LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011921\
Data File : VX020664.D
Acq On : 19 Jan 2021 17:17
Operator : JC/SP
Sample : M1125-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1693-94

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_X\METHOD\82X011921W.M
Title : SW846 8260

Signal : TIC: VX020664.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.471	59	63	69	rBV	115816	134309	2.11%	0.682%
2	2.111	158	168	197	rBV	1382952	3021843	47.45%	15.343%
3	2.325	197	203	213	rVV	313775	536345	8.42%	2.723%
4	2.416	213	218	229	rVB	64321	114626	1.80%	0.582%
5	3.959	452	471	485	rBV	1796577	6368825	100.00%	32.338%
6	5.464	706	718	733	rBV2	150891	435949	6.85%	2.214%
7	5.629	733	745	759	rVB	253283	715586	11.24%	3.633%
8	6.025	795	810	821	rBV	164193	435113	6.83%	2.209%
9	6.830	928	942	956	rBV	395698	940121	14.76%	4.773%
10	7.269	1006	1014	1031	rBV	156429	349871	5.49%	1.776%
11	8.696	1241	1248	1255	rBV	838299	1299228	20.40%	6.597%
12	10.092	1468	1477	1490	rBV	837646	1138187	17.87%	5.779%
13	11.122	1640	1646	1656	rVB	670918	867936	13.63%	4.407%
14	12.061	1794	1800	1807	rVB	934023	1140682	17.91%	5.792%
15	12.140	1807	1813	1822	rVB2	96280	130800	2.05%	0.664%
16	12.256	1826	1832	1846	rBV	701565	994851	15.62%	5.051%
17	13.548	2040	2044	2050	rVB	245593	321595	5.05%	1.633%
18	13.628	2051	2057	2064	rBV5	66990	127168	2.00%	0.646%
19	13.701	2064	2069	2077	rBV	372565	545922	8.57%	2.772%
20	14.676	2223	2229	2238	rVB	54404	75695	1.19%	0.384%

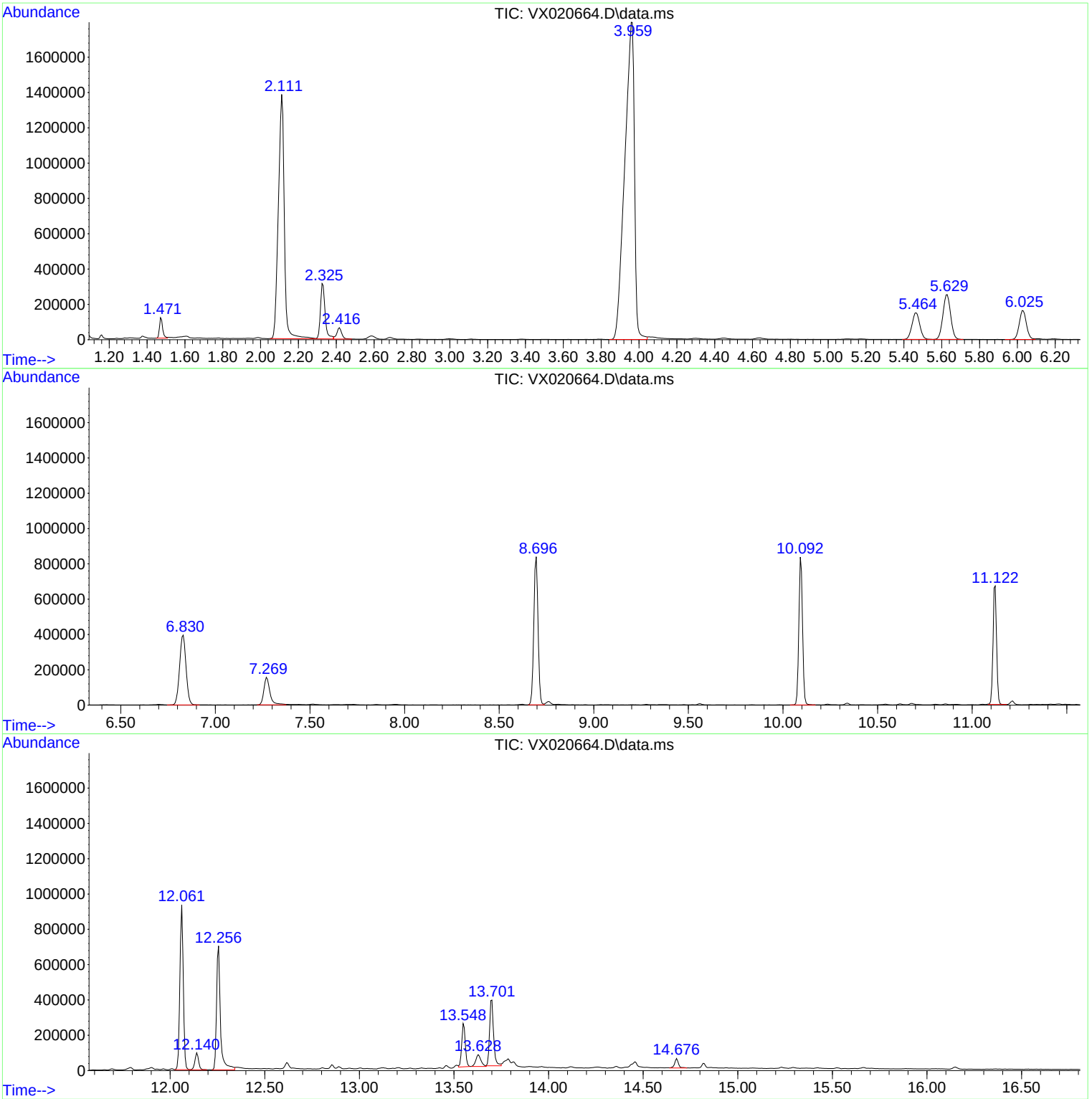
Sum of corrected areas: 19694652

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011921\
Data File : VX020664.D
Acq On : 19 Jan 2021 17:17
Operator : JC/SP
Sample : M1125-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1693-94

