LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX051920\
Data File : VX016342.D
Acq On : 19 May 2020 18:04
Operator : JC/SP
Sample : L2663-07
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1369

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\82X050420W.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	2.087	158	164	179	rBV	343330	532511	4.65%	1.572%
2	2.416	212	218	234	rVB	240386	409247	3.58%	1.208%
3	3.916	453	464	478	rBV	42893	118495	1.04%	0.350%
4	5.470	708	719	732	rBV2	130363	370751	3.24%	1.095%
5	5.635	734	746	760	rVB	233551	653164	5.71%	1.928%
6	6.031	798	811	822	rBV	140037	372478	3.25%	1.100%
7	6.830	933	942	957	rBV	362497	863819	7.55%	2.550%
8	7.958	1121	1127	1138	rVB	137688	268476	2.35%	0.793%
9	8.695	1241	1248	1255	rBV	776984	1202491	10.51%	3.550%
10	10.098	1472	1478	1491	rBV	797980	1068284	9.33%	3.154%
11	11.122	1641	1646	1653	rVB	686018	852582	7.45%	2.517%
12	11.963	1781	1784	1789	rVB	157032	194019	1.70%	0.573%
13	12.061	1795	1800	1807	rVB	889784	1092922	9.55%	3.227%
14	12.140	1807	1813	1820	rBV	1591964	2118765	18.51%	6.255%
15	12.256	1827	1832	1841	rBV	107866	170048	1.49%	0.502%
16	12.622	1885	1892	1904	rBV	78347	140919	1.23%	0.416%
17	12.896	1933	1937	1944	rVB	93965	116227	1.02%	0.343%
18	13.012	1951	1956	1967	rBV	1497324	2084734	18.21%	6.155%
19	13.109	1967	1972	1974	rVV	1939615	2370945	20.71%	7.000%
20	13.140	1974	1977	1992	rVB	4040481	5375264	46.96%	15.870%
21	13.463	2025	2030	2040	rBV	9859376	11445962	100.00%	33.793%
22	13.548	2040	2044	2054	rVB	902358	1293389	11.30%	3.819%
23	14.444	2187	2191	2195	rVB	243151	259087	2.26%	0.765%
24	14.505	2196	2201	2208	rBV2	131853	213931	1.87%	0.632%
25	14.609	2211	2218	2223	rBV2	88260	163424	1.43%	0.482%
26	14.731	2232	2238	2246	rBV3	57472	119255	1.04%	0.352%

Sum of corrected areas: 33871189

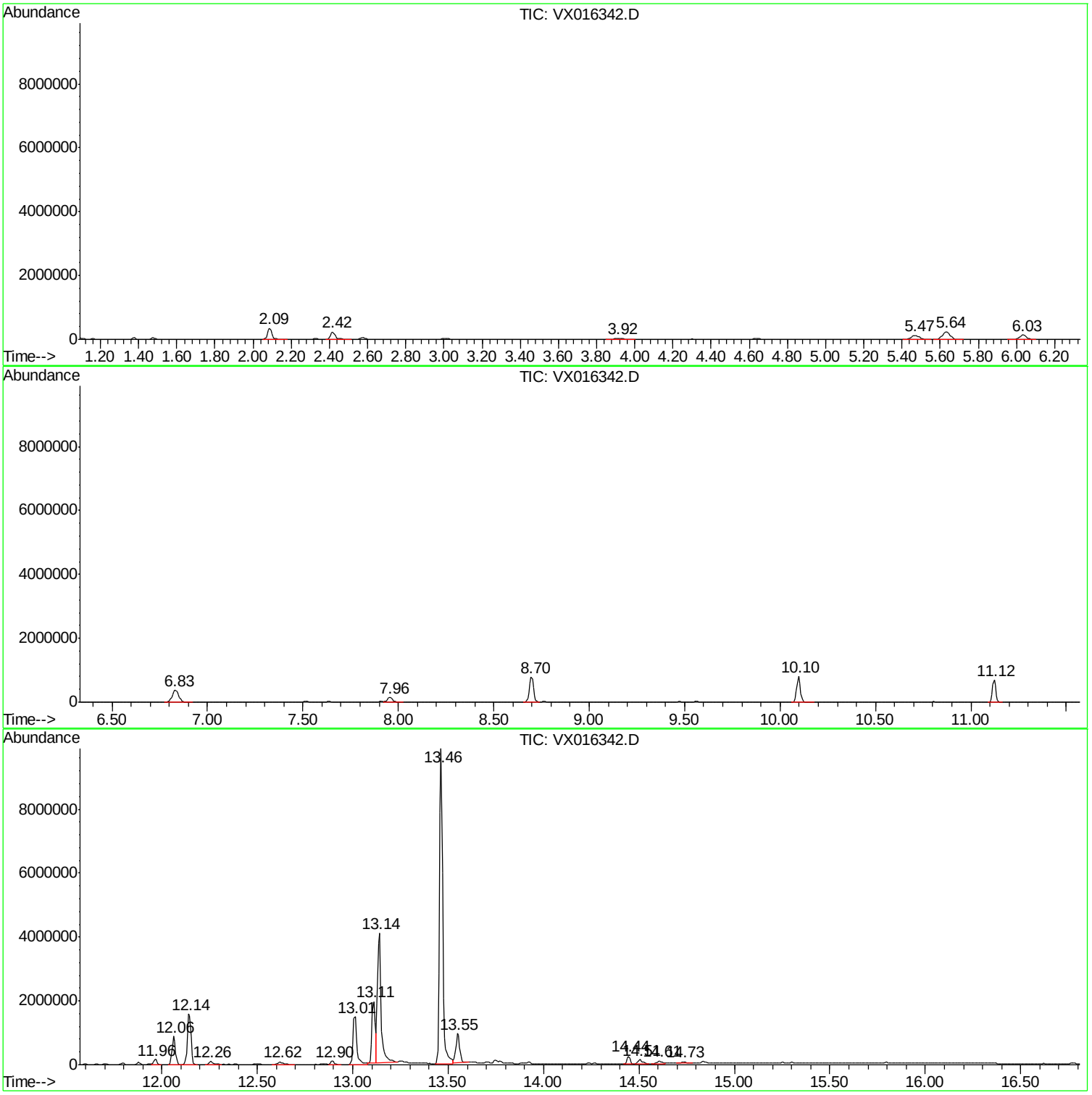
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX051920\
Data File : VX016342.D
Acq On : 19 May 2020 18:04
Operator : JC/SP
Sample : L2663-07
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1369

