LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030321\
Data File : VN066123.D
Acq On : 3 Mar 2021 14:41
Operator : JC/MD
Sample : M1489-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP-41071-72

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\82N030221W.M
Title : SW846 8260

Signal : TIC: VN066123.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.290	159	171	220	rBV	5862468	11705646	100.00%	64.155%
2	3.251	454	470	496	rVB2	61145	146211	1.25%	0.801%
3	3.669	583	600	625	rBV	298113	761411	6.50%	4.173%
4	4.290	773	793	819	rBV	54860	153892	1.31%	0.843%
5	5.968	1293	1315	1346	rBV2	45428	182044	1.56%	0.998%
6	6.499	1458	1480	1507	rBV	190627	572110	4.89%	3.136%
7	7.627	1819	1831	1851	rVB2	72253	170659	1.46%	0.935%
8	7.991	1926	1944	1967	rBV4	69415	192062	1.64%	1.053%
9	8.550	2104	2118	2133	rBV	118882	241649	2.06%	1.324%
10	10.058	2572	2587	2598	rBV	186676	352783	3.01%	1.933%
11	10.122	2598	2607	2629	rVB	105095	197119	1.68%	1.080%
12	11.376	2981	2997	3021	rBV2	223161	446309	3.81%	2.446%
13	11.511	3021	3039	3049	rVV3	57110	127950	1.09%	0.701%
14	11.585	3051	3062	3083	rVB	102346	203026	1.73%	1.113%
15	11.916	3154	3165	3176	rBV	83638	154049	1.32%	0.844%
16	12.373	3295	3307	3323	rVB	151625	263894	2.25%	1.446%
17	12.884	3455	3466	3486	rVB	102050	180698	1.54%	0.990%
18	13.074	3516	3525	3547	rVB	97839	189788	1.62%	1.040%
19	13.312	3588	3599	3618	rBV2	167798	321677	2.75%	1.763%
20	13.418	3618	3632	3650	rBV2	638295	1178826	10.07%	6.461%
21	14.096	3829	3843	3854	rBV	101411	171801	1.47%	0.942%
22	15.096	4139	4154	4164	rBV	172058	332390	2.84%	1.822%

Sum of corrected areas: 18245994

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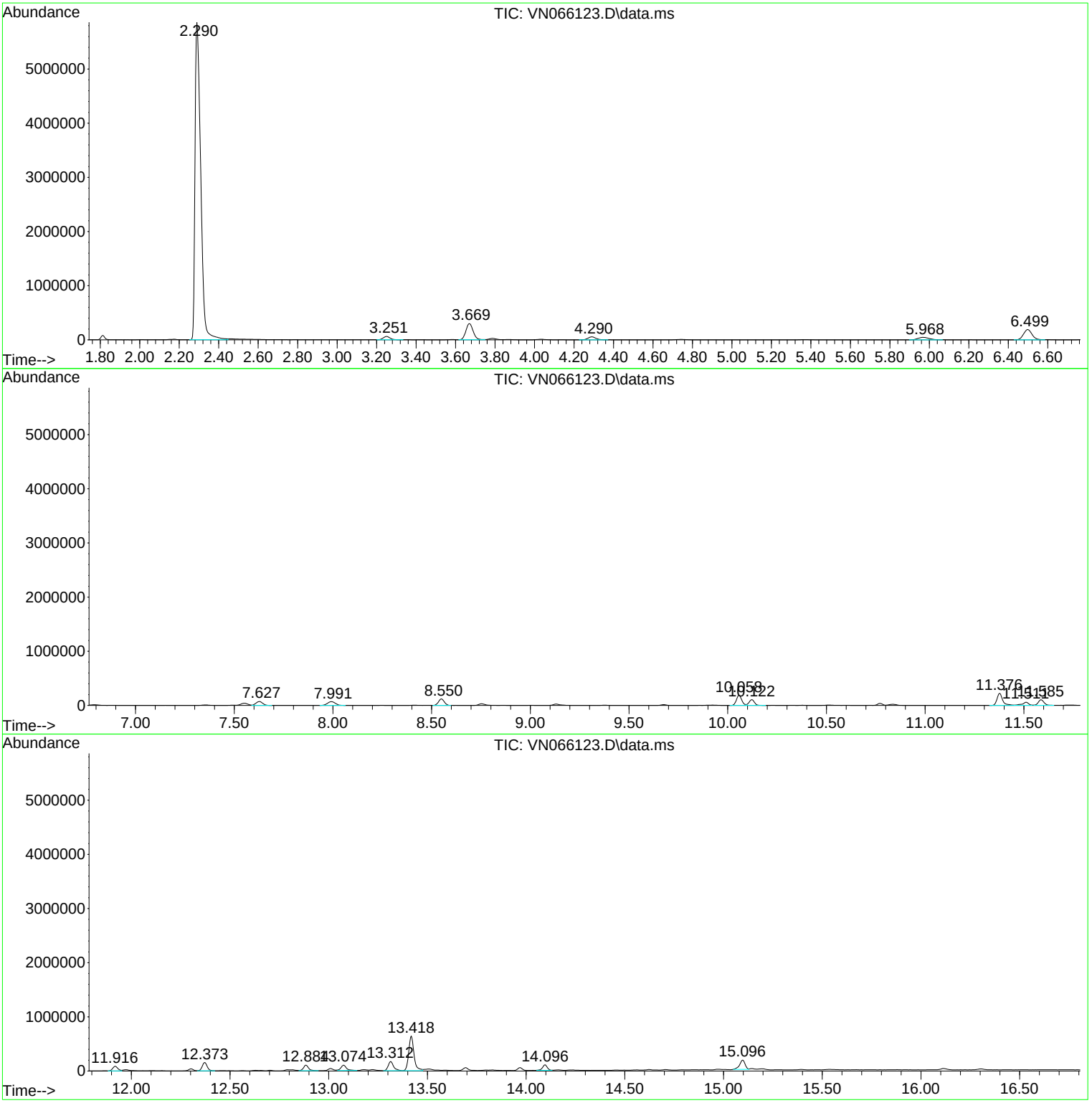
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP-41071-72

