LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX041219\
Data File : VX008914.D
Acq On : 13 Apr 2019 02:48
Operator : JC/SP
Sample : K2381-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CL-COMP-1

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\82X040319W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.483	50	54	71	rBV	5320228	6561582	100.00%	42.756%
2	2.123	154	159	170	rBV	92224	147650	2.25%	0.962%
3	2.446	205	212	225	rBV	104133	183203	2.79%	1.194%
4	2.611	233	239	249	rVB	44268	82564	1.26%	0.538%
5	2.776	258	266	275	rBV	92612	169363	2.58%	1.104%
6	4.336	512	522	535	rBV	107271	299098	4.56%	1.949%
7	5.501	702	713	725	rBV	107411	305870	4.66%	1.993%
8	5.659	728	739	753	rVB	197126	566274	8.63%	3.690%
9	6.062	795	805	814	rBV	139416	364504	5.56%	2.375%
10	6.860	926	936	950	rBV	322914	758607	11.56%	4.943%
11	7.299	998	1008	1027	rBV	101775	225017	3.43%	1.466%
12	8.714	1233	1240	1247	rBV	694179	1058154	16.13%	6.895%
13	9.293	1331	1335	1345	rBV	51794	80512	1.23%	0.525%
14	10.110	1462	1469	1479	rBV	628576	869601	13.25%	5.666%
15	10.207	1479	1485	1490	rBV	84505	120143	1.83%	0.783%
16	10.805	1578	1583	1592	rBV	109911	150504	2.29%	0.981%
17	11.134	1632	1637	1642	rBV	499241	645637	9.84%	4.207%
18	11.737	1731	1736	1744	rVB	204898	233639	3.56%	1.522%
19	11.920	1762	1766	1774	rVB	141526	183205	2.79%	1.194%
20	12.036	1778	1785	1788	rBV4	46065	87382	1.33%	0.569%
21	12.079	1788	1792	1799	rVB	592793	744144	11.34%	4.849%
22	12.268	1815	1823	1834	rBV	1128896	1433468	21.85%	9.341%
23	12.359	1834	1838	1850	rVB3	39382	76617	1.17%	0.499%

Sum of corrected areas: 15346738

LSC Report - Integrated Chromatogram

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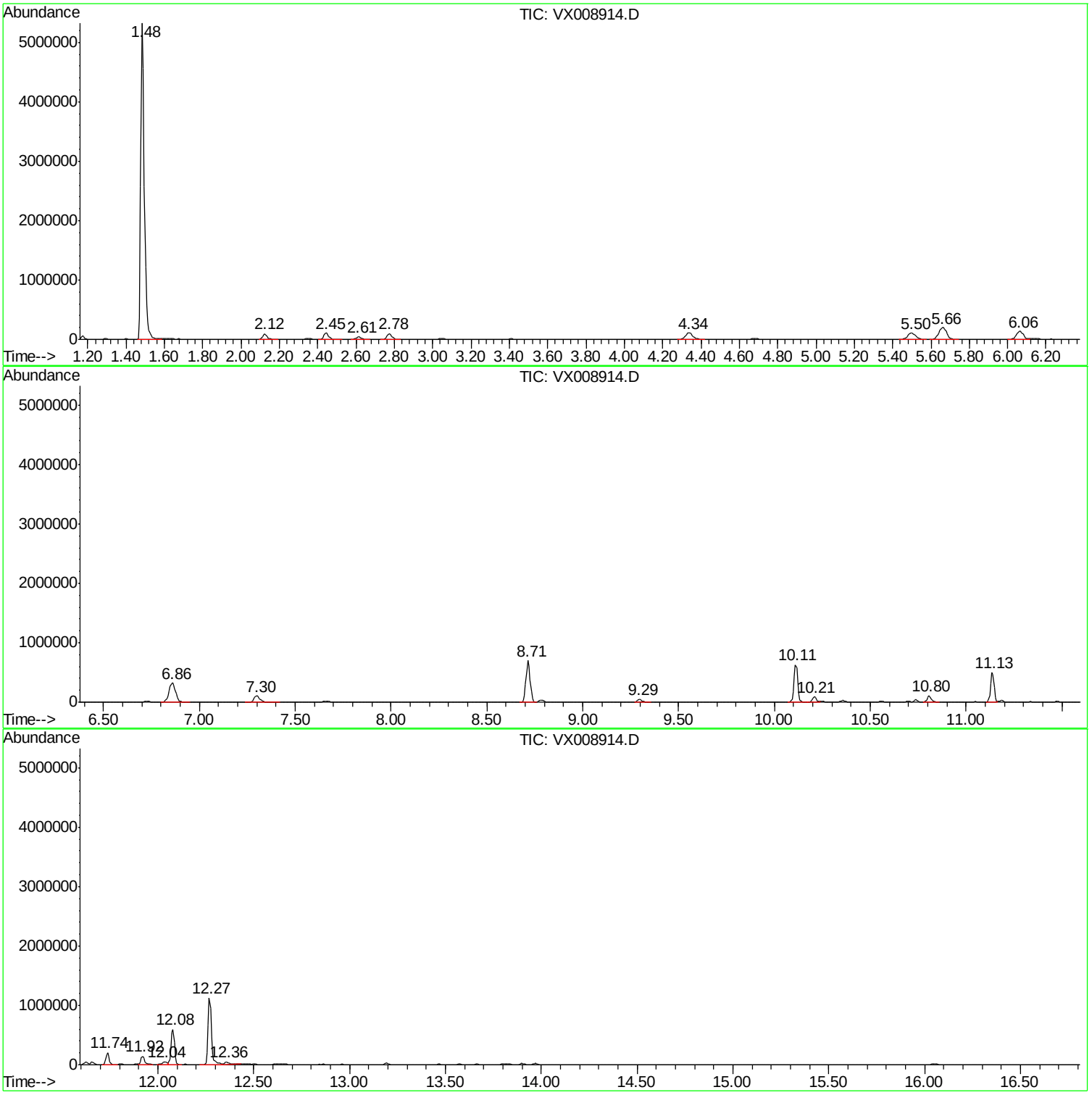
Data File : VX008914.D
Acq On : 13 Apr 2019 02:48
Operator : JC/SP
Sample : K2381-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CL-COMP-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X040319W.M
Quant Title : SW846 8260

