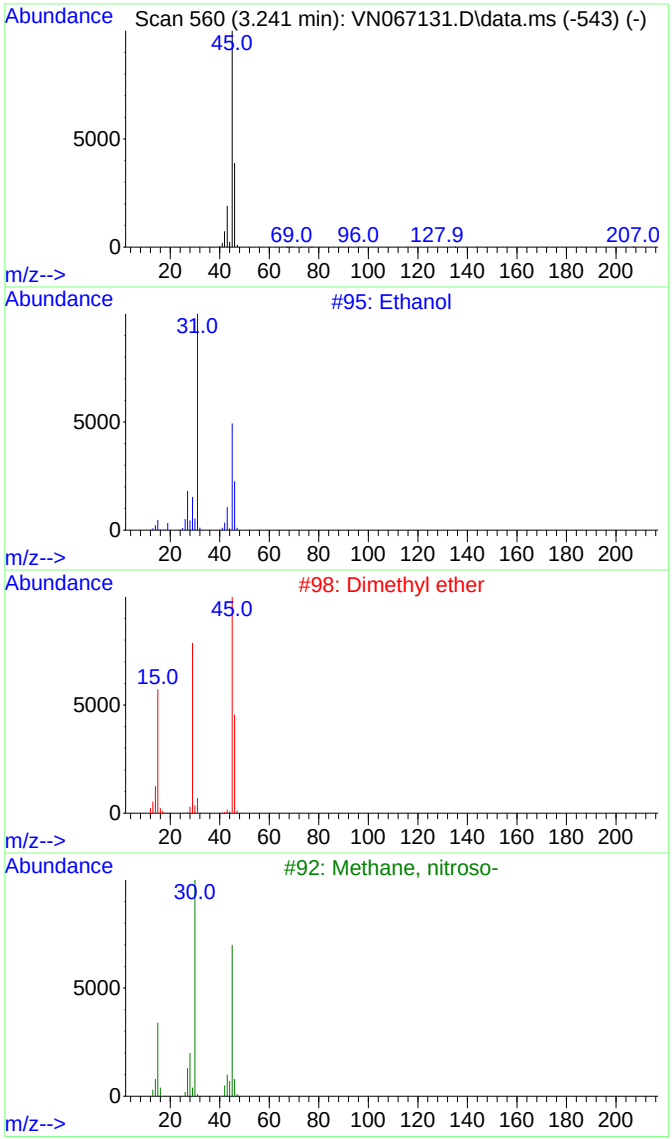
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

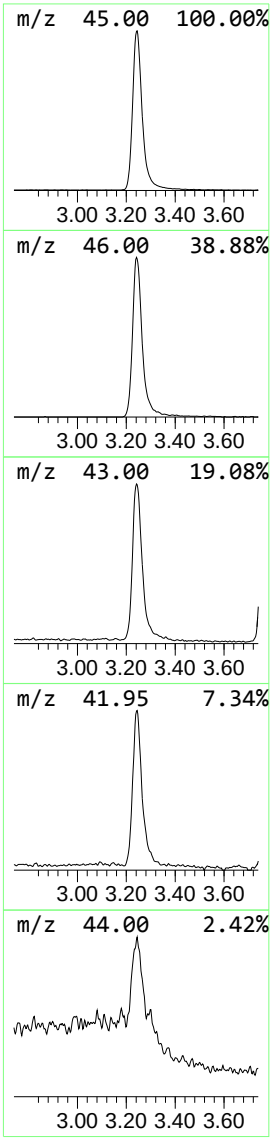
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.241	24.74 ug/l	798213	Pentafluorobenzene	7.600

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	78
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Formic acid	46	CH2O2	000064-18-6	4
5	Formamide	45	CH3NO	000075-12-7	3





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Data File : VN067131.D
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Operator : JC/MD
Sample : M2387-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 31055