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030221W.M
Quant Title : SW846 8260

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



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Data File : VN066123.D
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030221W.M
Quant Title : SW846 8260

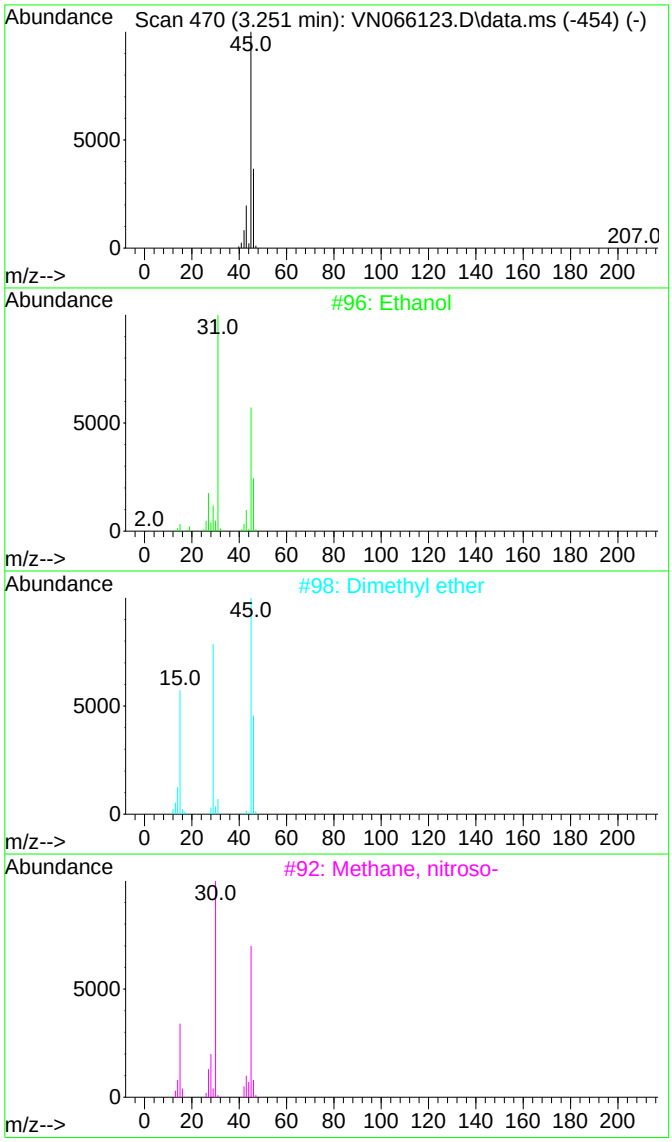
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

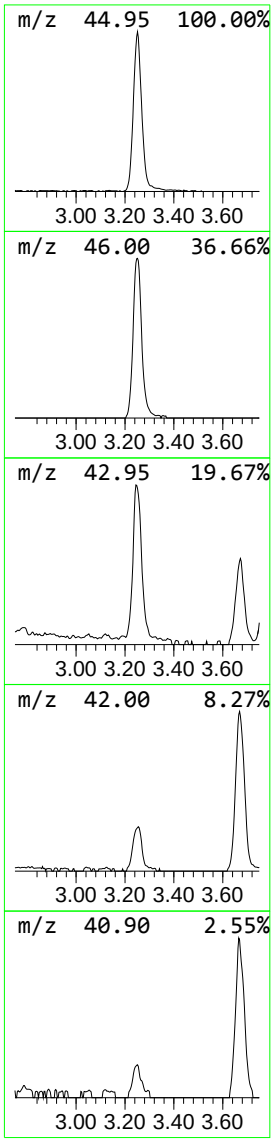
****

Peak Number 2 Ethanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.251	42.84 ug/l	146211	Pentafluorobenzene	7.627