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011921W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011921\
Data File : VX020664.D
Acq On : 19 Jan 2021 17:17
Operator : JC/SP
Sample : M1125-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1693-94

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011921W.M
Quant Title : SW846 8260

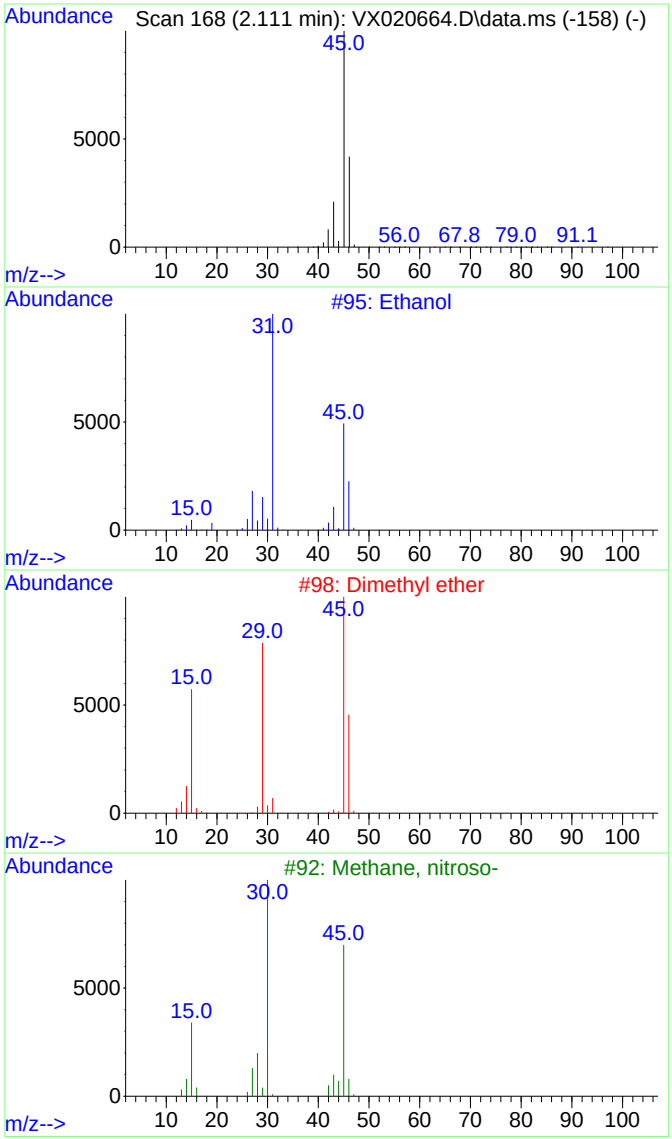
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

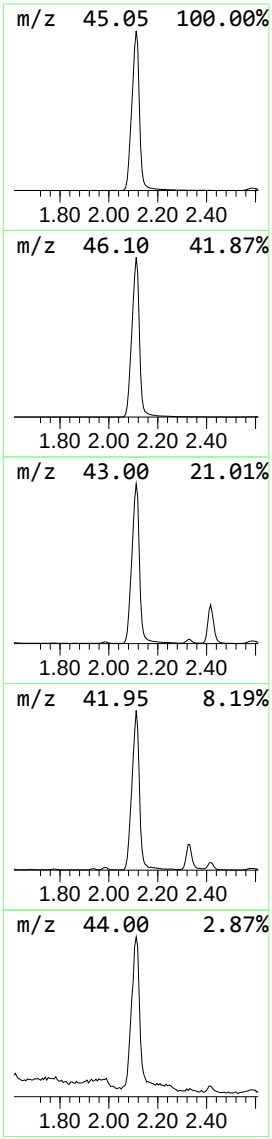
****

Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.111	211.15 ug/l	3021840	Pentafluorobenzene	5.629

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	Oxalic acid	90	C2H2O4	000144-62-7	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011921\
Data File : VX020664.D
Acq On : 19 Jan 2021 17:17
Operator : JC/SP
Sample : M1125-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1693-94

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011921W.M
Quant Title : SW846 8260