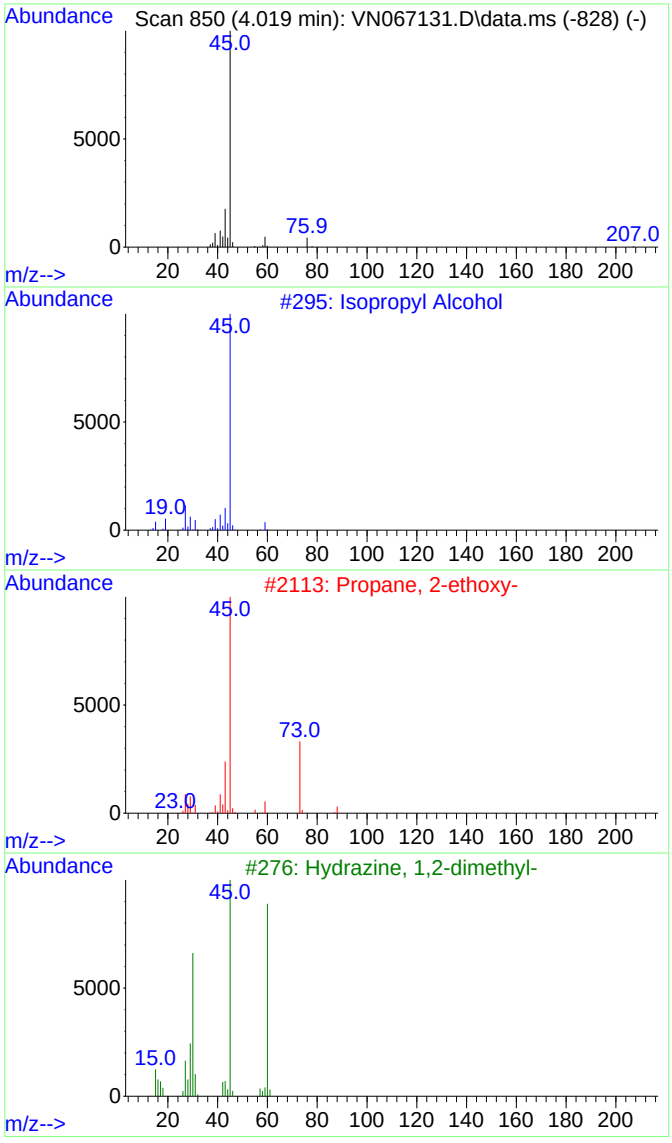
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

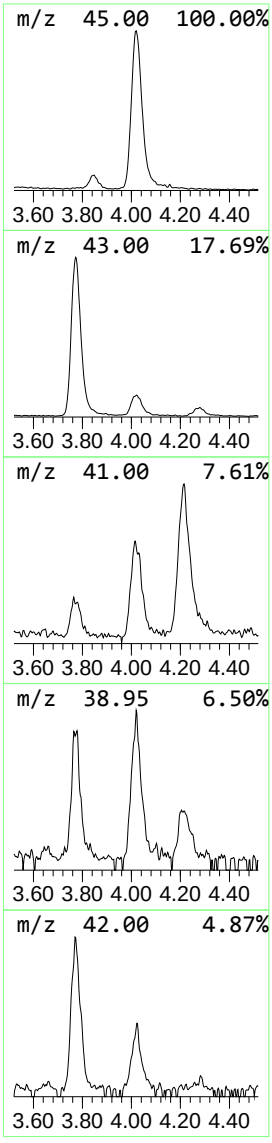
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Isopropyl Alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.019	5.54 ug/l	178585	Pentafluorobenzene	7.600

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	86
2	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	40
3	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4	(R)-(-)-2-Pentanol	88	C5H12O	031087-44-2	9
5	2-Pentanol	88	C5H12O	006032-29-7	9





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Operator : JC/MD
Sample : M2387-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 31055