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX051920\
Data File : VX016342.D
Acq On : 19 May 2020 18:04
Operator : JC/SP
Sample : L2663-07
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1369

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

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

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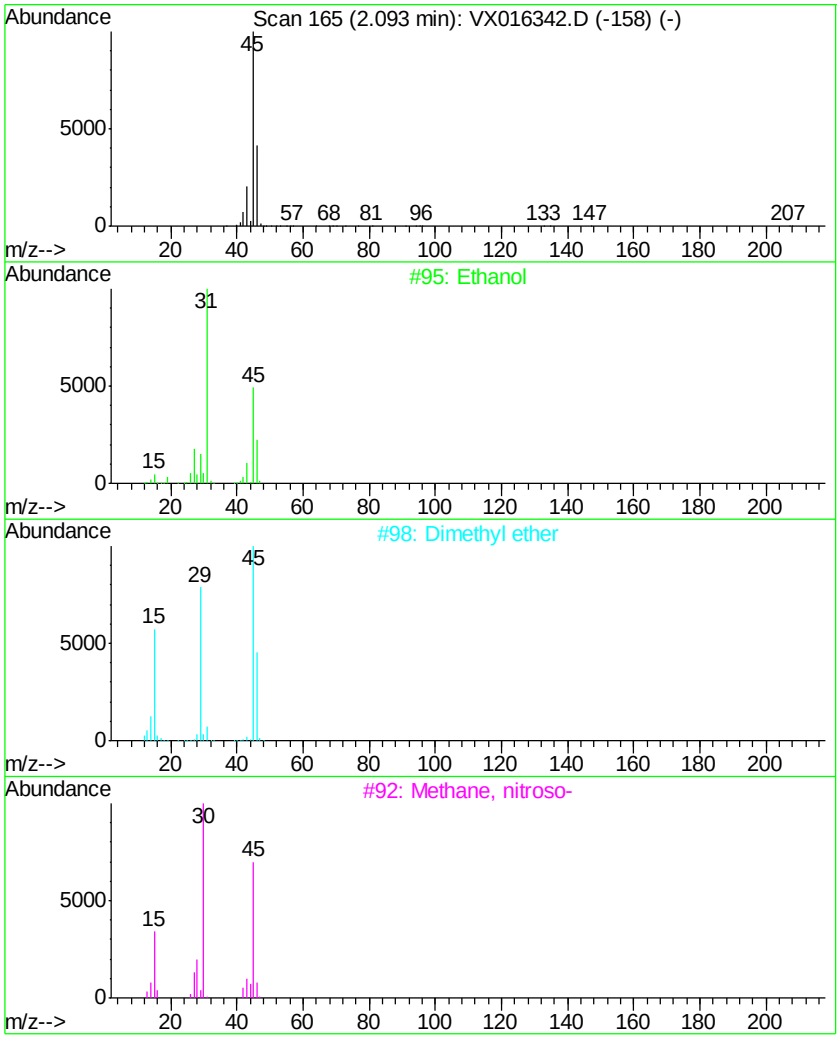
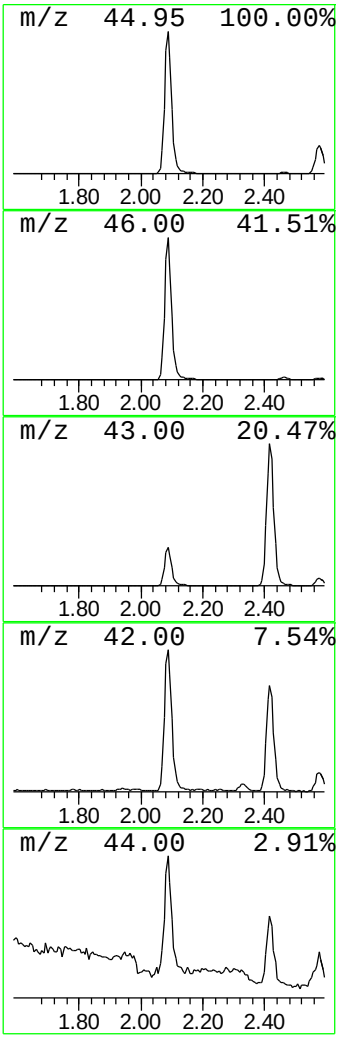
Peak Number 1 Ethanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.09	40.76 ug/l	532511	Pentafluorobenzene	5.64

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





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX051920\
Data File : VX016342.D
Acq On : 19 May 2020 18:04
Operator : JC/SP
Sample : L2663-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1369