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	83
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	L-Lactic acid	90	C3H6O3	000079-33-4	4





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Operator : JC/MD
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP-41071-72

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030221W.M
Quant Title : SW846 8260

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

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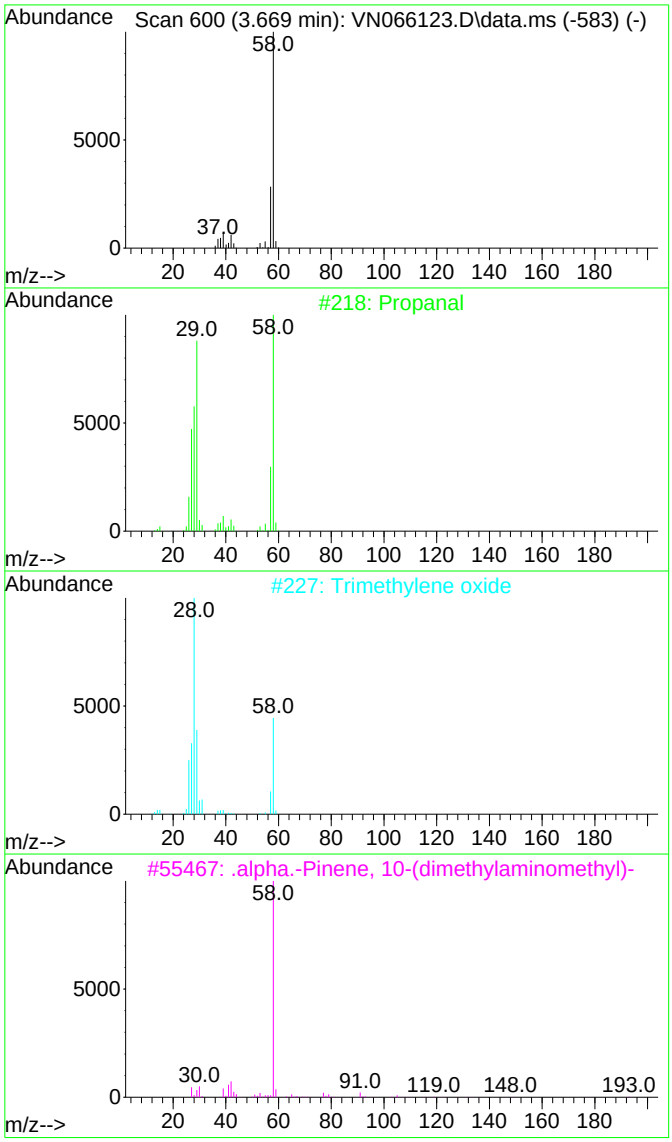
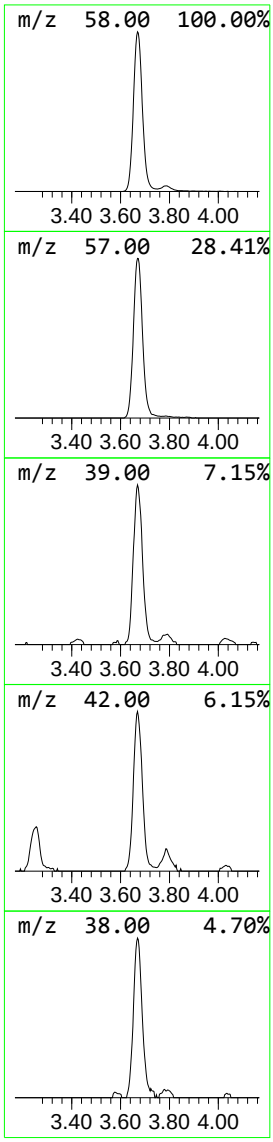
Peak Number 3 Propanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.669	223.08 ug/l	761411	Pentafluorobenzene	7.627

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal	58	C3H6O	000123-38-6	78
2	Trimethylene oxide	58	C3H6O	000503-30-0	9
3	.alpha.-Pinene, 10-(dimethylamin...	193	C13H23N	015063-97-5	9
4	Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7
5	Propylene oxide	58	C3H6O	000075-56-9	7





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Operator : JC/MD
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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP-41071-72