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

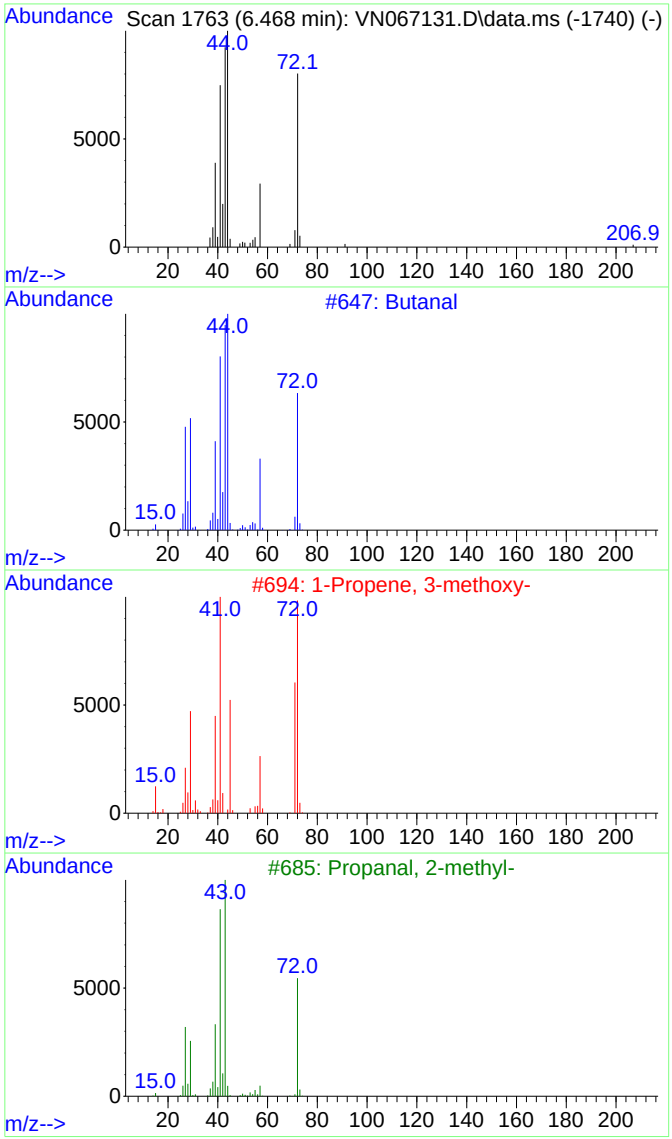
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

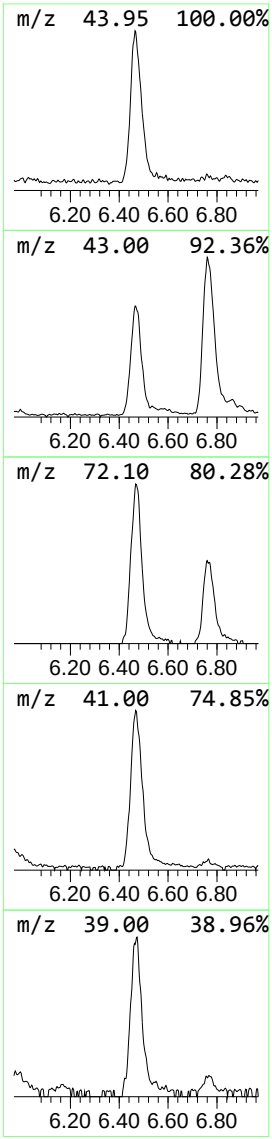
****

Peak Number 3 Butanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.468	5.77 ug/l	186192	Pentafluorobenzene	7.600

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	43
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4	Ethene, ethoxy-	72	C4H8O	000109-92-2	40
5	1-Propene, 1-methoxy-	72	C4H8O	007319-16-6	35





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Data File : VN067131.D
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Operator : JC/MD
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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 31055