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

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

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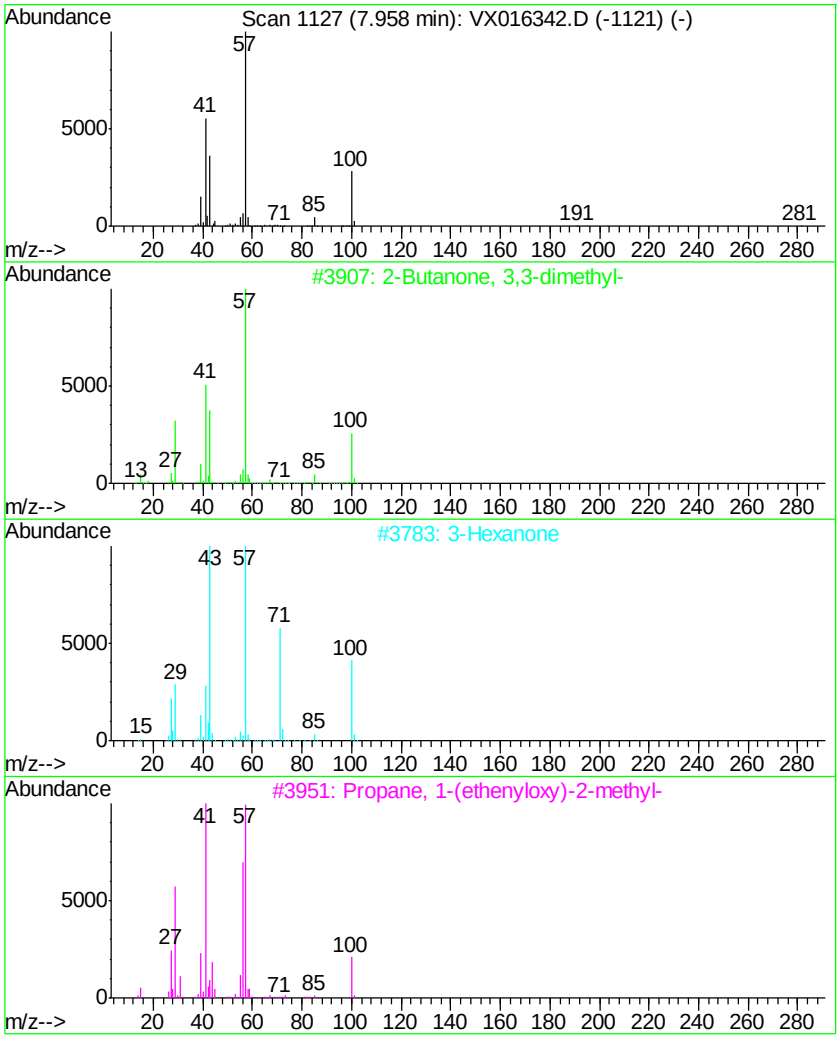
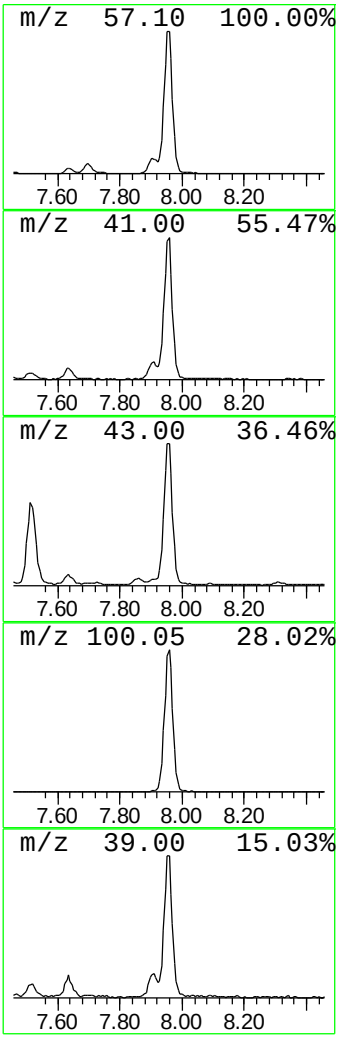
Peak Number 2 2-Butanone, 3,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.96	15.54 ug/l	268476	1,4-Difluorobenzene	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	91
2	3-Hexanone	100	C6H12O	000589-38-8	64
3	Propane, 1-(ethenyloxy)-2-methyl-	100	C6H12O	000109-53-5	64
4	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	59
5	trans-1-Ethoxy-1-butene	100	C6H12O	1000139-43-9	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX051920\
Data File : VX016342.D
Acq On : 19 May 2020 18:04
Operator : JC/SP
Sample : L2663-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1369