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



Library Search Compound Report

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Data File : VX008914.D
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Sample : K2381-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CL-COMP-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X040319W.M
Quant Title : SW846 8260

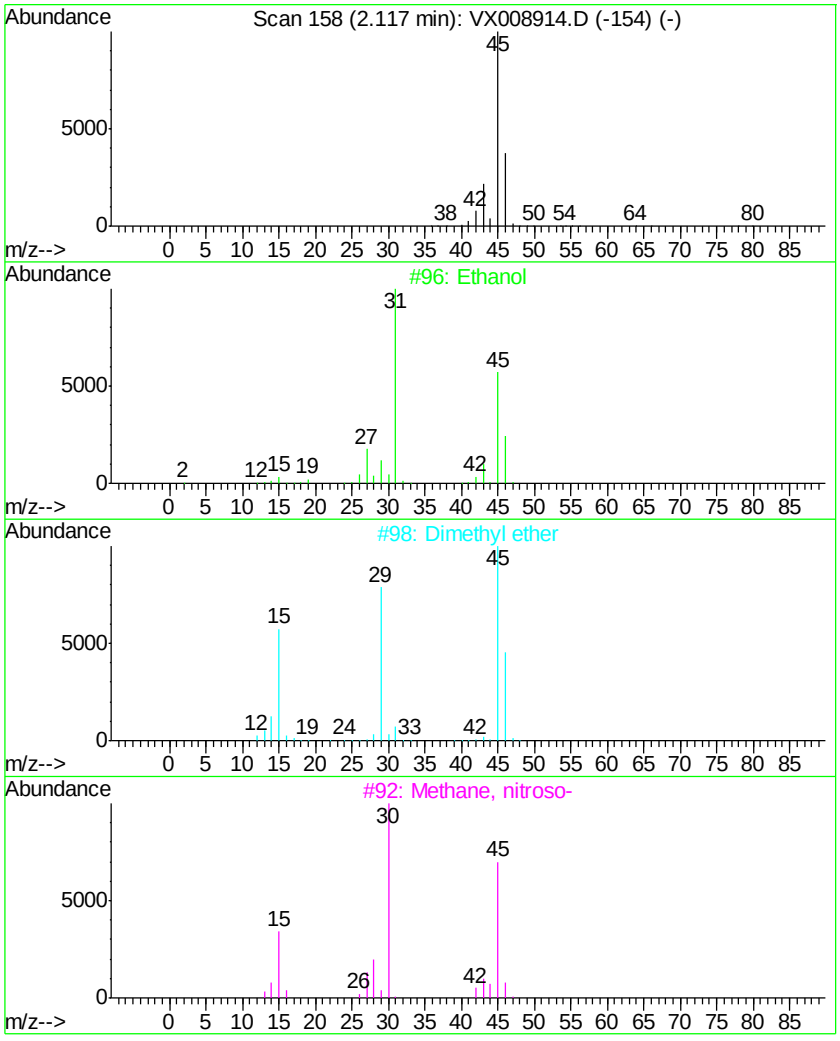
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

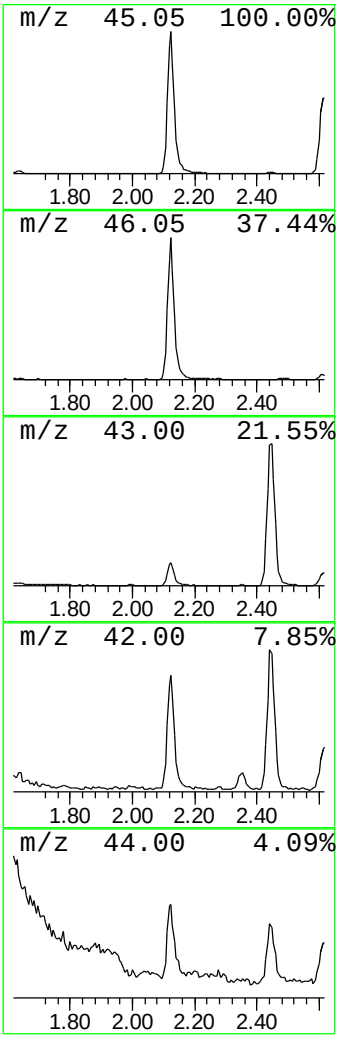
****

Peak Number 2 Ethanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	13.04 ug/l	147650	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	64
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





Library Search Compound Report

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Data File : VX008914.D
Acq On : 13 Apr 2019 02:48
Operator : JC/SP
Sample : K2381-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CL-COMP-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X040319W.M
Quant Title : SW846 8260