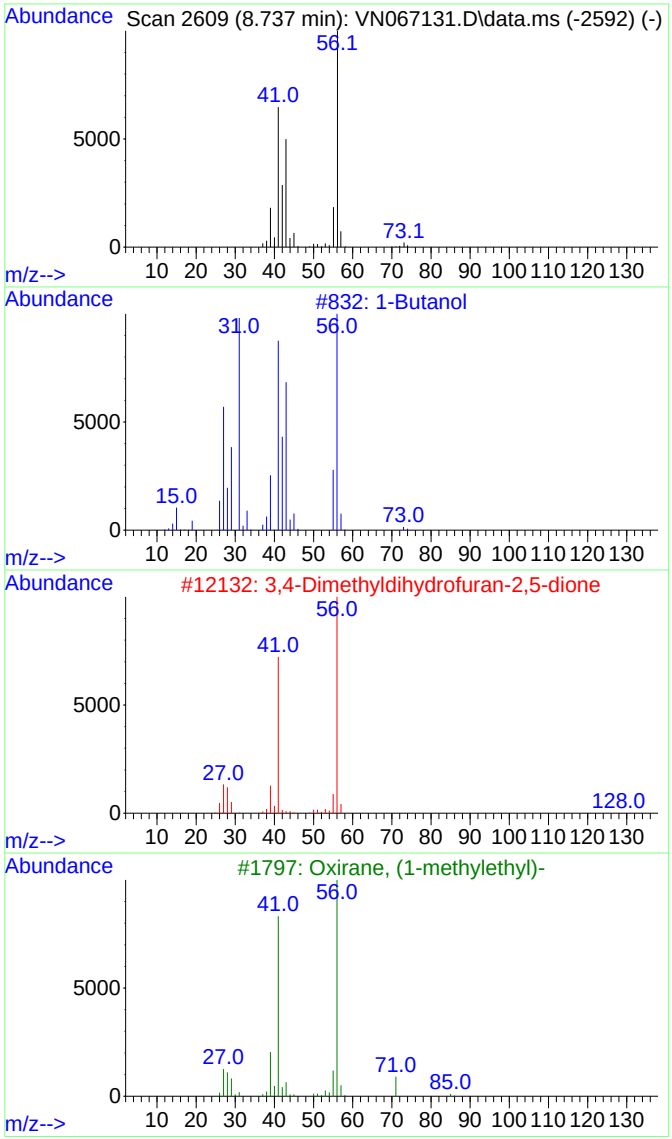
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

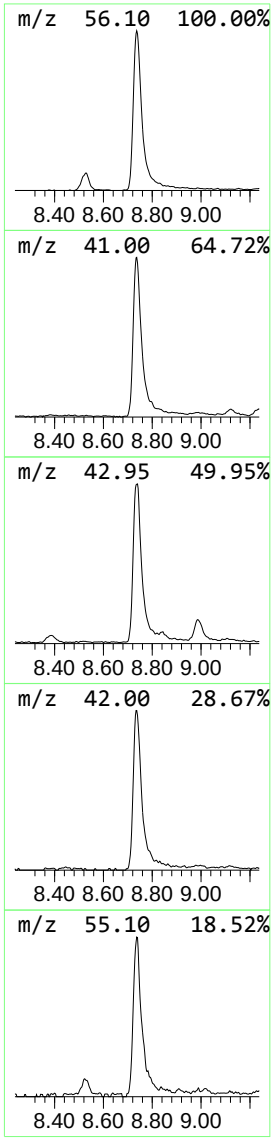
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Butanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.737	12.58 ug/l	472746	1,4-Difluorobenzene	8.525

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	90
2	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	33
3	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	9
4	3-Butenoic acid, 2-amino-	101	C4H7NO2	056512-51-7	9
5	Formic acid, butyl ester	102	C5H10O2	000592-84-7	9





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Operator : JC/MD
Sample : M2387-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 31055