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

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

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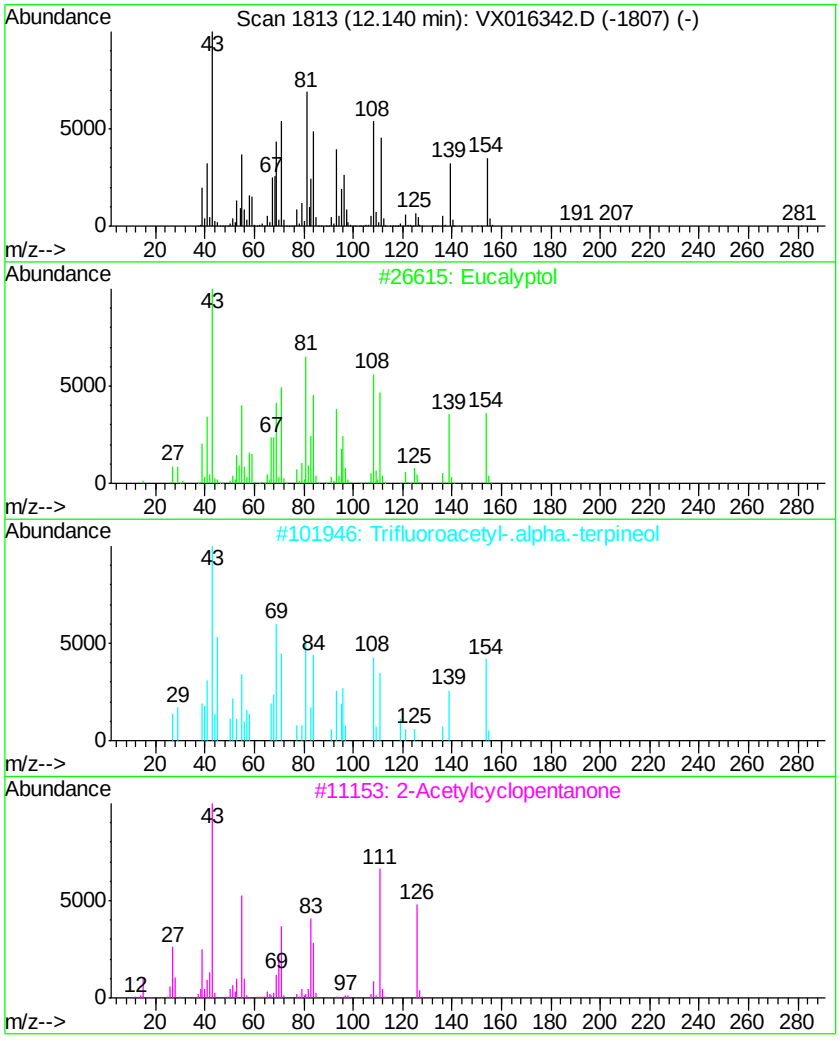
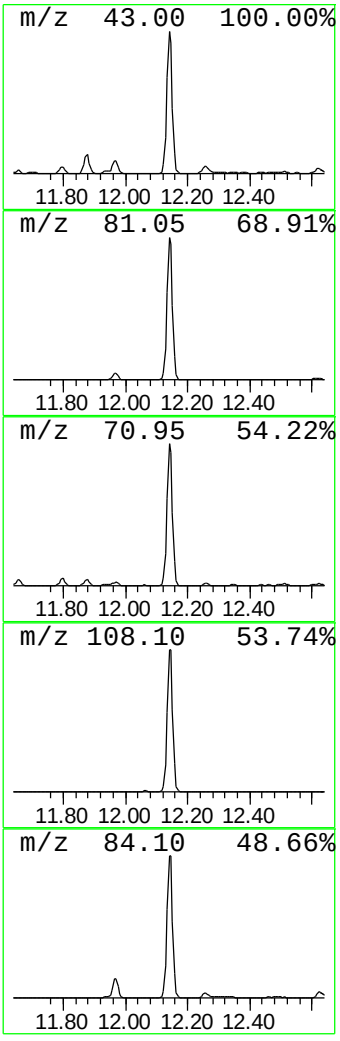
Peak Number 3 Eucalyptol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.14	96.93 ug/l	2118770	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eucalyptol	154	C10H18O	000470-82-6	99
2	Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	52
3	2-Acetylcyclopentanone	126	C7H10O2	001670-46-8	27
4	5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	27
5	3-Cyclohexen-1-ol, 4-methyl-1-(1...	154	C10H18O	020126-76-5	25





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX051920\
Data File : VX016342.D
Acq On : 19 May 2020 18:04
Operator : JC/SP
Sample : L2663-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1369