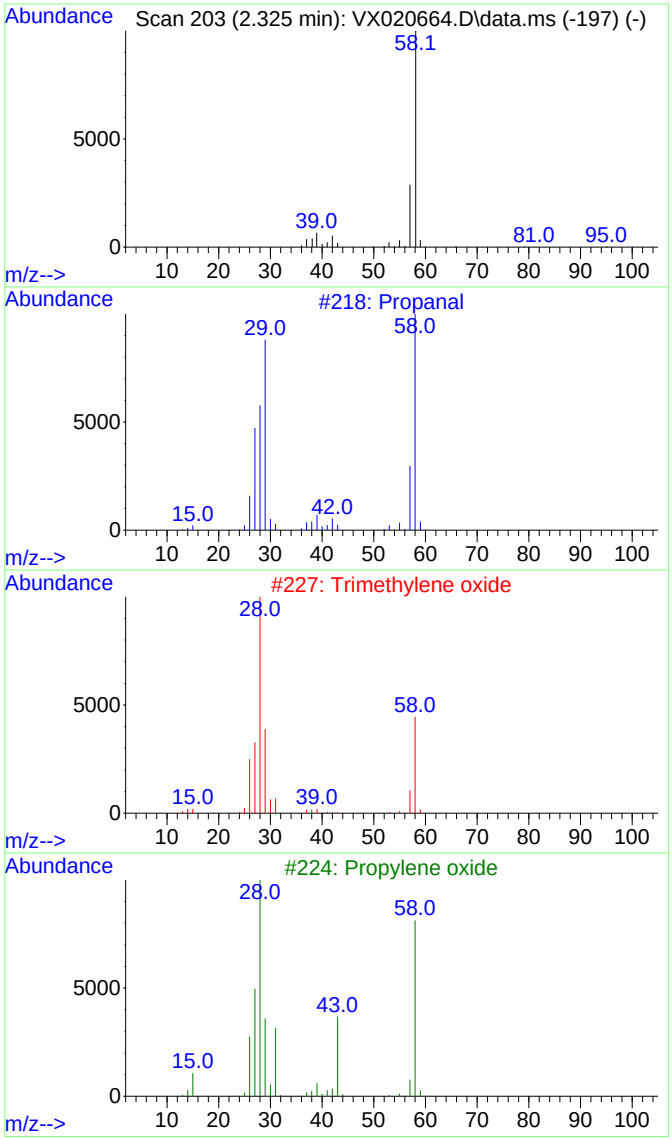
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

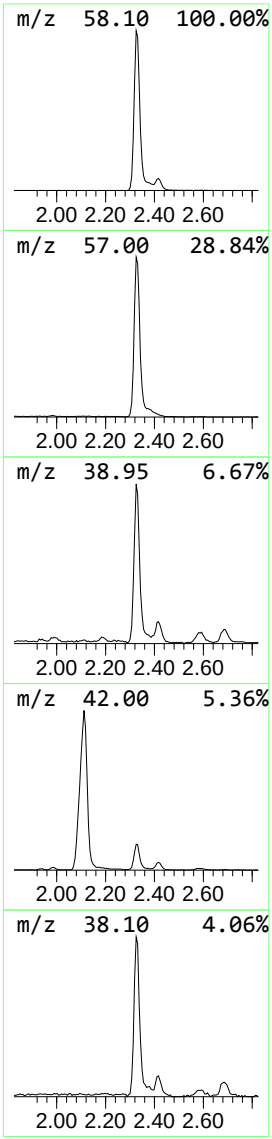
****

Peak Number 3 Propanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.325	37.48 ug/l	536345	Pentafluorobenzene	5.629

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	Propylene oxide	58	C3H6O	000075-56-9	7
4	Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	5
5	.alpha.-Pinene, 10-(dimethylamin...	193	C13H23N	015063-97-5	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011921\
Data File : VX020664.D
Acq On : 19 Jan 2021 17:17
Operator : JC/SP
Sample : M1125-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1693-94

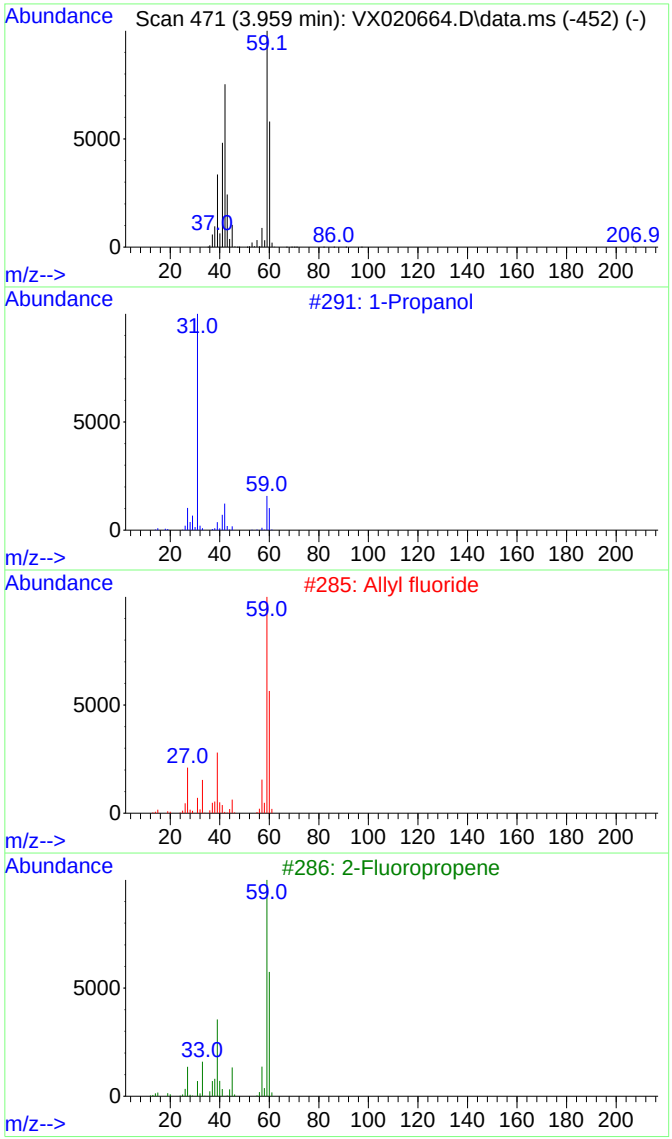
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011921W.M
Quant Title : SW846 8260