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

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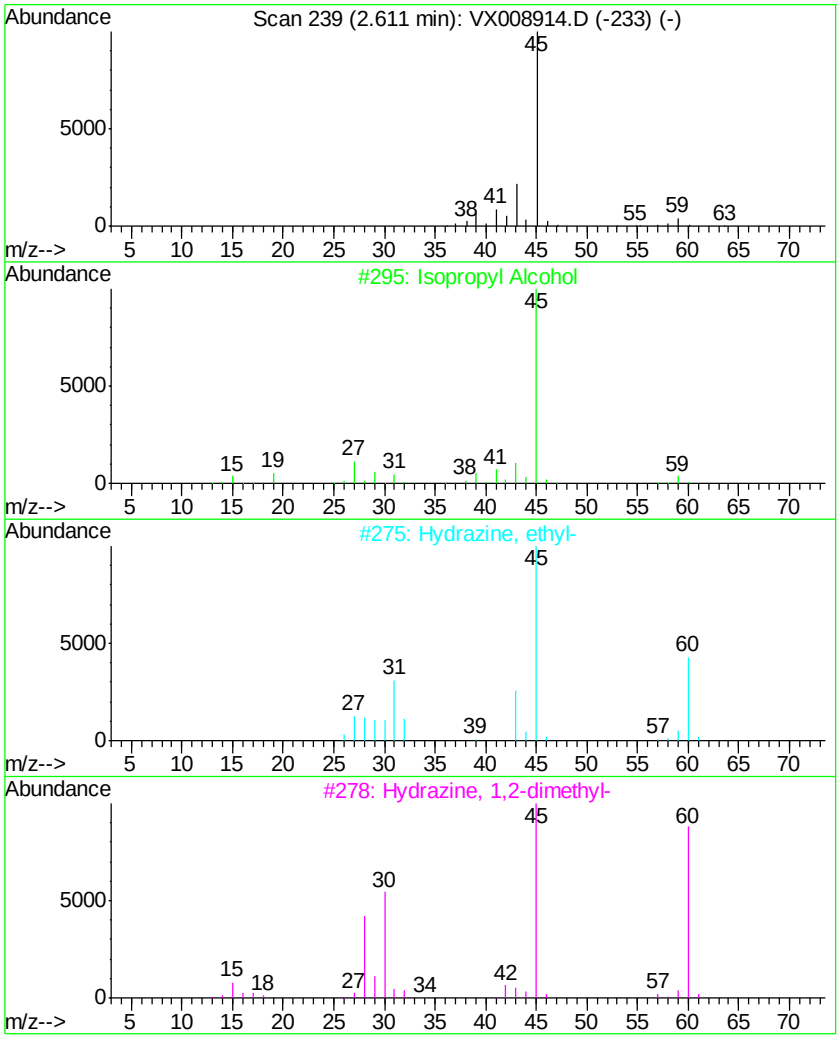
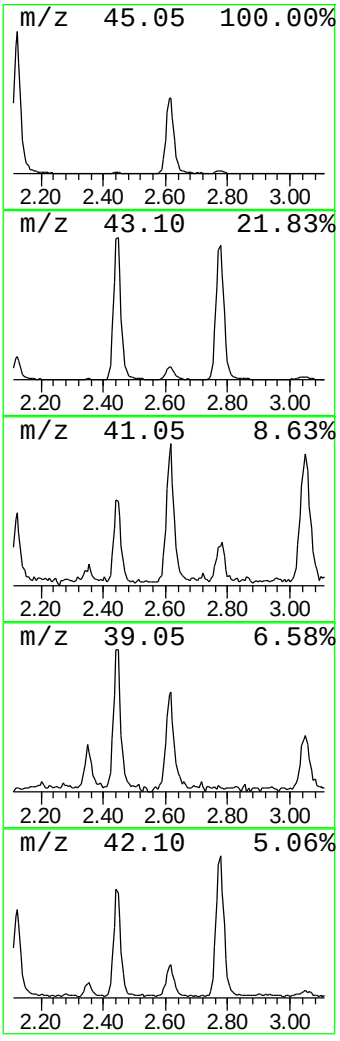
Peak Number 3 Isopropyl Alcohol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.61	7.29 ug/l	82564	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	86
2	Hydrazine, ethyl-	60	C2H8N2	000624-80-6	40
3	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4	4-Penten-2-ol	86	C5H10O	000625-31-0	9
5	Formamide	45	CH3NO	000075-12-7	5





Library Search Compound Report

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Data File : VX008914.D
Acq On : 13 Apr 2019 02:48
Operator : JC/SP
Sample : K2381-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CL-COMP-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X040319W.M
Quant Title : SW846 8260

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

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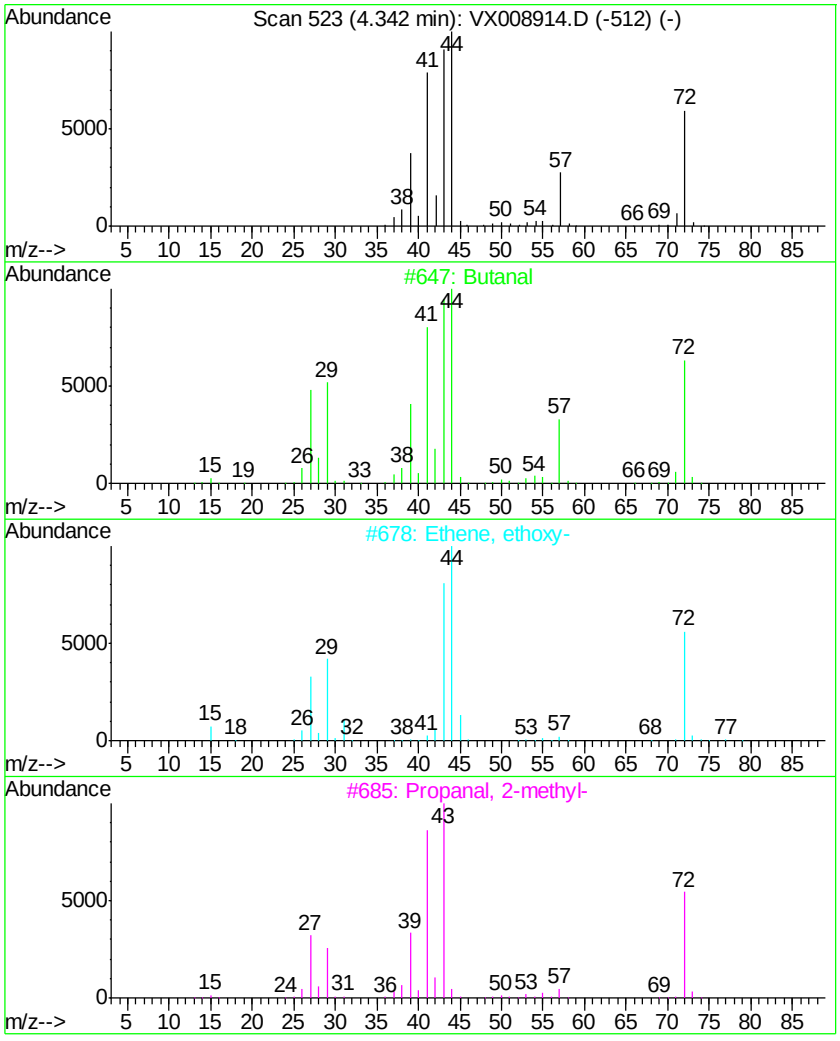
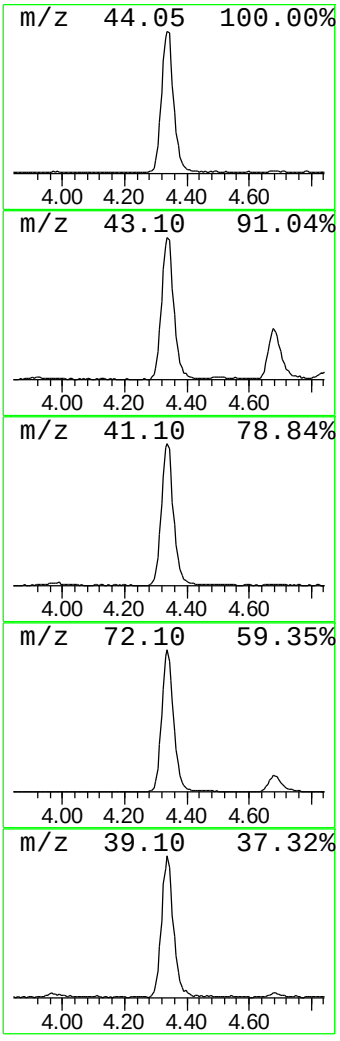
Peak Number 4 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.34	26.41 ug/l	299098	Pentafluorobenzene	5.67