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

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

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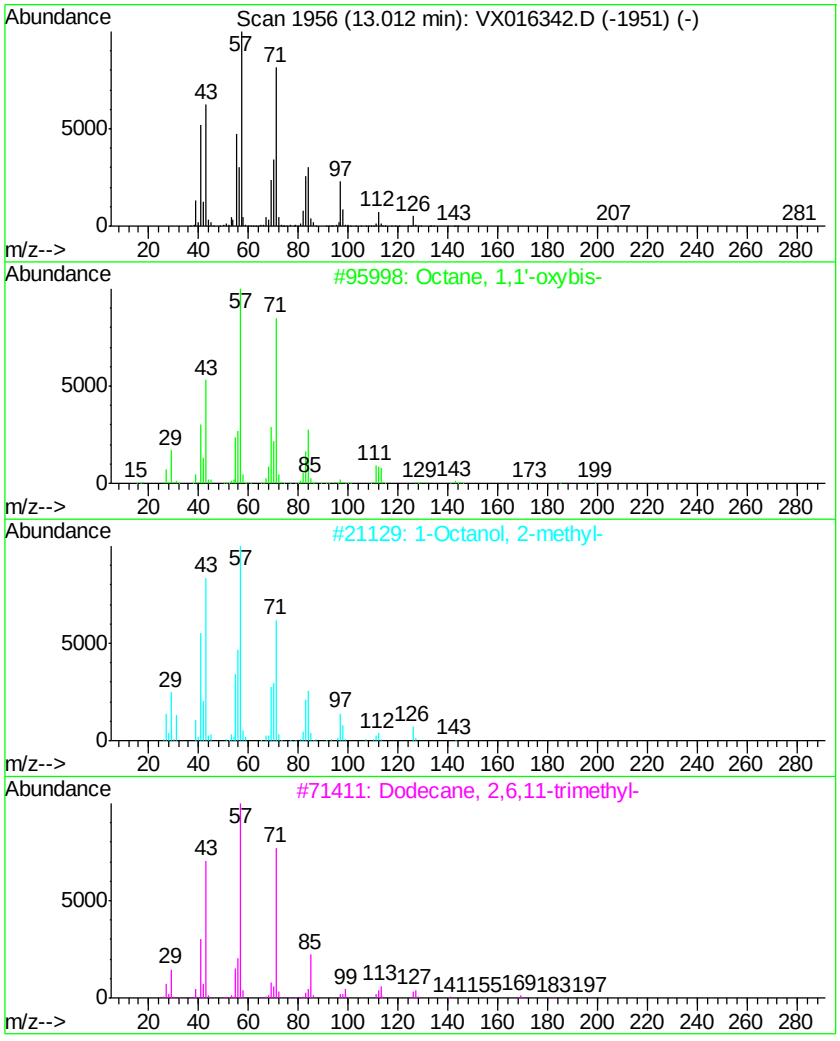
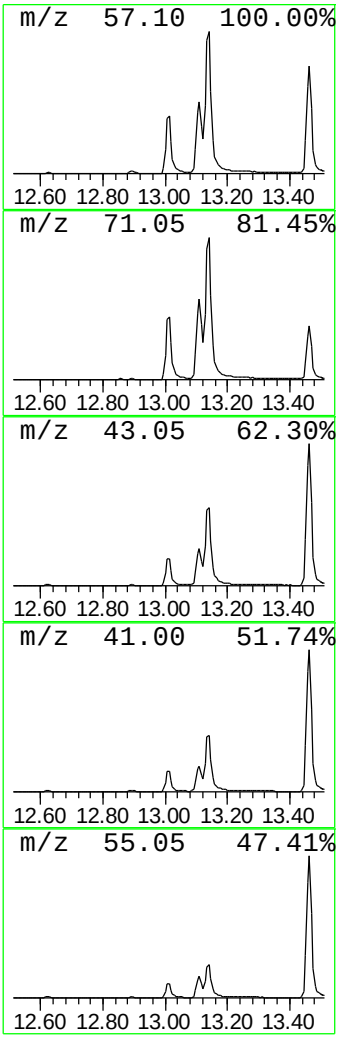
Peak Number 4 Octane, 1,1'-oxybis- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.01	95.37 ug/l	2084730	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	64
2	1-Octanol, 2-methyl-	144	C9H20O	000818-81-5	53
3	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	50
4	Octane, 2,3,7-trimethyl-	156	C11H24	062016-34-6	47
5	4-Methyl-3-heptanol, pentafluoro...	276	C11H17F5O2	1000365-51-7	47





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX051920\
Data File : VX016342.D
Acq On : 19 May 2020 18:04
Operator : JC/SP
Sample : L2663-07
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1369

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

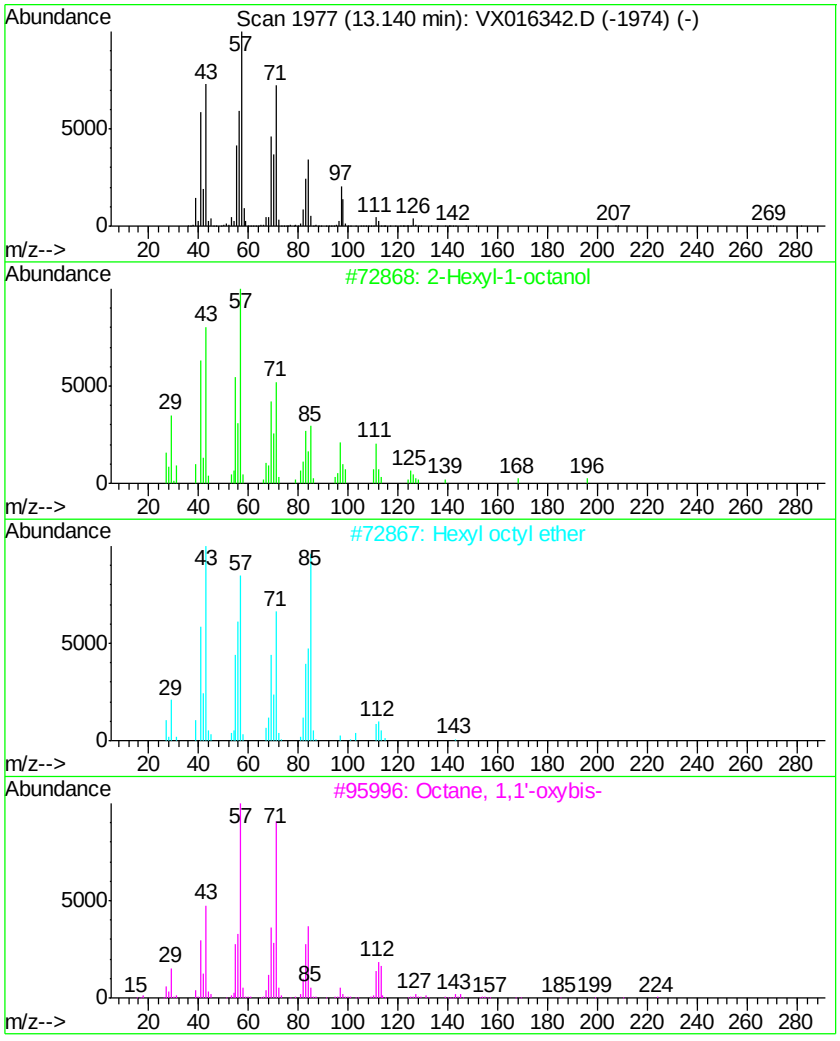
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