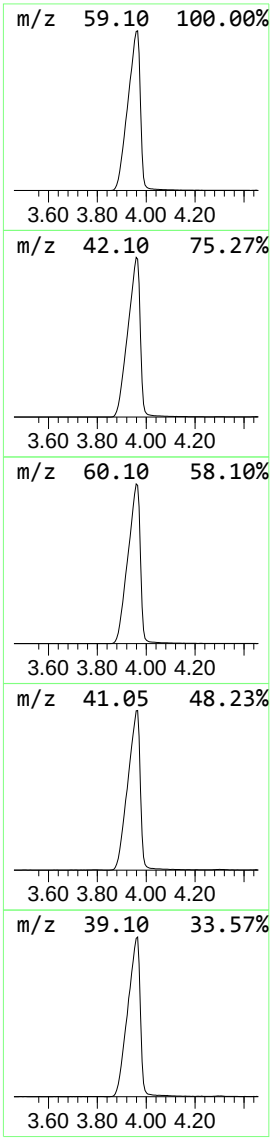
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.959	445.01 ug/l	6368830	Pentafluorobenzene	5.629

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	78
2	Allyl fluoride	60	C3H5F	000818-92-8	38
3	2-Fluoropropene	60	C3H5F	001184-60-7	37
4	Methanamine, N-hydroxy-N-methyl-	61	C2H7NO	005725-96-2	25
5	Acetaldoxime	59	C2H5NO	000107-29-9	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011921\
Data File : VX020664.D
Acq On : 19 Jan 2021 17:17
Operator : JC/SP
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1693-94

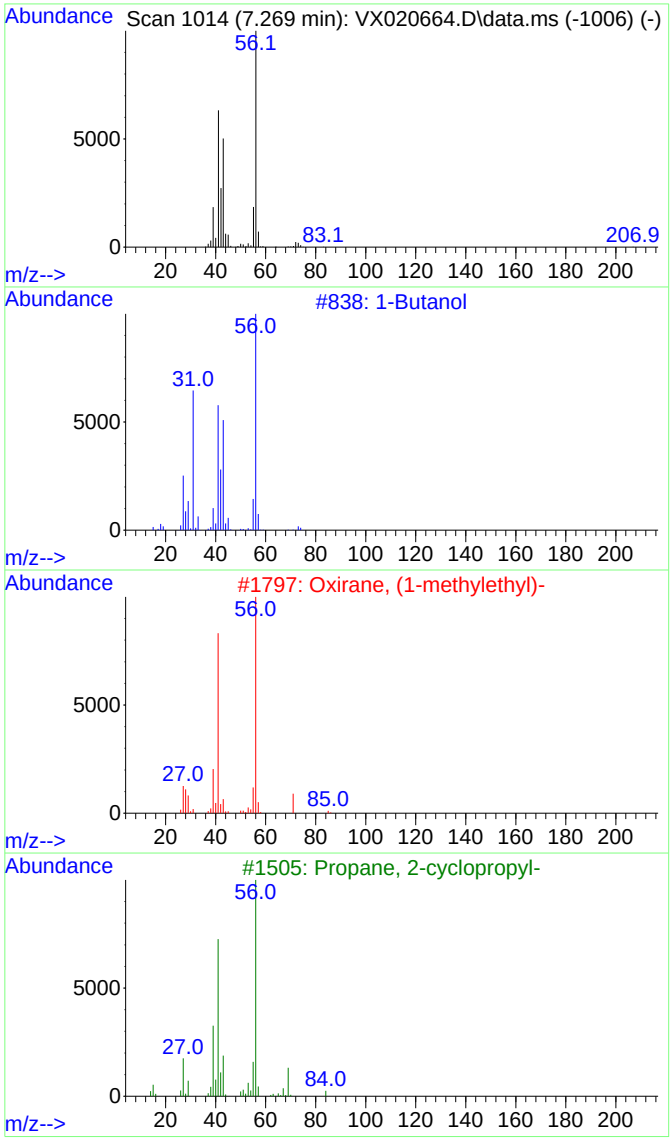
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011921W.M
Quant Title : SW846 8260

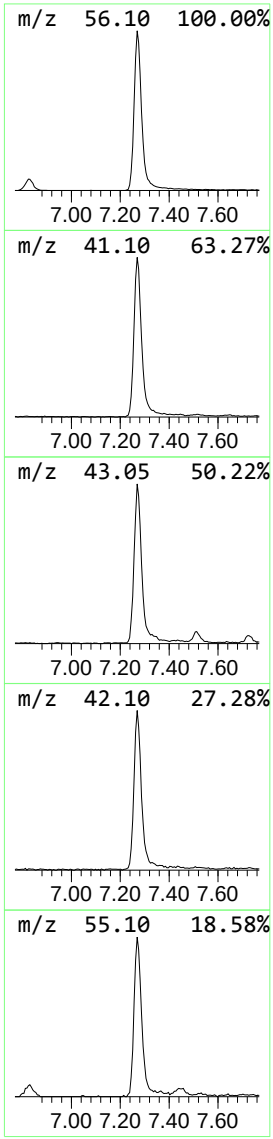
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Butanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.269	18.61 ug/l	349871	1,4-Difluorobenzene	6.830