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	52
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	52
4	Cyclopropyl carbinol	72	C4H8O	002516-33-8	17
5	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	17





Library Search Compound Report

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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CL-COMP-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X040319W.M
Quant Title : SW846 8260

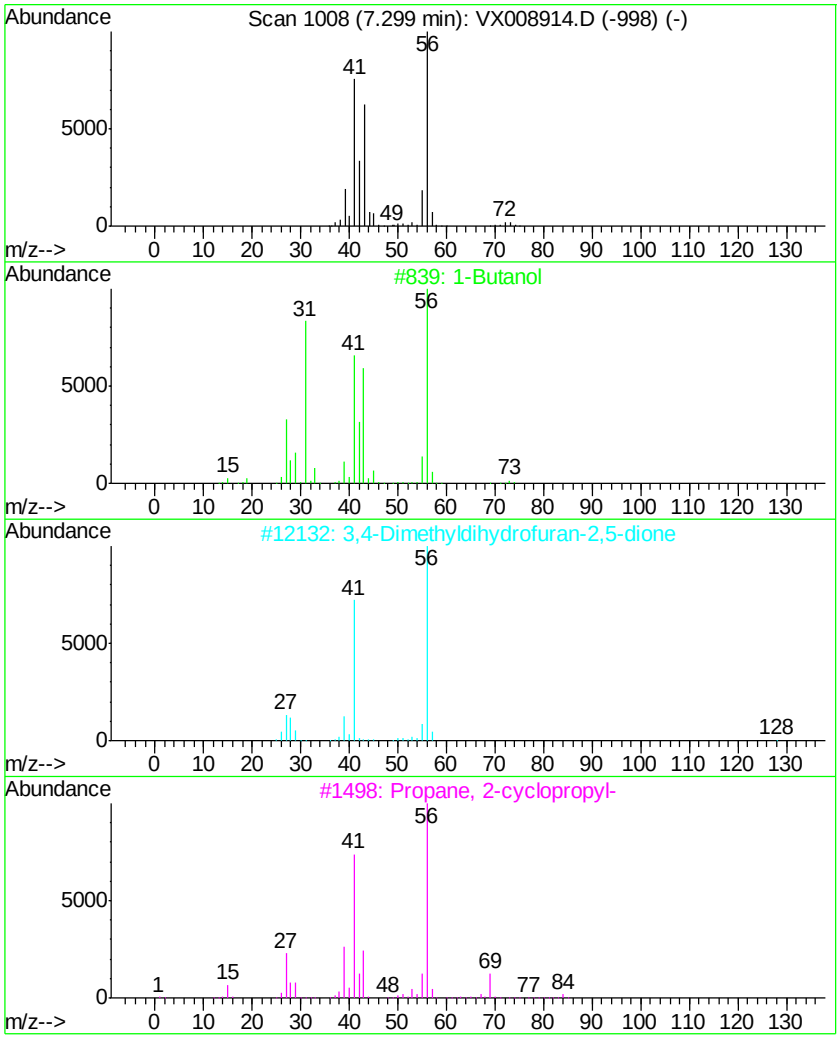
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

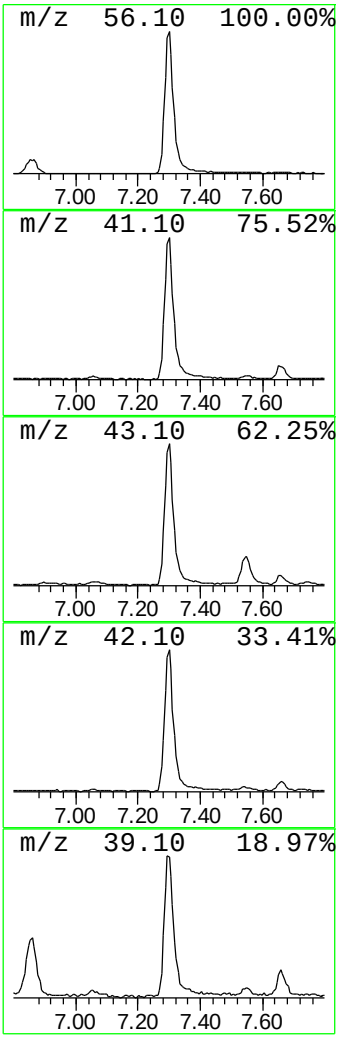
****

Peak Number 5 1-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.30	14.83 ug/l	225017	1,4-Difluorobenzene	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	91
2	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	45
3	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	39
4	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	9
5	Formic acid, butyl ester	102	C5H10O2	000592-84-7	9