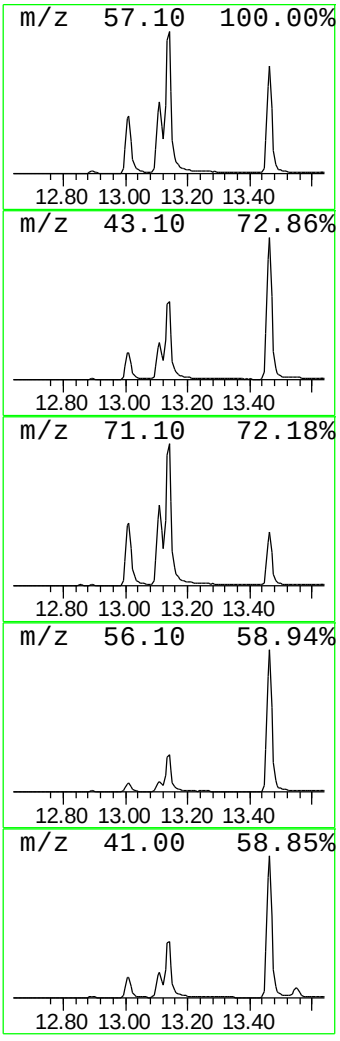
****

Peak Number 6 2-Hexyl-1-octanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.14	245.91 ug/l	5375260	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexyl-1-octanol	214	C14H30O	019780-79-1	64
2	Hexyl octyl ether	214	C14H30O	017071-54-4	59
3	Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	53
4	Acetic acid, trichloro-, octyl e...	274	C10H17Cl3O2	016958-78-4	50
5	1-Nonene	126	C9H18	000124-11-8	47





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX051920\
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Sample : L2663-07
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1369

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

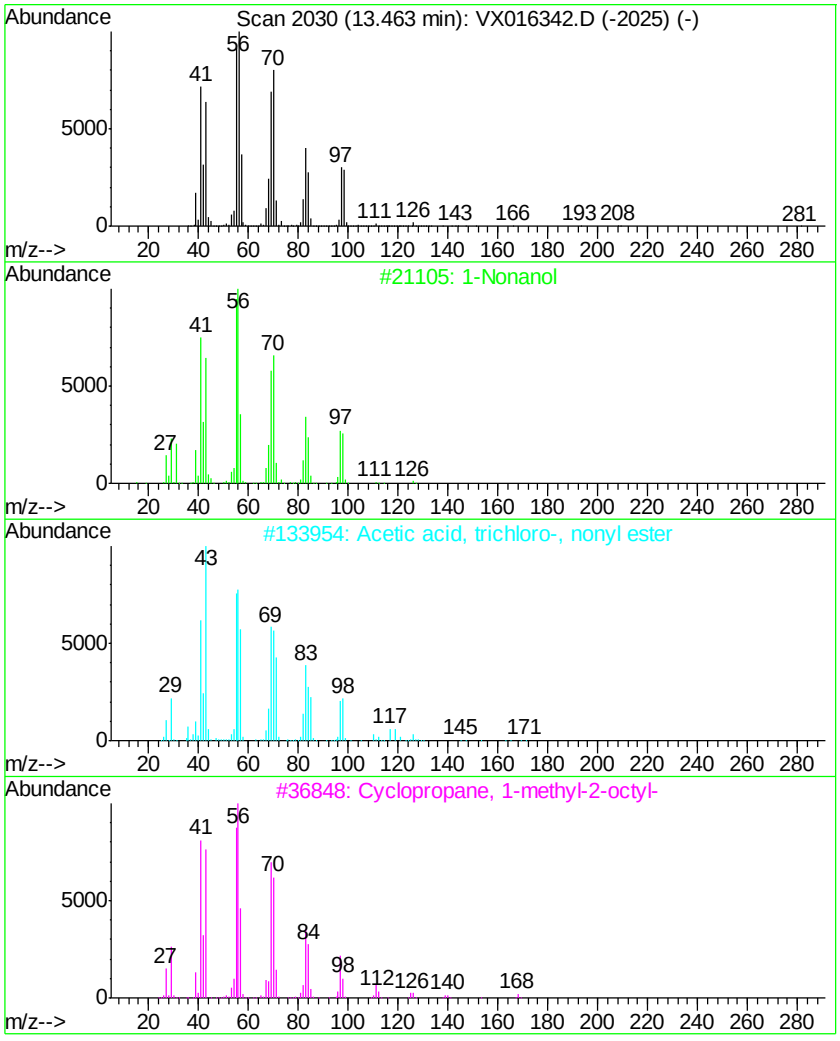
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