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	90
2	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	33
3	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	9
4	Formic acid, butyl ester	102	C5H10O2	000592-84-7	9
5	Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011921\
Data File : VX020664.D
Acq On : 19 Jan 2021 17:17
Operator : JC/SP
Sample : M1125-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1693-94

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011921W.M
Quant Title : SW846 8260

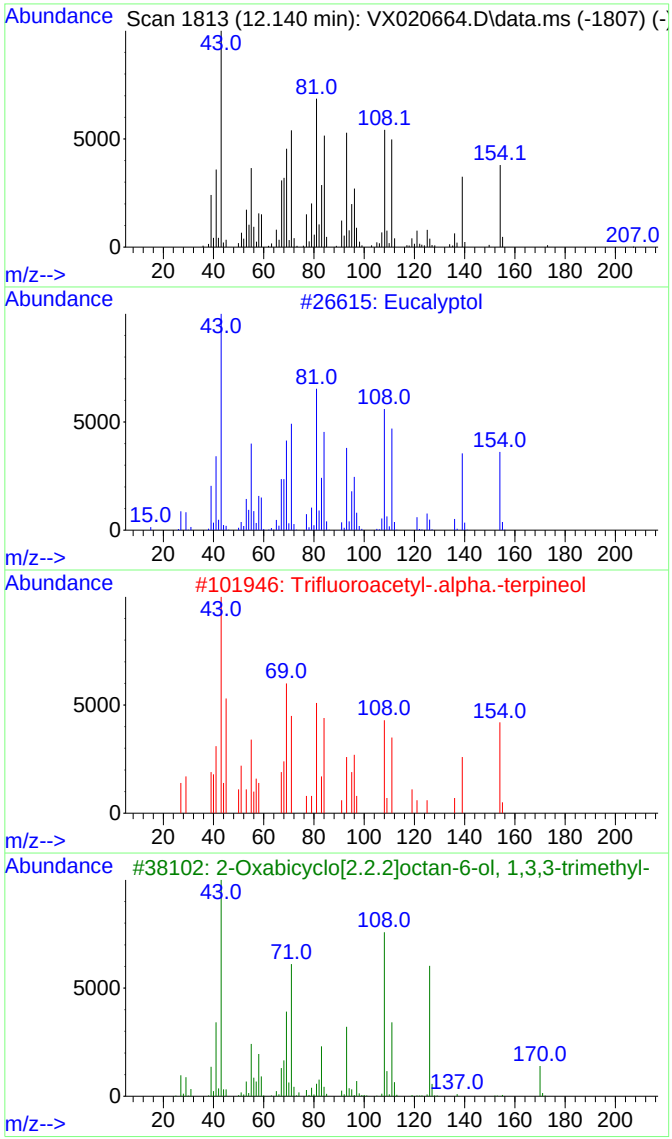
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

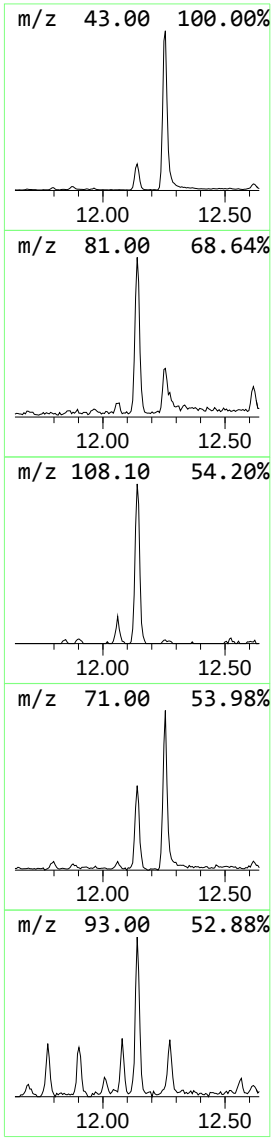
****

Peak Number 6 Eucalyptol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.140	5.73 ug/l	130800	1,4-Dichlorobenzene-d4	12.061

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eucalyptol	154	C10H18O	000470-82-6	98
2	Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	74
3	2-Oxabicyclo[2.2.2]octan-6-ol, 1...	170	C10H18O2	018679-48-6	27
4	trans-Cyclohexane-1,4-dimethanol...	228	C12H20O4	010412-78-9	22
5	1-Methyl-3-(1'-methylcyclopropyl...	136	C10H16	103240-53-5	15





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011921\
Data File : VX020664.D
Acq On : 19 Jan 2021 17:17
Operator : JC/SP
Sample : M1125-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1693-94