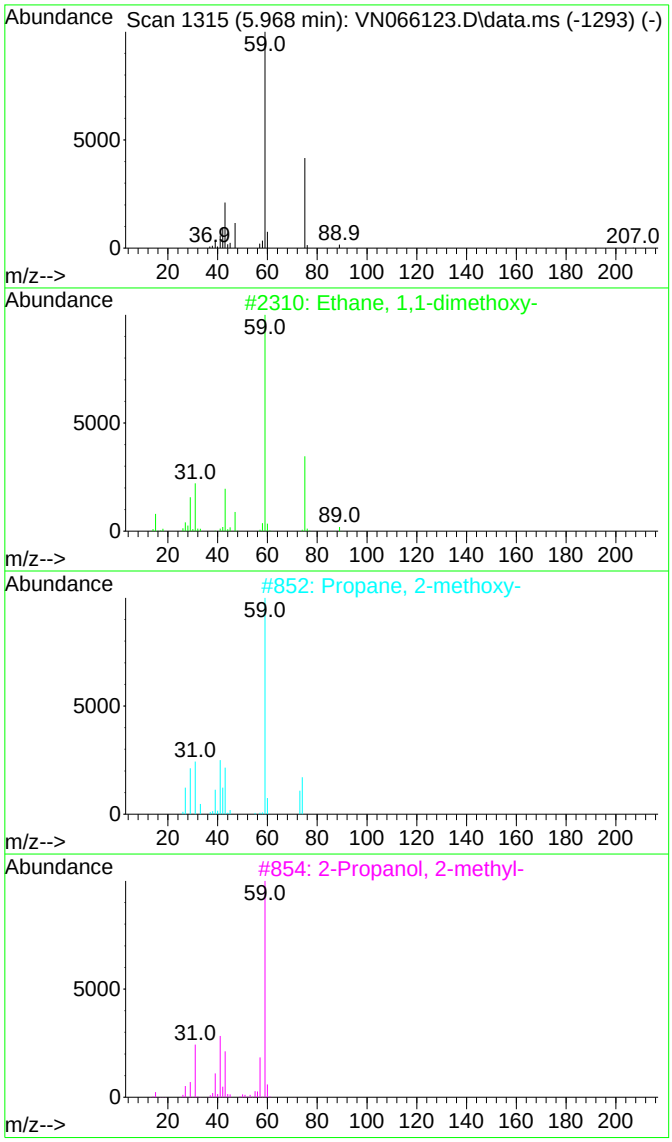
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030221W.M
Quant Title : SW846 8260

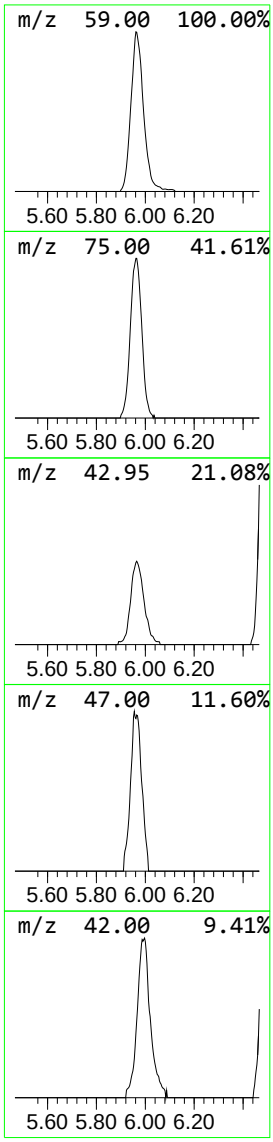
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.968	53.34 ug/l	182044	Pentafluorobenzene	7.627

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethane, 1,1-dimethoxy-	90	C4H10O2	000534-15-6	78
2	Propane, 2-methoxy-	74	C4H10O	000598-53-8	28
3	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	9
4	2-Hydroxy-2,4-dimethyl-3-pentanone	130	C7H14O2	003212-67-7	9
5	1,2-Butanediol	90	C4H10O2	000584-03-2	9





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ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP-41071-72

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030221W.M
Quant Title : SW846 8260