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Operator : JC/SP
Sample : K2381-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CL-COMP-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X040319W.M
Quant Title : SW846 8260

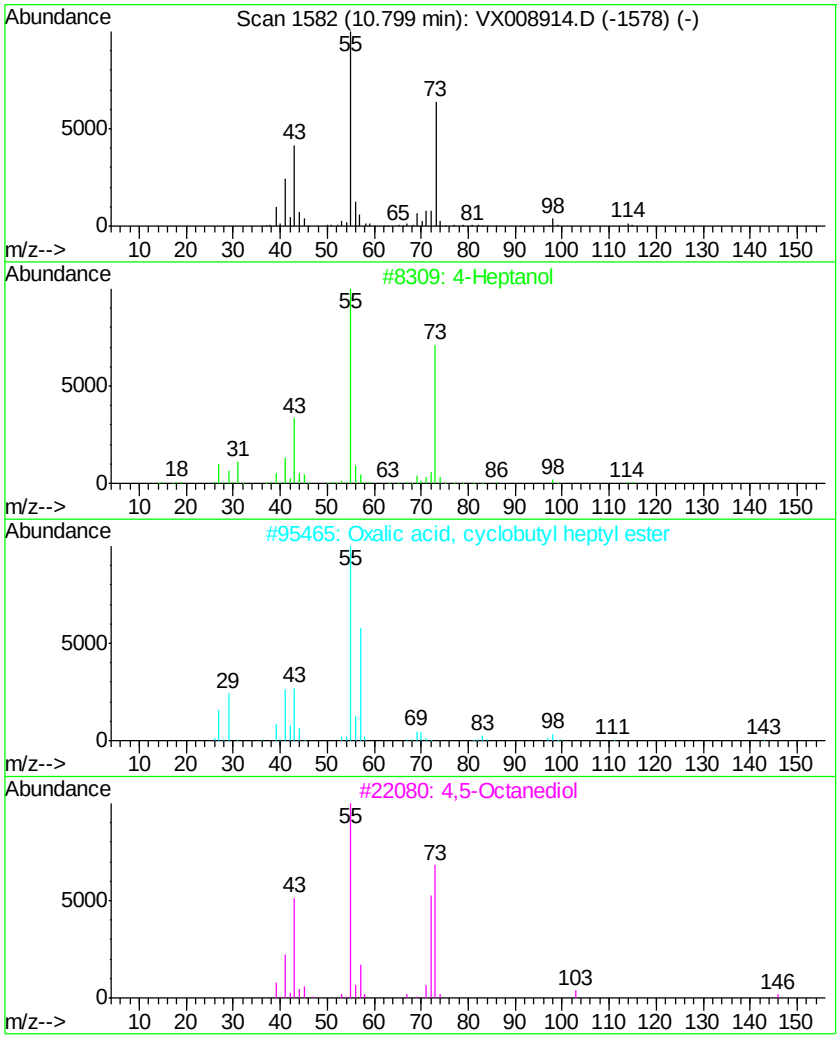
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

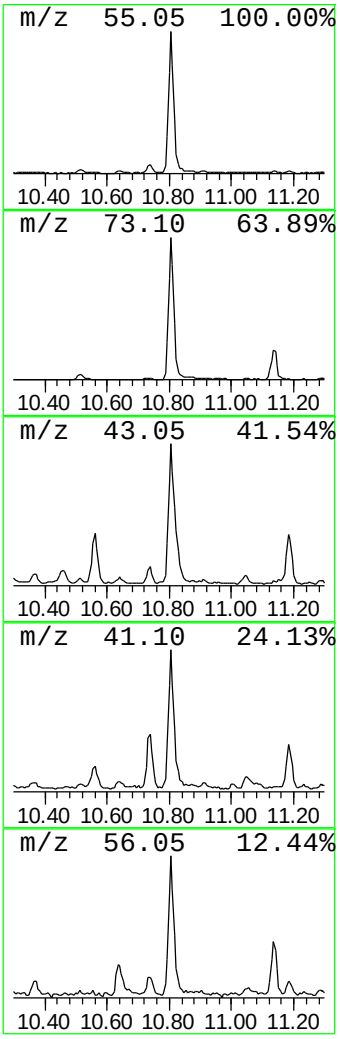
****

Peak Number 6 4-Heptanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	8.65 ug/l	150504	Chlorobenzene-d5	10.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol	116	C7H16O	000589-55-9	78
2	Oxalic acid, cyclobutyl heptyl e...	242	C13H22O4	1000309-69-8	37
3	4,5-Octanediol	146	C8H18O2	022607-10-9	33
4	5-Hydroxy-4-octanone	144	C8H16O2	000496-77-5	33
5	DL-4,5-Octanediol	146	C8H18O2	022520-40-7	33





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ALS Vial : 44 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CL-COMP-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X040319W.M
Quant Title : SW846 8260