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

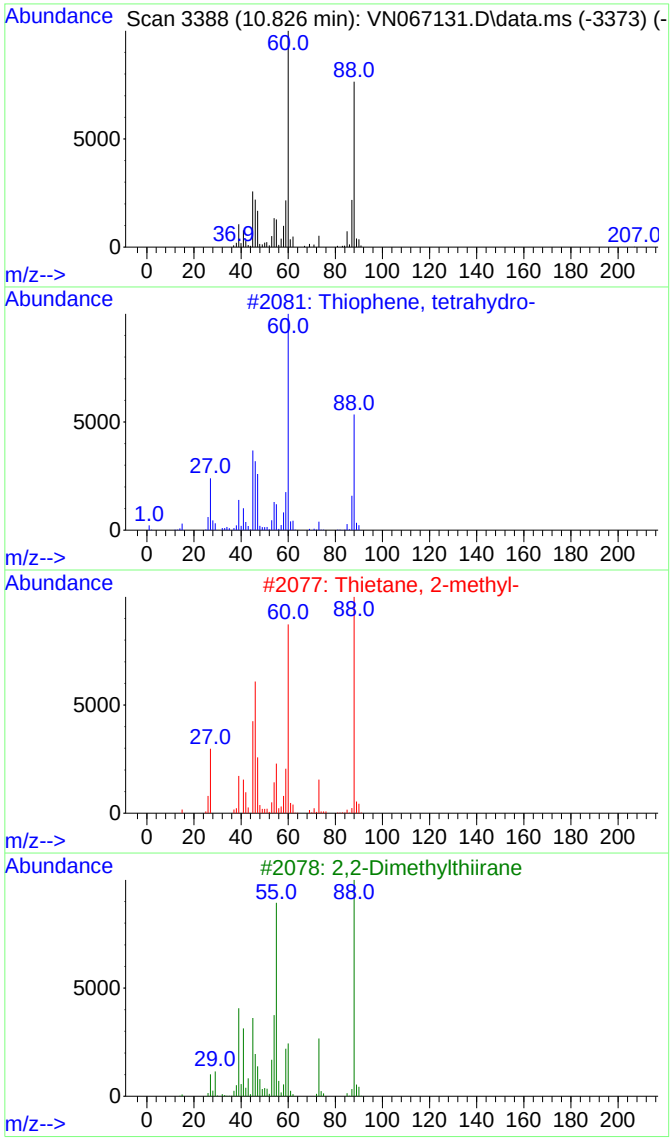
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

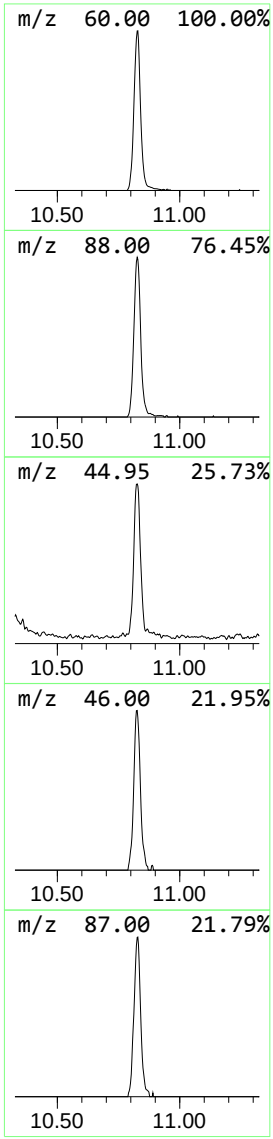
****

Peak Number 5 Thiophene, tetrahydro- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.826	5.38 ug/l	225537	Chlorobenzene-d5	11.360

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-	88	C4H8S	000110-01-0	95
2	Thietane, 2-methyl-	88	C4H8S	017837-41-1	72
3	2,2-Dimethylthiirane	88	C4H8S	003772-13-2	47
4	1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	36
5	Sulfide, allyl methyl	88	C4H8S	010152-76-8	32





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ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 31055