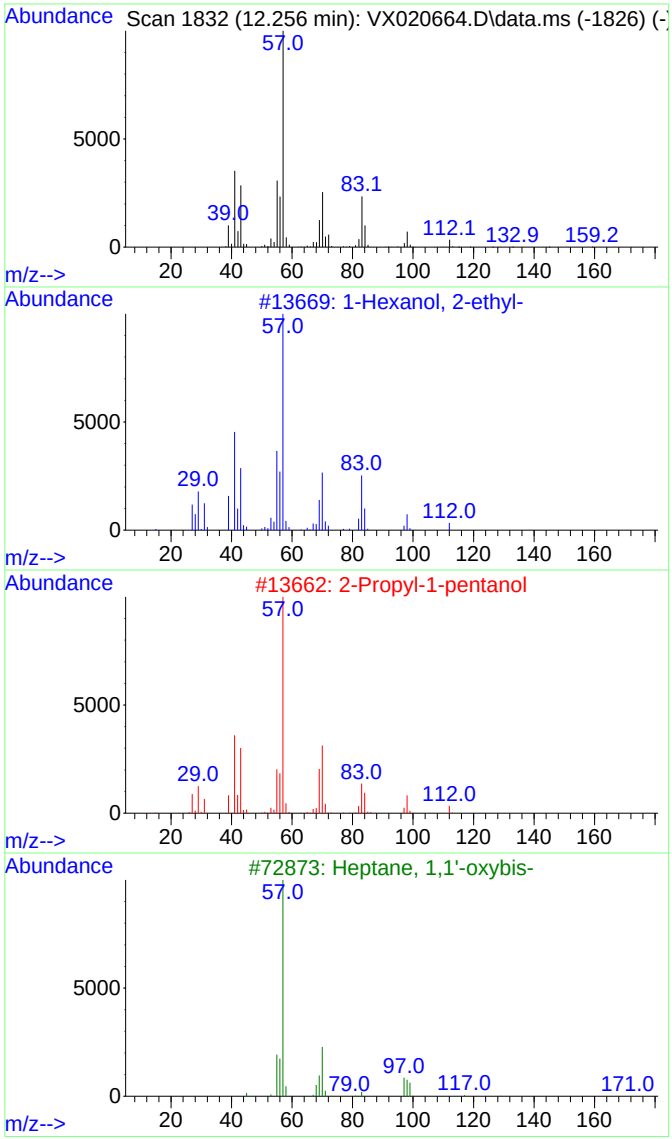
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011921W.M
Quant Title : SW846 8260

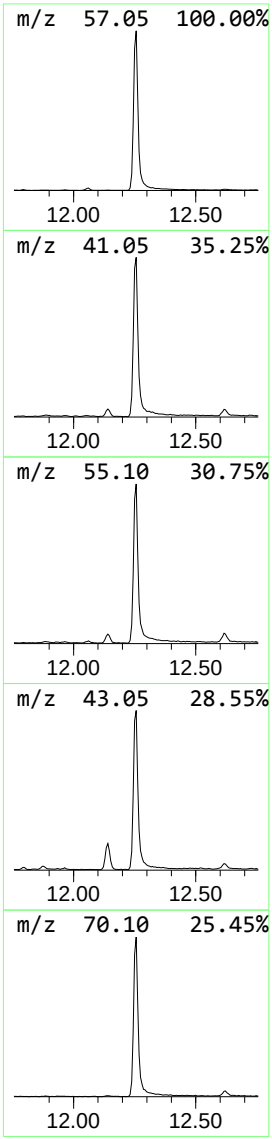
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.256	43.61 ug/l	994851	1,4-Dichlorobenzene-d4	12.061

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
4	Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	45
5	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011921\
Data File : VX020664.D
Acq On : 19 Jan 2021 17:17
Operator : JC/SP
Sample : M1125-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1693-94

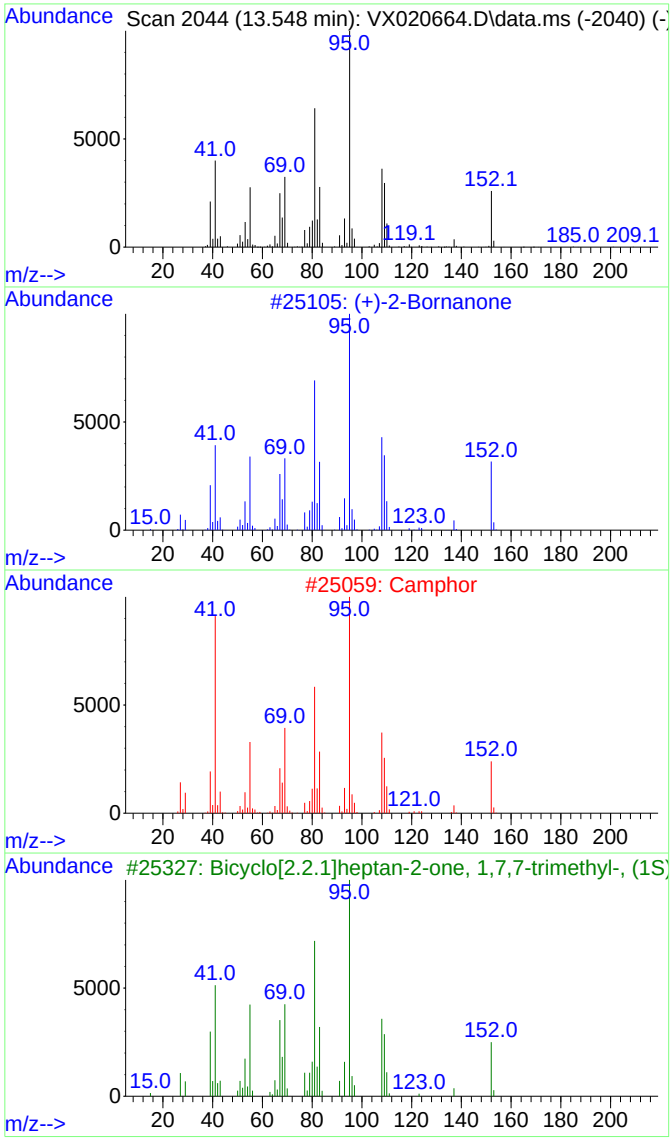
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011921W.M
Quant Title : SW846 8260