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

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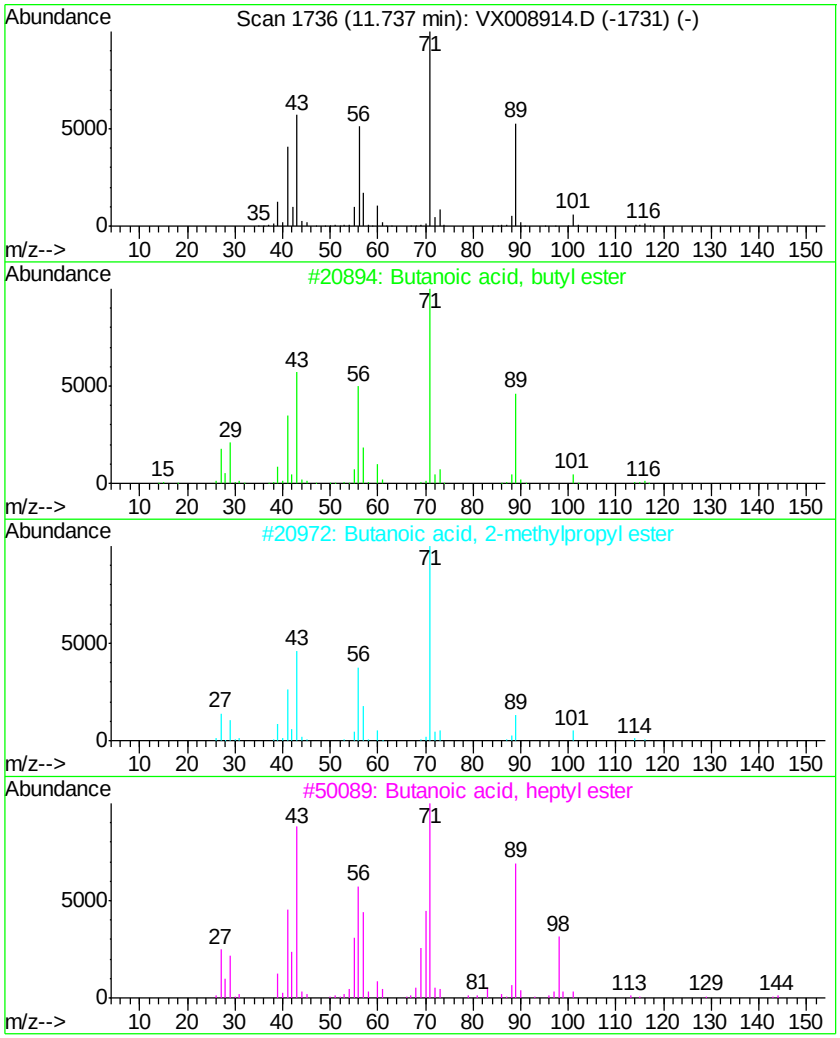
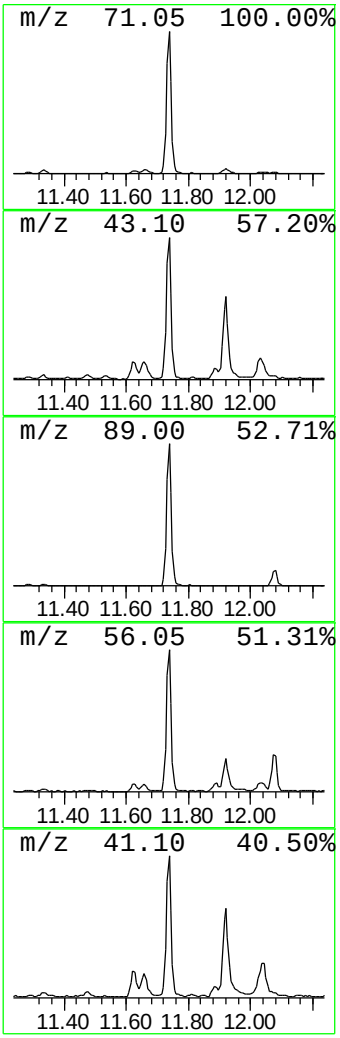
Peak Number 7 Butanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.74	15.70 ug/l	233639	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
3	Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	72
4	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
5	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	59





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Instrument : MSVOA_X
ClientSampleId : CL-COMP-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X040319W.M
Quant Title : SW846 8260

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

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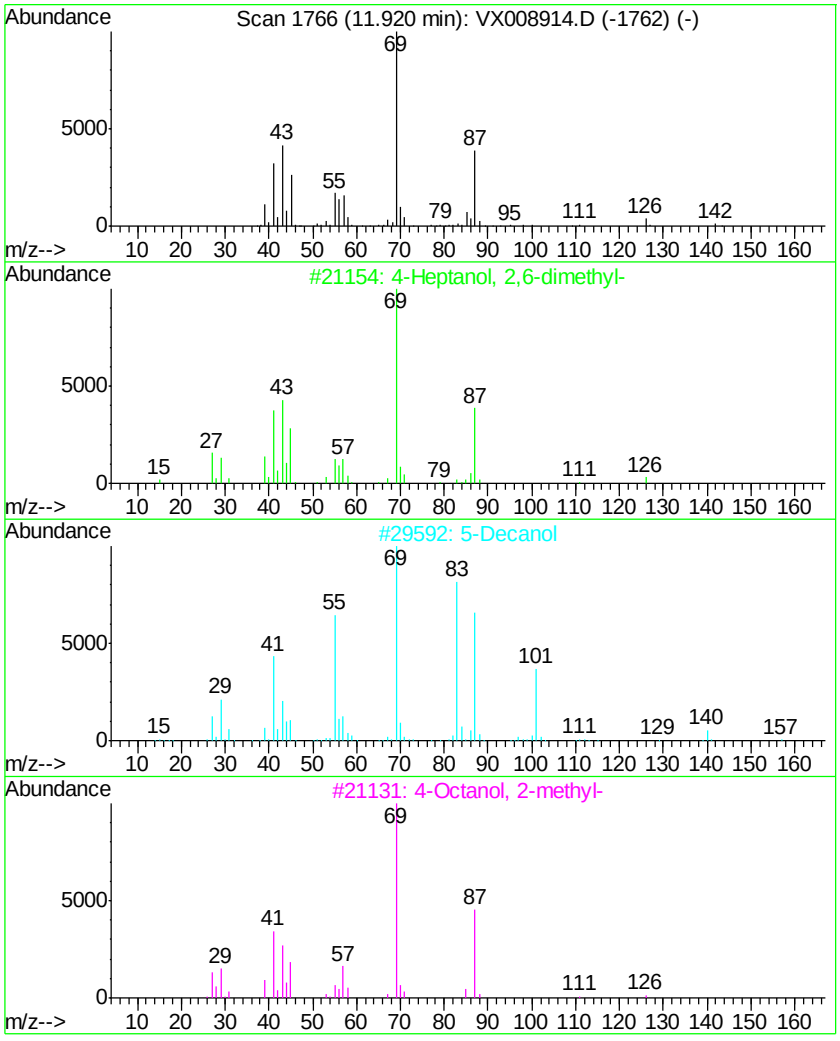
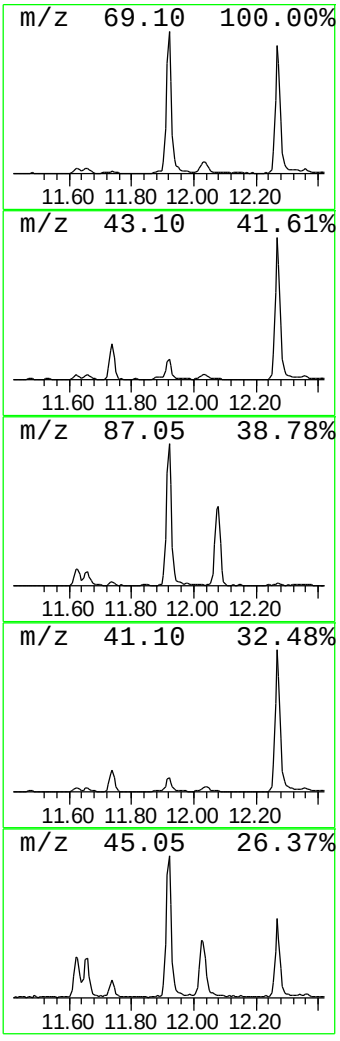
Peak Number 8 4-Heptanol, 2,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	12.31 ug/l	183205	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	90
2	5-Decanol	158	C10H22O	005205-34-5	72
3	4-Octanol, 2-methyl-	144	C9H20O	040575-41-5	72
4	3-Hexanol, 2,5-dimethyl-	130	C8H18O	019550-07-3	64
5	2-Butenoic acid, 1-methylpropyl ...	142	C8H14O2	010371-45-6	64