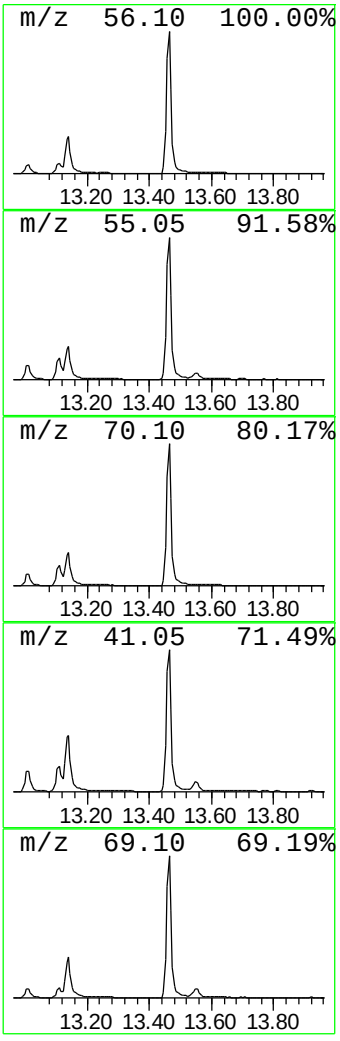
****

Peak Number 7 1-Nonanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.46	523.64 ug/l	11446000	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonanol	144	C9H20O	000143-08-8	91
2	Acetic acid, trichloro-, nonyl e...	288	C11H19Cl3O2	065611-32-7	83
3	Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	78
4	1-Octanol	130	C8H18O	000111-87-5	72
5	Cycloheptane	98	C7H14	000291-64-5	64





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX051920\
Data File : VX016342.D
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ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1369

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

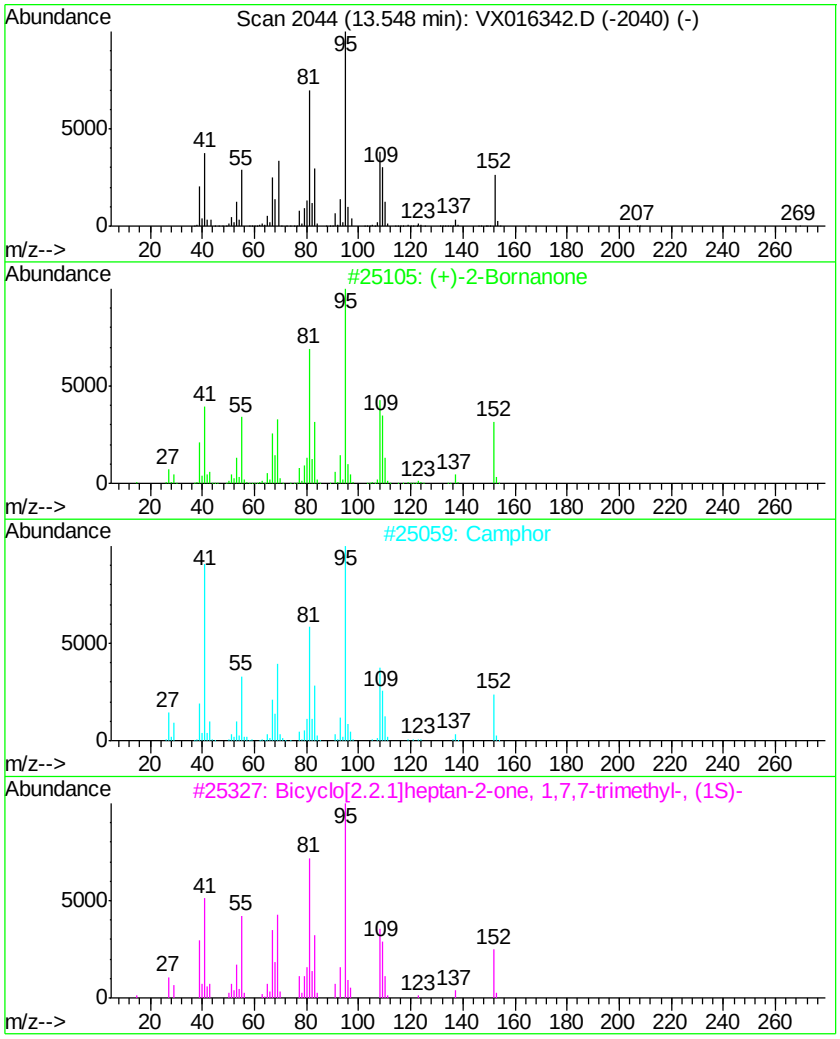
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

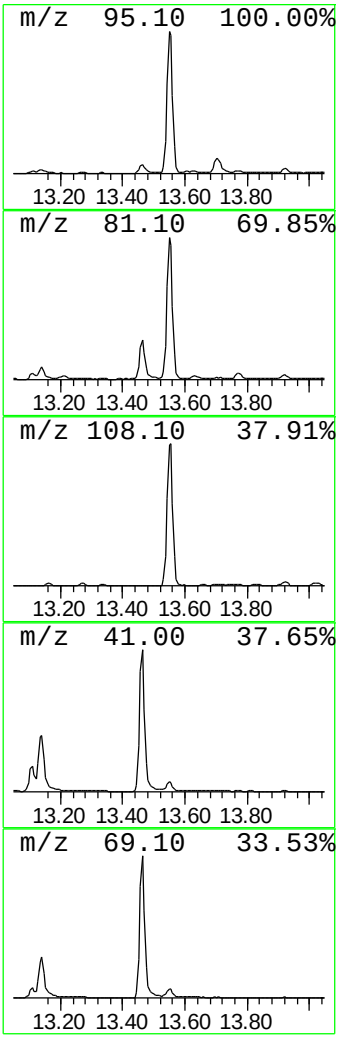
****

Peak Number 8 (+)-2-Bornanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	59.17 ug/l	1293390	1,4-Dichlorobenzene-d4	12.06

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	2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	49
5	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	41





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Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1369