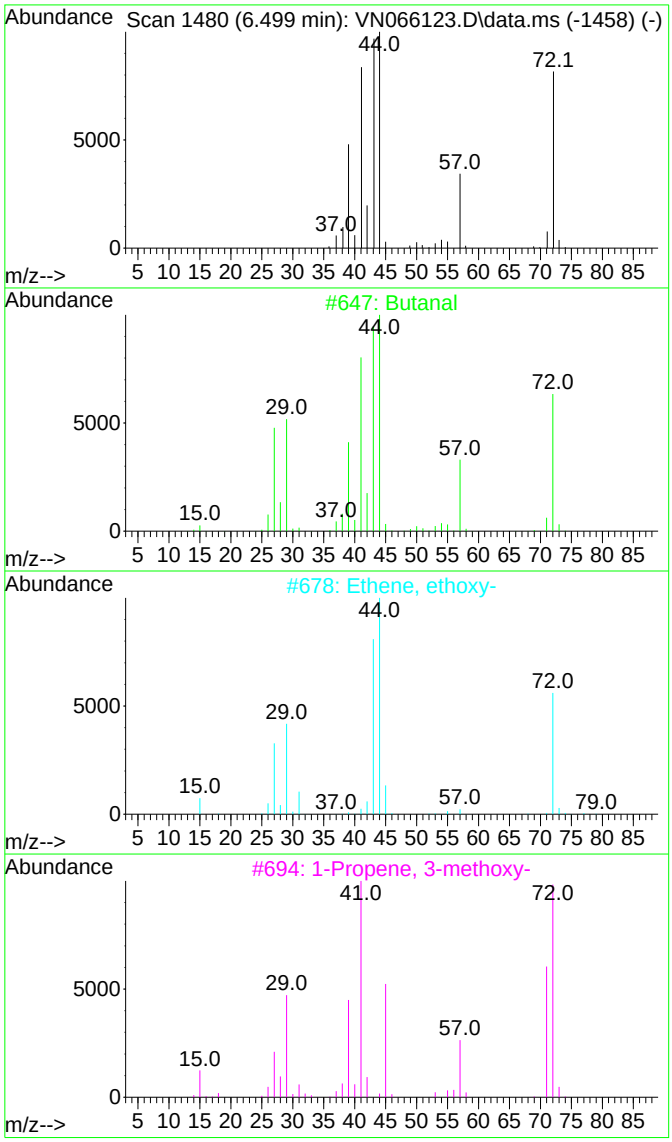
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

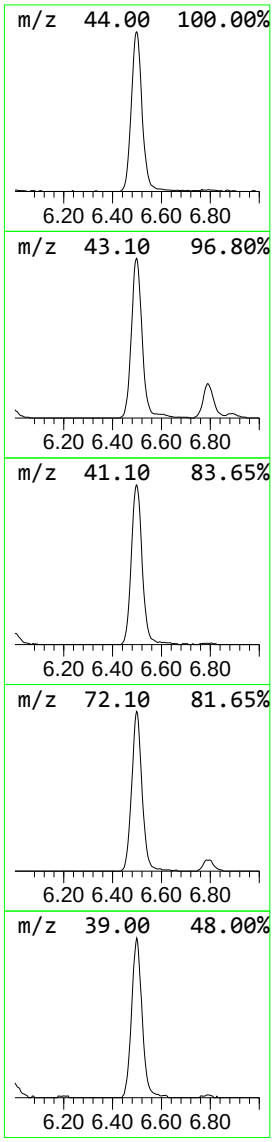
****

Peak Number 5 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.499	167.62 ug/l	572110	Pentafluorobenzene	7.627

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	50
3	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	43
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
5	Isobutylene epoxide	72	C4H8O	000558-30-5	27





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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP-41071-72

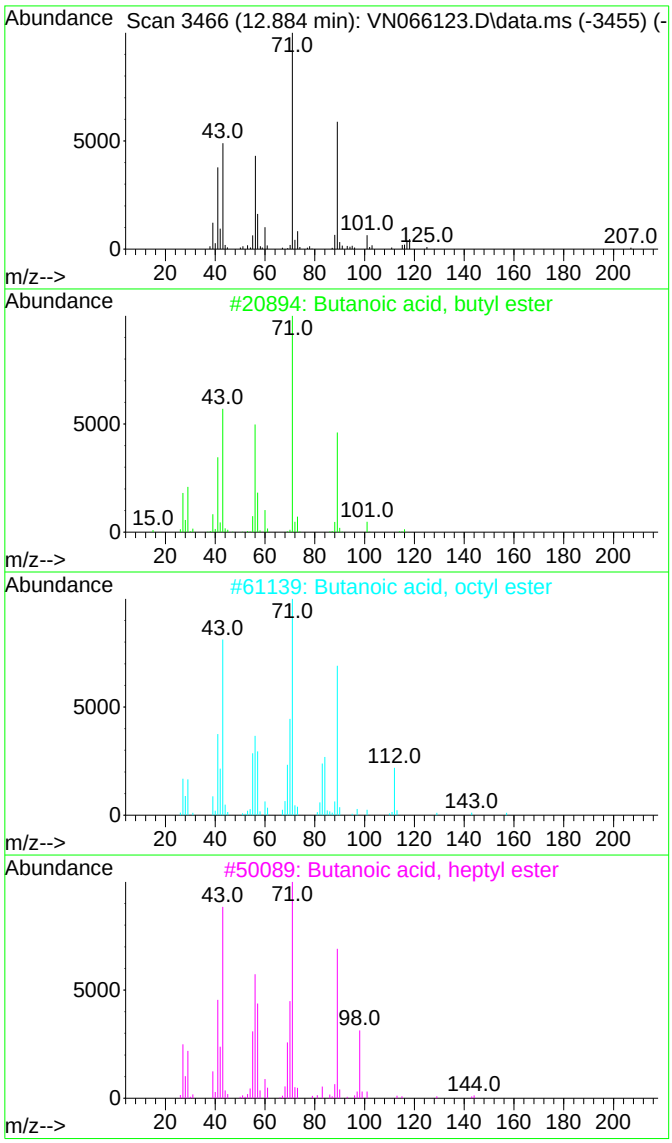
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030221W.M
Quant Title : SW846 8260