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Operator : JC/SP
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CL-COMP-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X040319W.M
Quant Title : SW846 8260

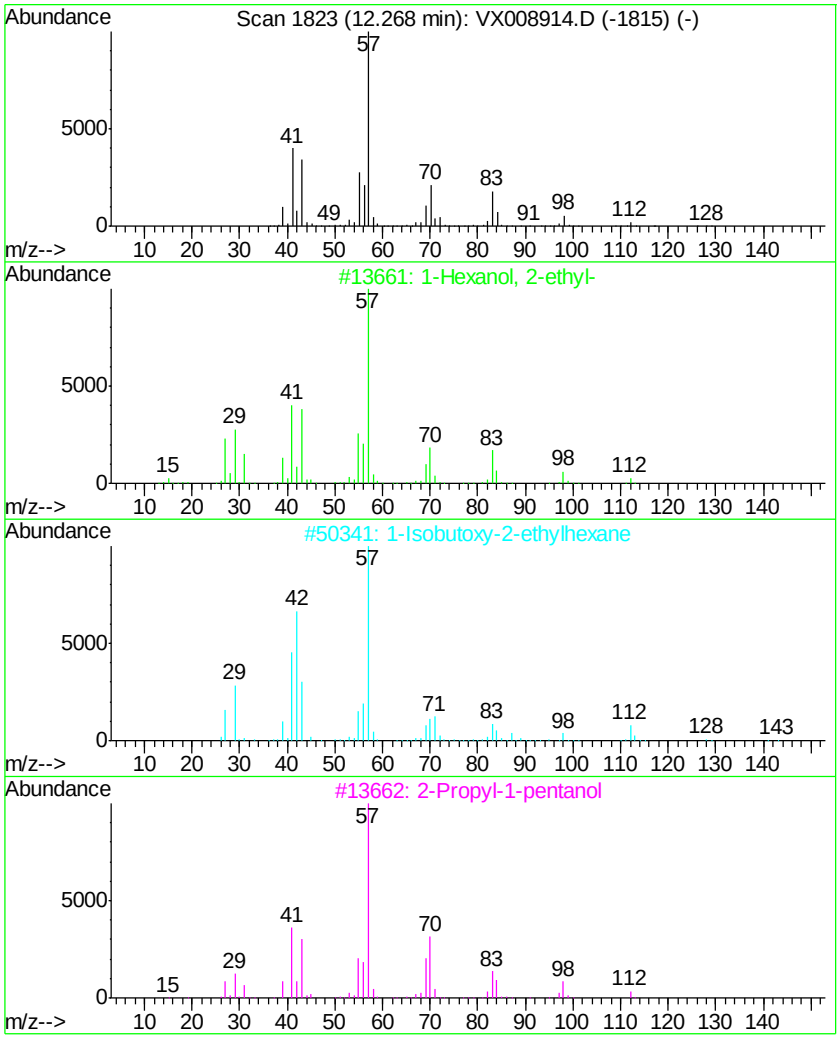
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

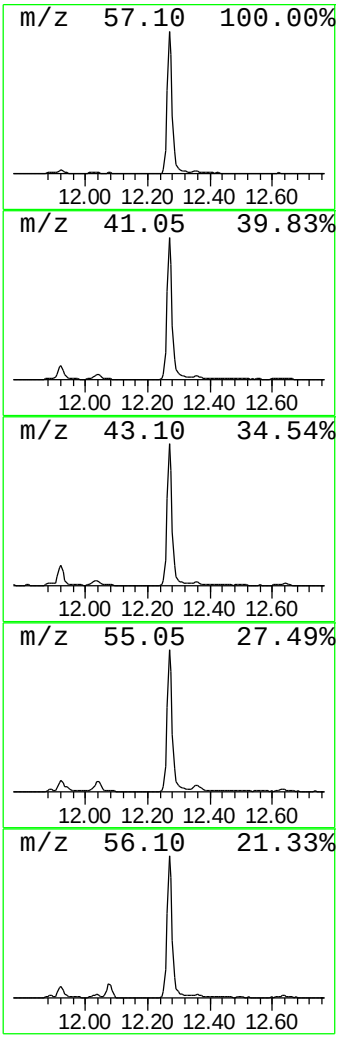
****

Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.27	96.32 ug/l	1433470	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50
5	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	45