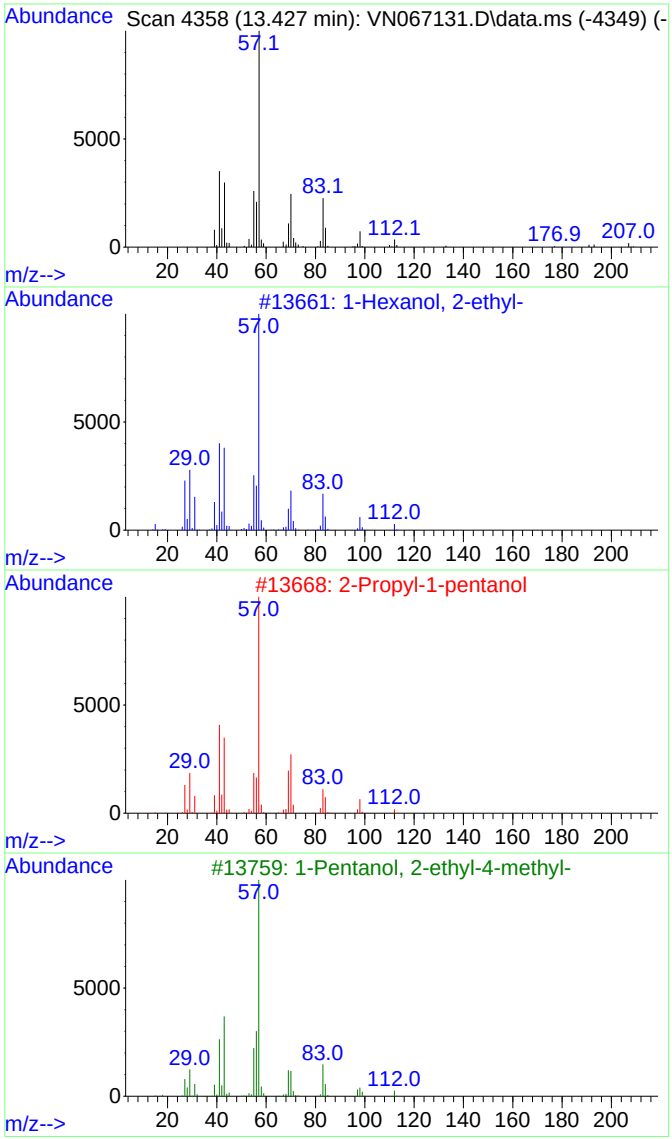
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

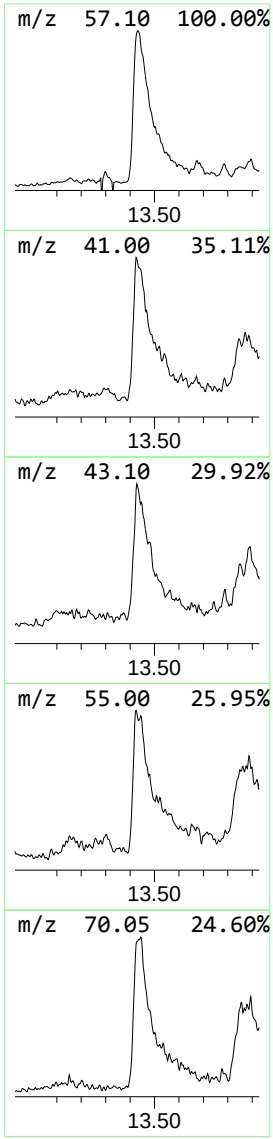
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.428	5.87 ug/l	202316	1,4-Dichlorobenzene-d4	13.301

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
4	Isobutyl octyl carbonate	230	C13H26O3	1000372-74-6	47
5	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	42