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

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

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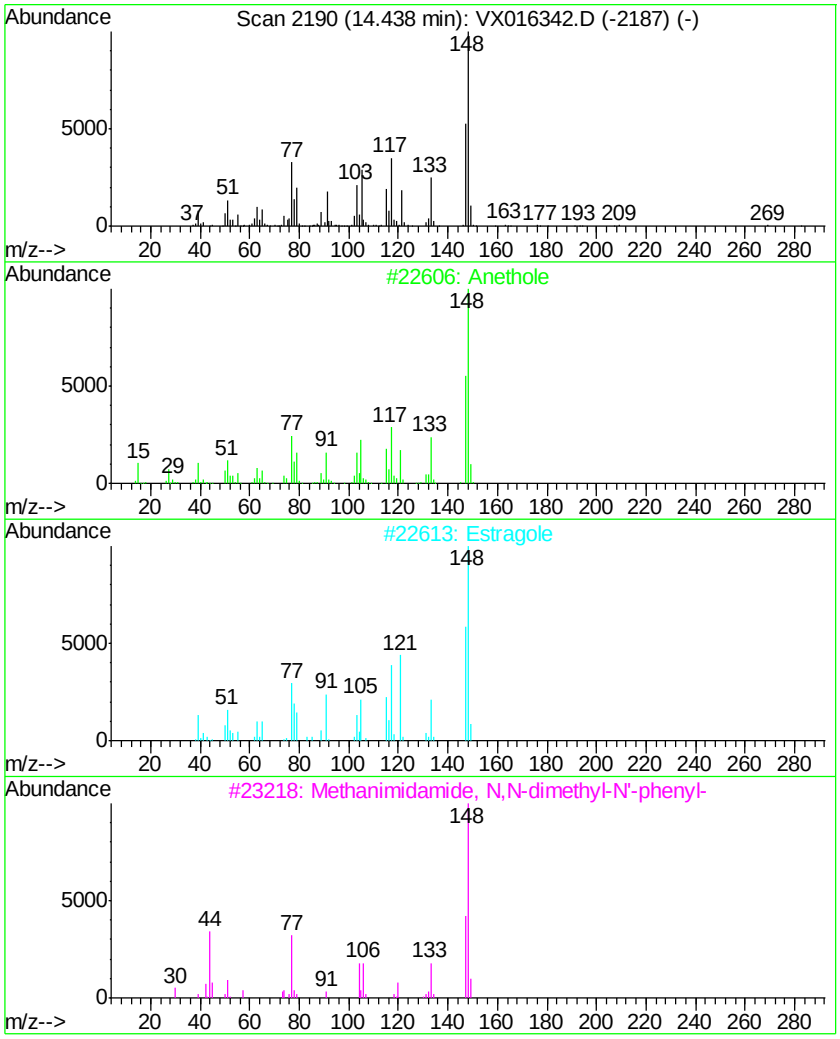
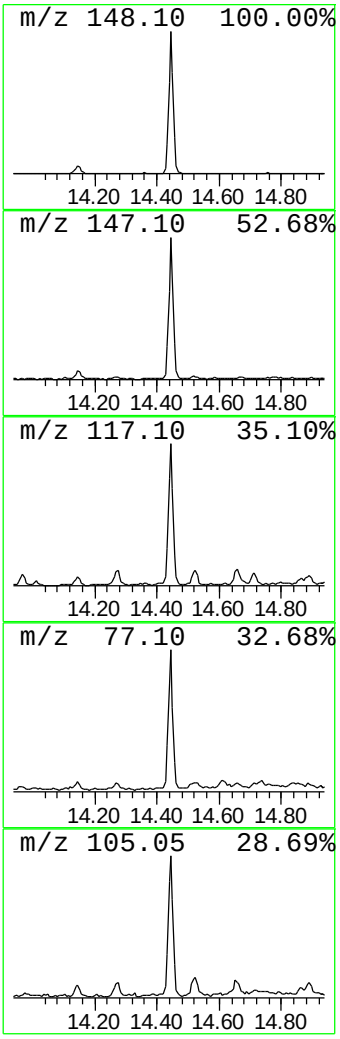
Peak Number 9 Anethole Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.44	11.85 ug/l	259087	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anethole	148	C10H12O	000104-46-1	95
2	Estragole	148	C10H12O	000140-67-0	93
3	Methanimidamide, N,N-dimethyl-N'...	148	C9H12N2	001783-25-1	58
4	5-Methoxyindane	148	C10H12O	1000342-73-8	52
5	3H-Indazol-3-one, 1,2-dihydro-1-...	148	C8H8N2O	001006-19-5	52





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX051920\
Data File : VX016342.D
Acq On : 19 May 2020 18:04
Operator : JC/SP
Sample : L2663-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1369

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.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	2.09	40.8	ug/l	532511	1	5.64	653164	50.0
2-Butanone, 3,3-d...	7.96	15.5	ug/l	268476	2	6.83	863819	50.0
Eucalyptol	12.14	96.9	ug/l	2118770	4	12.06	1092920	50.0
Octane, 1,1'-oxybis-	13.01	95.4	ug/l	2084730	4	12.06	1092920	50.0
2-Hexyl-1-octanol	13.14	245.9	ug/l	5375260	4	12.06	1092920	50.0
1-Nonanol	13.46	523.6	ug/l	11446000	4	12.06	1092920	50.0
(+)-2-Bornanone	13.55	59.2	ug/l	1293390	4	12.06	1092920	50.0
Anethole	14.44	11.9	ug/l	259087	4	12.06	1092920	50.0