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ClientSampleId : CL-COMP-1

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Quant Title : SW846 8260

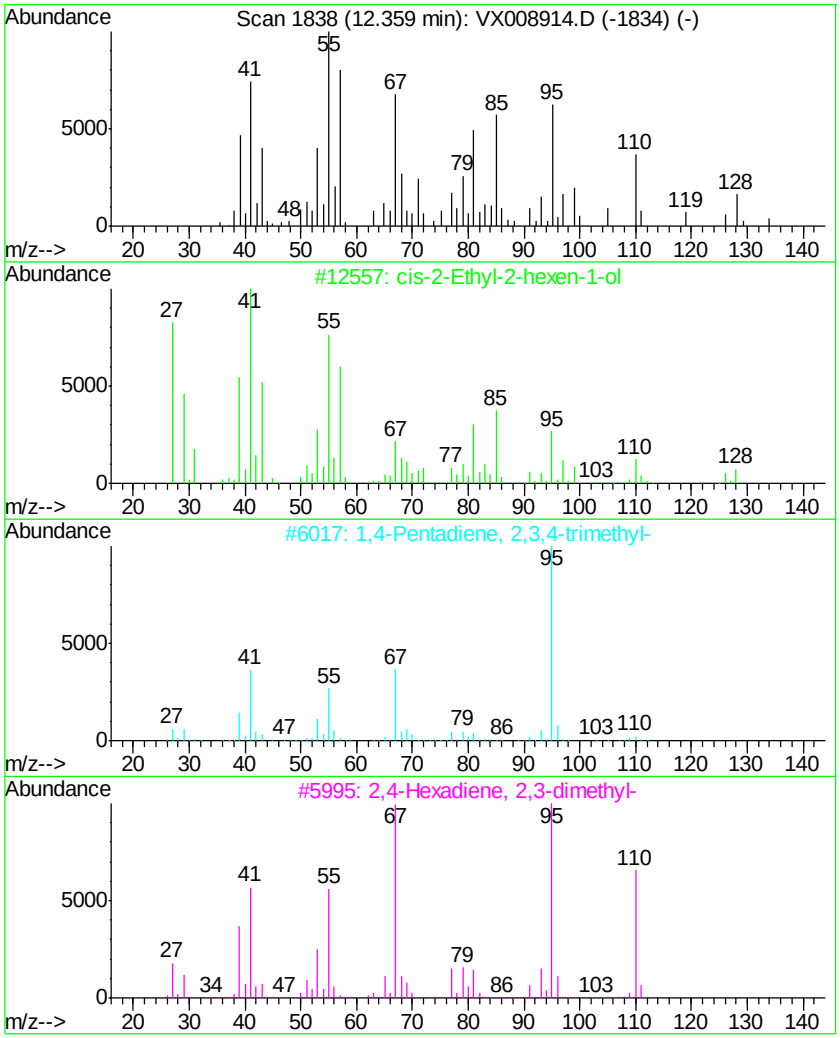
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

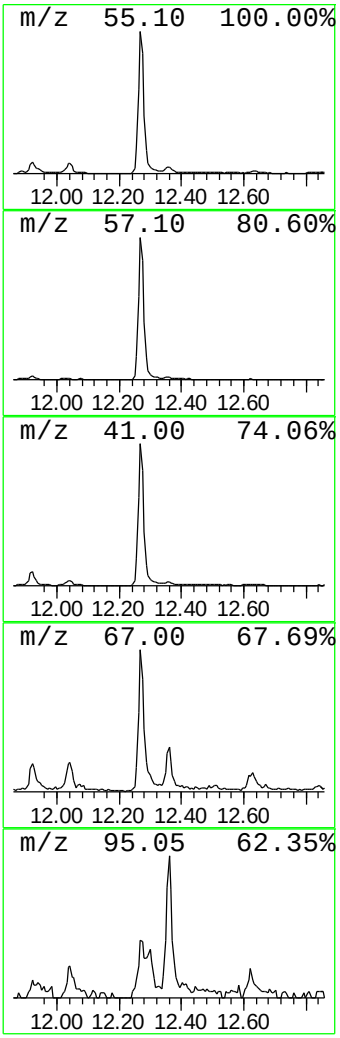
****

Peak Number 10 cis-2-Ethyl-2-hexen-1-ol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.36	5.15 ug/l	76617	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-2-Ethyl-2-hexen-1-ol	128	C8H16O	1000139-52-4	72
2	1,4-Pentadiene, 2,3,4-trimethyl-	110	C8H14	072014-90-5	50
3	2,4-Hexadiene, 2,3-dimethyl-	110	C8H14	005678-98-8	50
4	2,3-Hexadiene, 2-methyl-	96	C7H12	029212-09-7	38
5	Cyclohexene, 1,6-dimethyl-	110	C8H14	001759-64-4	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX041219\
Data File : VX008914.D
Acq On : 13 Apr 2019 02:48
Operator : JC/SP
Sample : K2381-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CL-COMP-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X040319W.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	2.12	13.0	ug/l	147650	1	5.67	566274	50.0
Isopropyl Alcohol	2.61	7.3	ug/l	82564	1	5.67	566274	50.0
Butanal	4.34	26.4	ug/l	299098	1	5.67	566274	50.0
1-Butanol	7.30	14.8	ug/l	225017	2	6.86	758607	50.0
4-Heptanol	10.80	8.7	ug/l	150504	3	10.11	869601	50.0
Butanoic acid, bu...	11.74	15.7	ug/l	233639	4	12.08	744144	50.0
4-Heptanol, 2,6-d...	11.92	12.3	ug/l	183205	4	12.08	744144	50.0
1-Hexanol, 2-ethyl-	12.27	96.3	ug/l	1433470	4	12.08	744144	50.0
cis-2-Ethyl-2-hex...	12.36	5.2	ug/l	76617	4	12.08	744144	50.0