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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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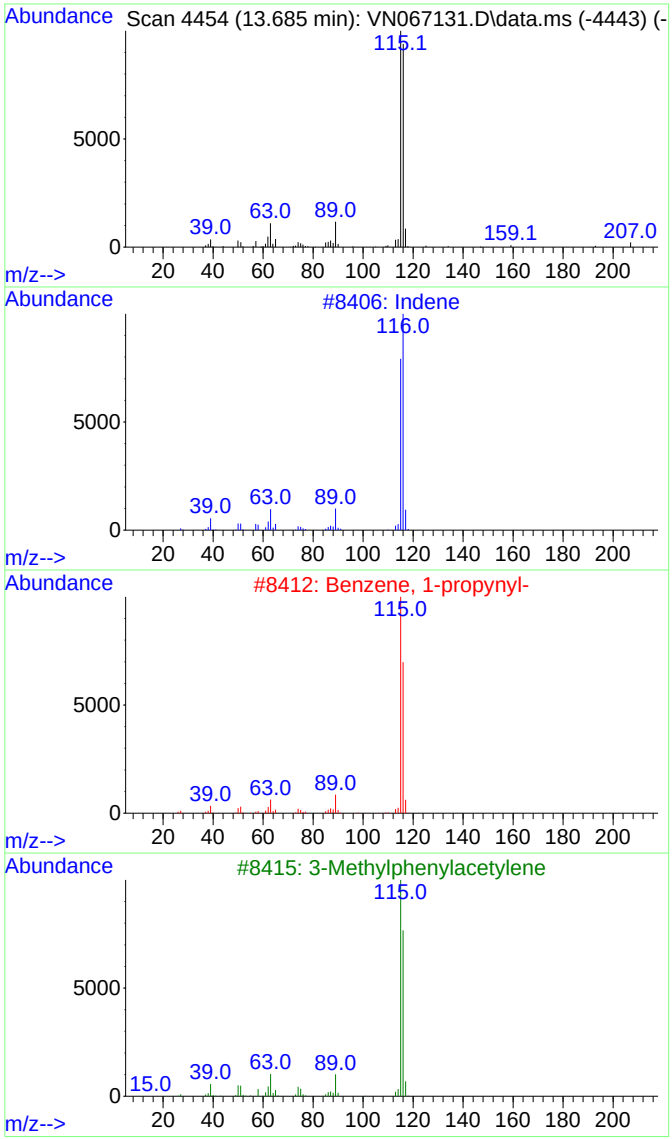
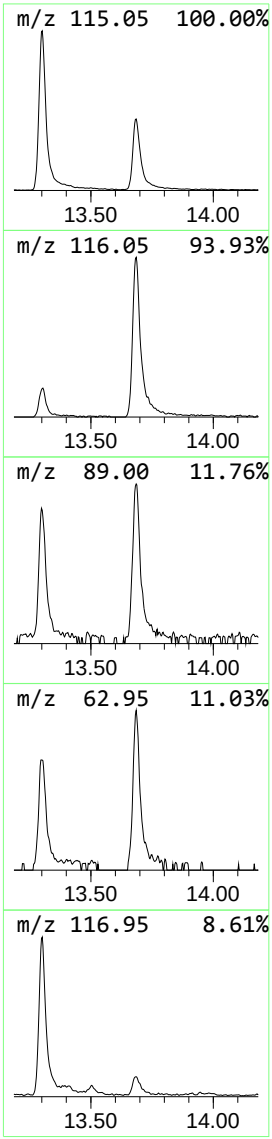
****
Peak Number 7 Indene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.685	6.35 ug/l	219087	1,4-Dichlorobenzene-d4	13.301

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	97
2	Benzene, 1-propynyl-	116	C9H8	000673-32-5	95
3	3-Methylphenylacetylene	116	C9H8	000766-82-5	94
4	Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91
5	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90