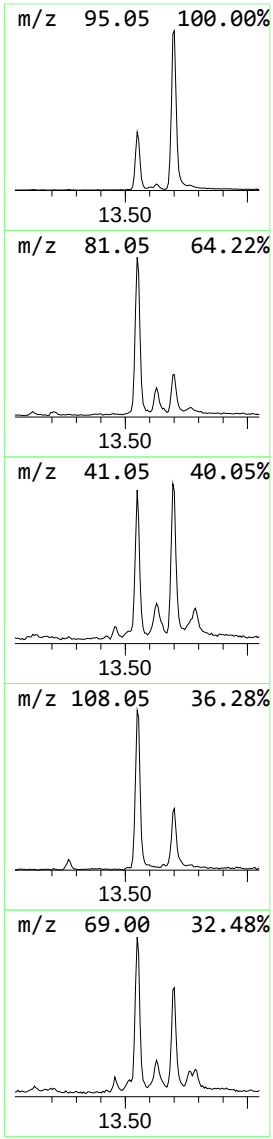
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 (+)-2-Bornanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.548	14.10 ug/l	321595	1,4-Dichlorobenzene-d4	12.061

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-2-Bornanone	152	C10H16O	000464-49-3	98
2	Camphor	152	C10H16O	000076-22-2	98
3	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	98
4	5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	58
5	2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	46





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Operator : JC/SP
Sample : M1125-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1693-94

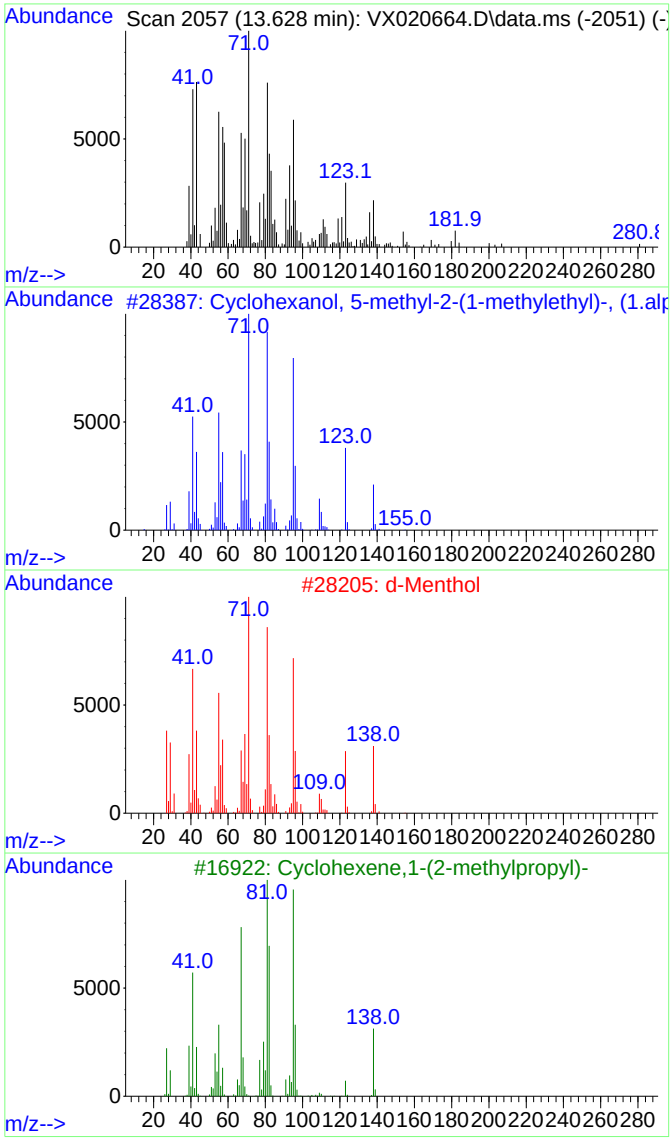
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011921W.M
Quant Title : SW846 8260

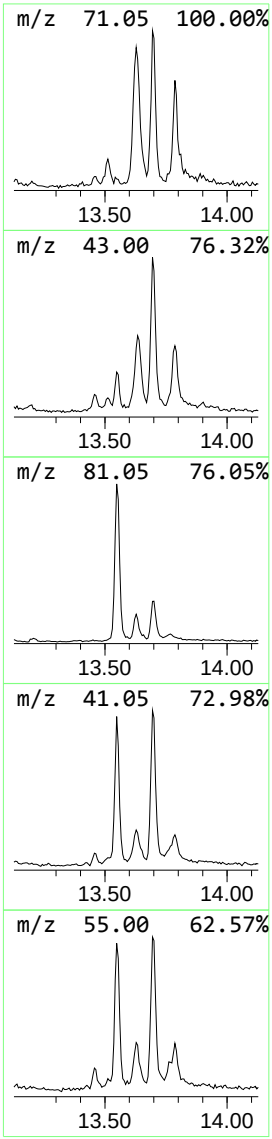
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Cyclohexanol, 5-methyl-2-(1... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.628	5.57 ug/l	127168	1,4-Dichlorobenzene-d4	12.061