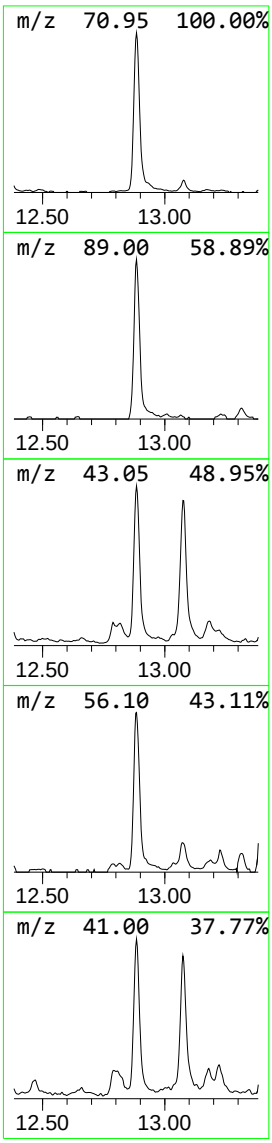
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Butanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.884	28.09 ug/l	180698	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2	Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	64
3	Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	64
4	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	59
5	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	59





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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP-41071-72

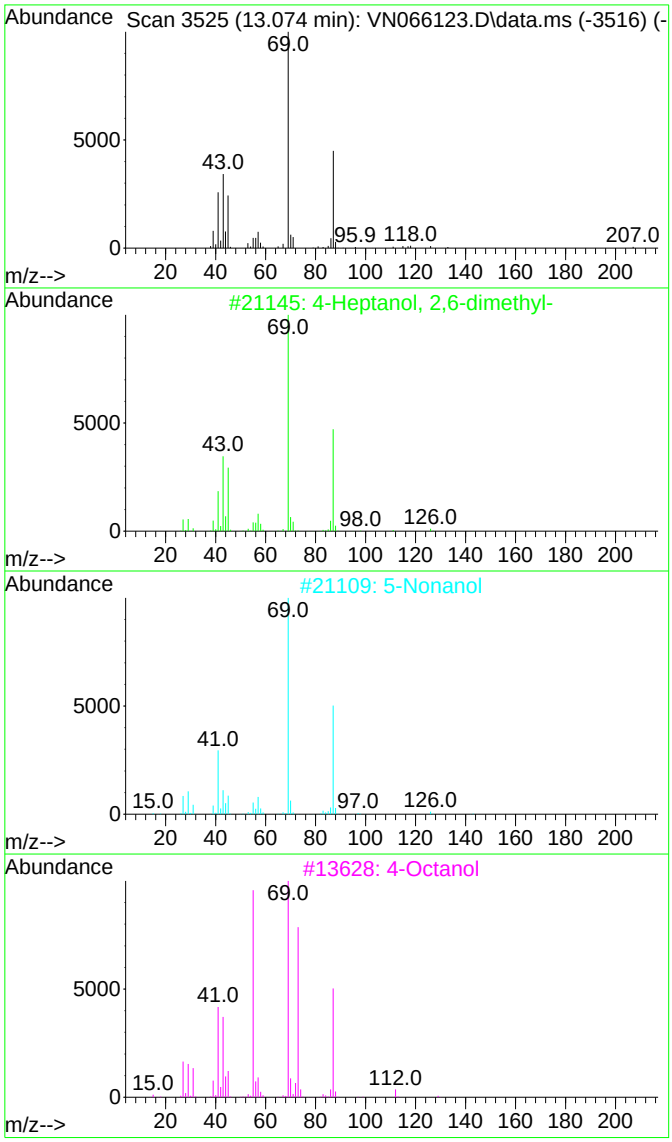
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030221W.M
Quant Title : SW846 8260