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Quant Title : SW846 8260

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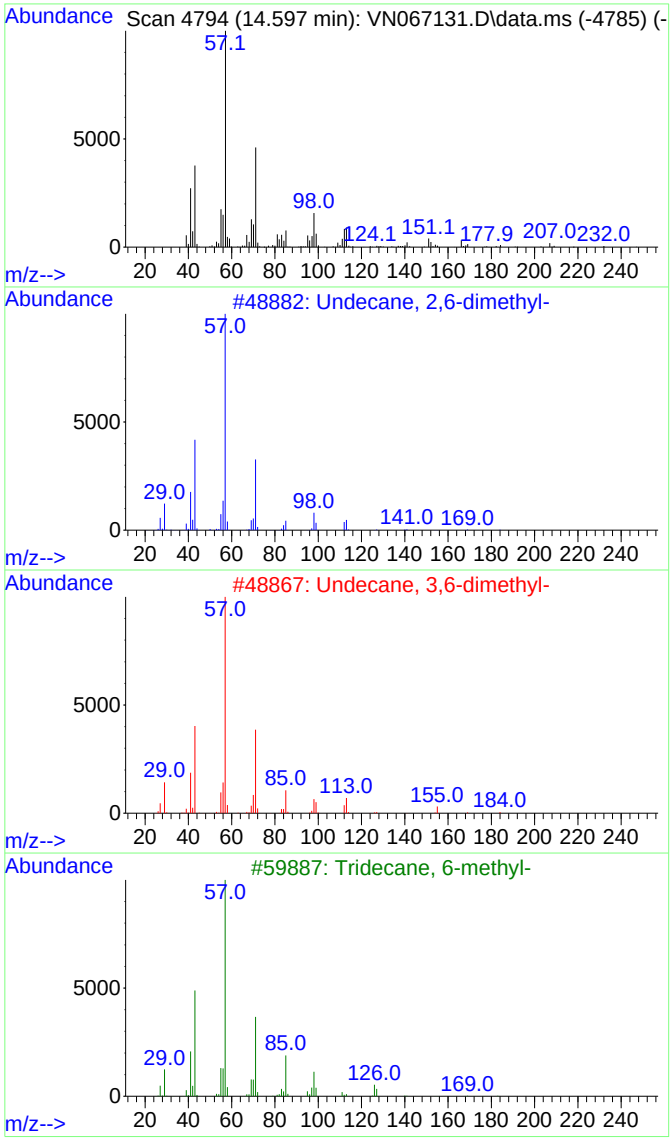
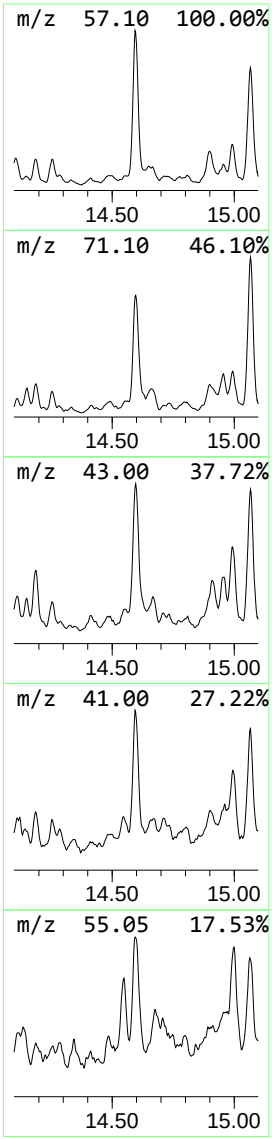
****
Peak Number 8 Undecane, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.597	10.95 ug/l	377480	1,4-Dichlorobenzene-d4	13.301

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	90
2	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	74
3	Tridecane, 6-methyl-	198	C14H30	013287-21-3	64
4	Dodecane, 6-methyl-	184	C13H28	006044-71-9	60
5	Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	53





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethanol	3.241	24.7	ug/l	798213	1	7.600	1613200	50.0
Isopropyl Alcohol	4.019	5.5	ug/l	178585	1	7.600	1613200	50.0
Butanal	6.468	5.8	ug/l	186192	1	7.600	1613200	50.0
1-Butanol	8.737	12.6	ug/l	472746	2	8.525	1879230	50.0
Thiophene, tetr...	10.826	5.4	ug/l	225537	3	11.360	2094360	50.0
1-Hexanol, 2-et...	13.428	5.9	ug/l	202316	4	13.301	1724040	50.0
Indene	13.685	6.3	ug/l	219087	4	13.301	1724040	50.0
Undecane, 2,6-d...	14.597	10.9	ug/l	377480	4	13.301	1724040	50.0