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	015356-70-4	74
2	d-Menthol	156	C10H20O	015356-60-2	64
3	Cyclohexene,1-(2-methylpropyl)-	138	C10H18	003983-03-7	60
4	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	000491-02-1	49
5	L-Menthyl chloroformate	218	C11H19ClO2	014602-86-9	46





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

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MSVOA_X
ClientSampleId :
1693-94

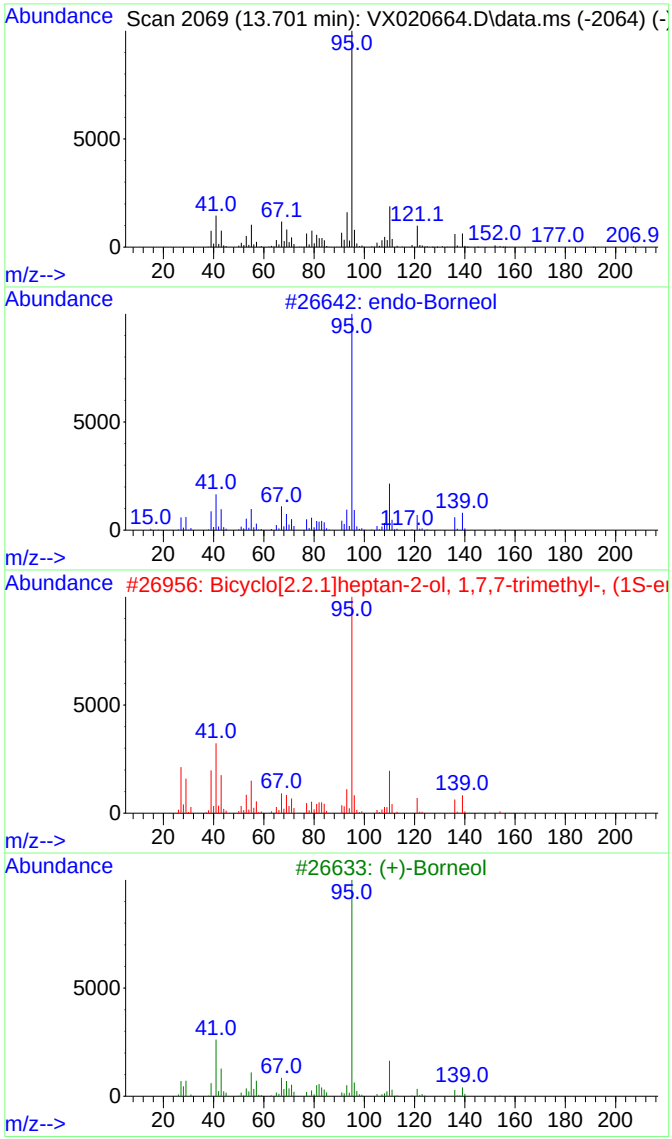
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011921W.M
Quant Title : SW846 8260

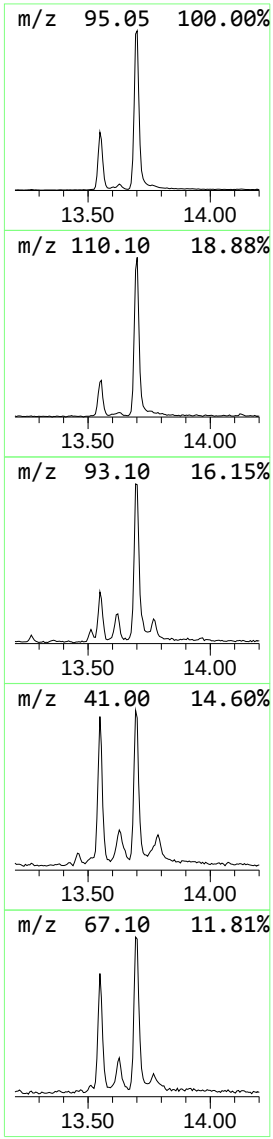
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 endo-Borneol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.701	23.93 ug/l	545922	1,4-Dichlorobenzene-d4	12.061

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	endo-Borneol	154	C10H18O	000507-70-0	93
2	Bicyclo[2.2.1]heptan-2-ol, 1,7,7...	154	C10H18O	000464-45-9	91
3	(+)-Borneol	154	C10H18O	1000150-76-3	80
4	Isoborneol	154	C10H18O	000124-76-5	64
5	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	64





Tentatively Identified Compound (LSC) summary

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Data File : VX020664.D
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Operator : JC/SP
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1693-94

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011921W.M
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	2.111	211.2	ug/l	3021840	1	5.629	715586	50.0
Propanal	2.325	37.5	ug/l	536345	1	5.629	715586	50.0
1-Propanol	3.959	445.0	ug/l	6368830	1	5.629	715586	50.0
1-Butanol	7.269	18.6	ug/l	349871	2	6.830	940121	50.0
Eucalyptol	12.140	5.7	ug/l	130800	4	12.061	1140680	50.0
1-Hexanol, 2-et...	12.256	43.6	ug/l	994851	4	12.061	1140680	50.0
(+)-2-Bornanone	13.548	14.1	ug/l	321595	4	12.061	1140680	50.0
Cyclohexanol, 5...	13.628	5.6	ug/l	127168	4	12.061	1140680	50.0
endo-Borneol	13.701	23.9	ug/l	545922	4	12.061	1140680	50.0