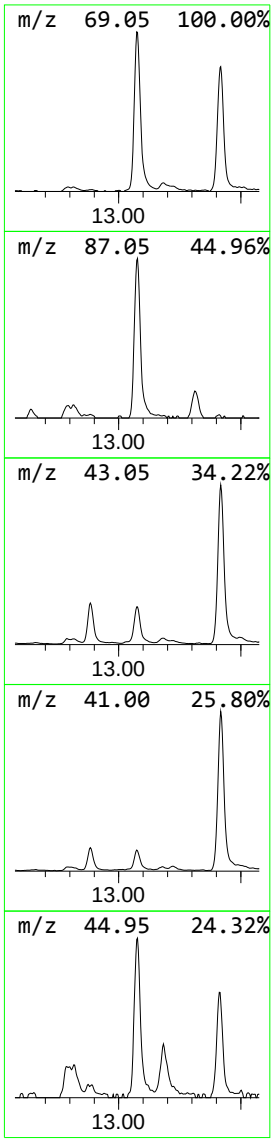
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 4-Heptanol, 2,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.074	29.50 ug/l	189788	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	90
2	5-Nonanol	144	C9H20O	000623-93-8	72
3	4-Octanol	130	C8H18O	000589-62-8	72
4	2-Butenoic acid, 2-methylpropyl ...	142	C8H14O2	073545-15-0	64
5	2-Propenoic acid, 2-methyl-, pro...	128	C7H12O2	002210-28-8	64





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Instrument :
MSVOA_N
ClientSampleId :
COMP-41071-72

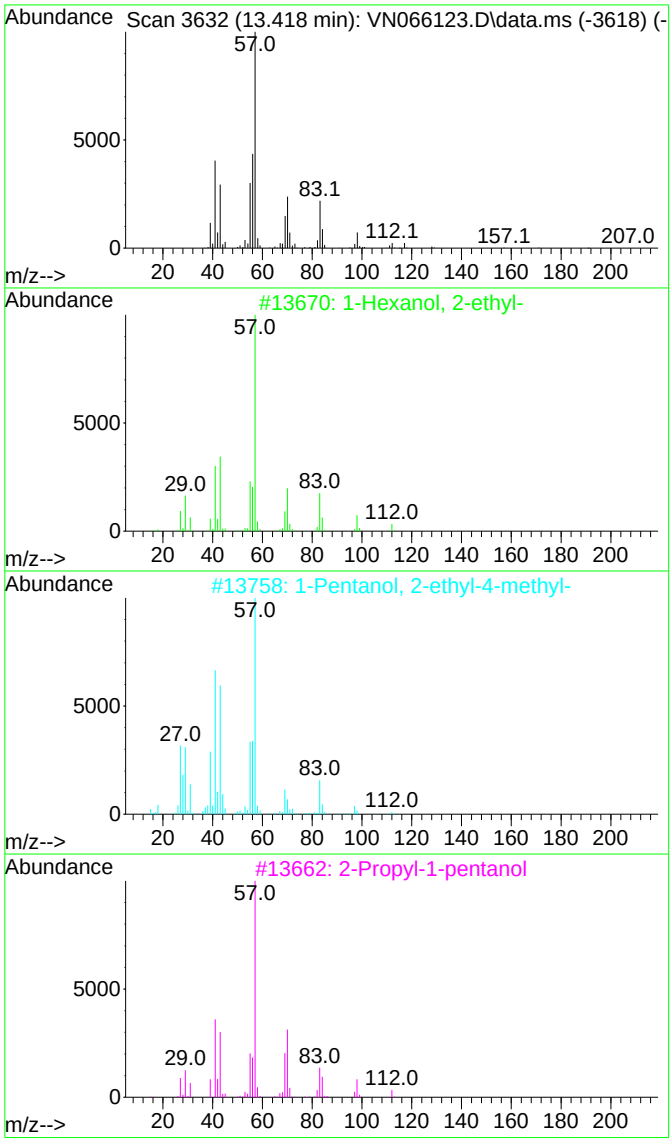
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030221W.M
Quant Title : SW846 8260

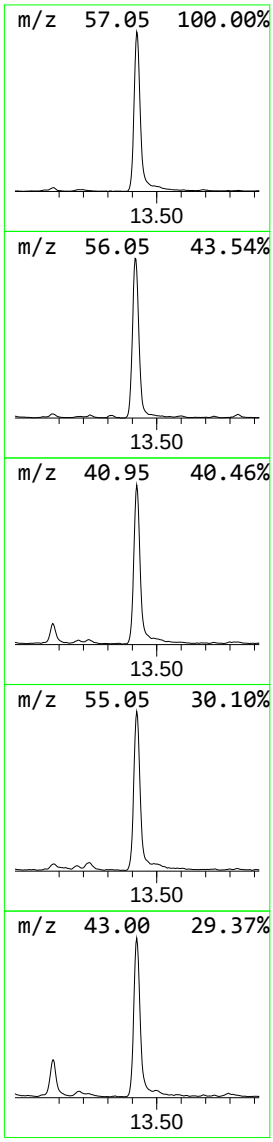
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.418	183.23 ug/l	1178830	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	49
5	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47





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MSVOA_N
ClientSampleId :
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Quant Title : SW846 8260

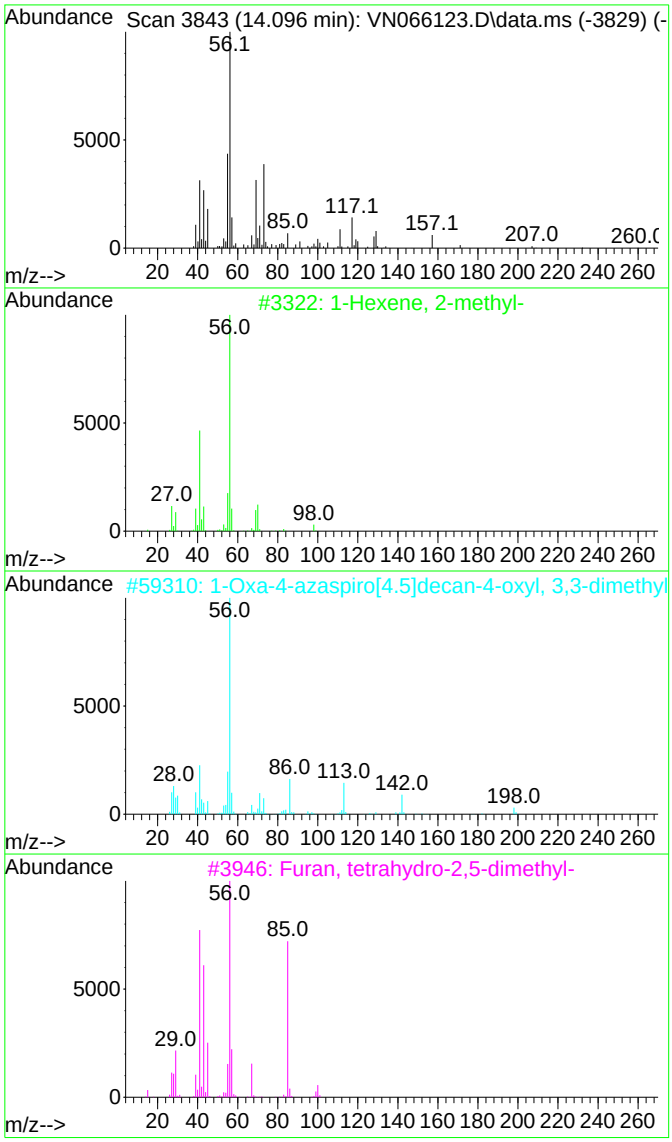
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

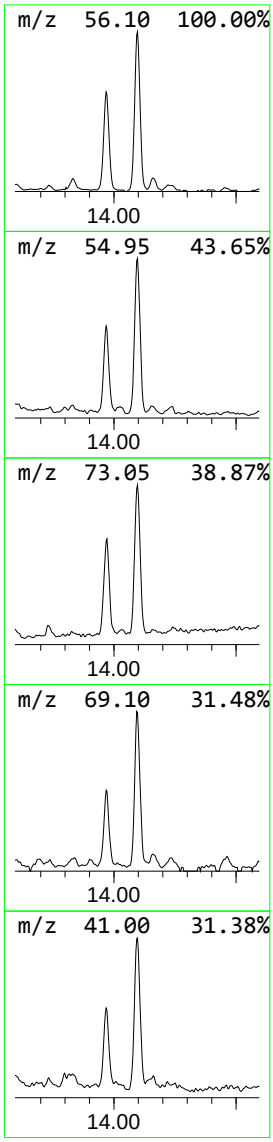
****

Peak Number 9 unknown14.096 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.096	26.70 ug/l	171801	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	47
2	1-Oxa-4-azaspiro[4.5]decan-4-oxy...	198	C10H16NO3	1000115-84-0	47
3	Furan, tetrahydro-2,5-dimethyl-	100	C6H12O	001003-38-9	47
4	Oxirane, (1-methylbutyl)-	114	C7H14O	053229-39-3	47
5	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	40





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	3.251	42.8	ug/l	146211	1	7.627	170659	50.0
Propanal	3.669	223.1	ug/l	761411	1	7.627	170659	50.0
Ethane, 1,1-dim...	5.968	53.3	ug/l	182044	1	7.627	170659	50.0
Butanal	6.499	167.6	ug/l	572110	1	7.627	170659	50.0
Butanoic acid, ...	12.884	28.1	ug/l	180698	4	13.315	321677	50.0
4-Heptanol, 2,6...	13.074	29.5	ug/l	189788	4	13.315	321677	50.0
1-Hexanol, 2-et...	13.418	183.2	ug/l	1178830	4	13.315	321677	50.0
unknown14.096	14.096	26.7	ug/l	171801	4	13.315	321677	50.0