LSC Area Percent Report

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX050518\
Data File : VX001433.D
Acq On : 05 May 2018 21:55
Operator : JC/MD
Sample : J2695-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CS-DRUM-2

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 : W:\HPCHEM1\MSVOA_X\METHOD\82X050518W.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	1.069	76	79	92	rBV	1234366	1555870	28.14%	6.931%
2	1.489	144	148	153	rBV	63065	71987	1.30%	0.321%
3	2.123	246	252	262	rBV	182796	284406	5.14%	1.267%
4	2.453	299	306	317	rBV	625909	1056131	19.10%	4.705%
5	2.629	329	335	342	rVB	53081	98180	1.78%	0.437%
6	4.105	569	577	589	rVB3	27374	70680	1.28%	0.315%
7	4.721	668	678	687	rBV	147284	424129	7.67%	1.889%
8	5.214	746	759	771	rBV3	24305	78178	1.41%	0.348%
9	5.513	796	808	822	rBV	152577	432255	7.82%	1.926%
10	5.672	822	834	851	rBV	226478	641918	11.61%	2.859%
11	6.080	889	901	912	rBV	164297	437459	7.91%	1.949%
12	6.775	998	1015	1021	rBV	25044	70291	1.27%	0.313%
13	6.867	1021	1030	1048	rVB	315331	746849	13.51%	3.327%
14	7.562	1138	1144	1156	rBV	106996	216283	3.91%	0.963%
15	8.659	1317	1324	1329	rBV	415397	650953	11.77%	2.900%
16	8.720	1329	1334	1342	rVV	759003	1223268	22.12%	5.449%
17	8.793	1342	1346	1353	rVB2	41064	78315	1.42%	0.349%
18	9.506	1457	1463	1471	rBV	74399	109225	1.98%	0.487%
19	9.592	1471	1477	1490	rVB	61623	99225	1.79%	0.442%
20	10.116	1555	1563	1577	rBV	614413	881532	15.94%	3.927%
21	10.835	1675	1681	1688	rBV	82778	116364	2.10%	0.518%
22	11.140	1726	1731	1739	rVB	635991	819127	14.81%	3.649%
23	11.543	1792	1797	1807	rVB	110620	156414	2.83%	0.697%
24	11.817	1836	1842	1851	rVB2	56761	88410	1.60%	0.394%
25	11.902	1851	1856	1861	rBV	139295	181579	3.28%	0.809%
26	11.988	1867	1870	1875	rVB2	47131	56479	1.02%	0.252%
27	12.085	1880	1886	1892	rVB	760407	970233	17.55%	4.322%
28	12.164	1892	1899	1913	rBV	224336	317335	5.74%	1.414%
29	12.280	1913	1918	1925	rBV	160964	247415	4.47%	1.102%
30	12.640	1974	1977	1990	rVB	44004	80207	1.45%	0.357%
31	12.920	2019	2023	2030	rVB	91432	118505	2.14%	0.528%
32	13.030	2036	2041	2053	rBV	281594	442827	8.01%	1.973%
33	13.134	2053	2058	2059	rBV	412671	490110	8.86%	2.183%
34	13.158	2059	2062	2076	rVB	1071117	1597829	28.89%	7.118%

LSC Area Percent Report

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX050518\
Data File : VX001433.D
Acq On : 05 May 2018 21:55
Operator : JC/MD
Sample : J2695-07
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CS-DRUM-2

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 : W:\HPCHEM1\MSVOA_X\METHOD\82X050518W.M
Title : SW846 8260

35	13.487	2110	2116	2127	rBV	4411445	5529955	100.00%	24.634%
36	13.579	2127	2131	2139	rVV	180603	367422	6.64%	1.637%
37	13.658	2139	2144	2154	rVV	372467	602463	10.89%	2.684%
38	13.768	2158	2162	2171	rVB	126534	167683	3.03%	0.747%
39	14.469	2272	2277	2282	rVB	167171	195342	3.53%	0.870%
40	14.627	2299	2303	2309	rBV	88072	123173	2.23%	0.549%
41	14.755	2318	2324	2336	rBV2	87511	131248	2.37%	0.585%
42	14.859	2336	2341	2354	rBV	172166	258153	4.67%	1.150%
43	15.322	2413	2417	2425	rVB2	114777	163267	2.95%	0.727%

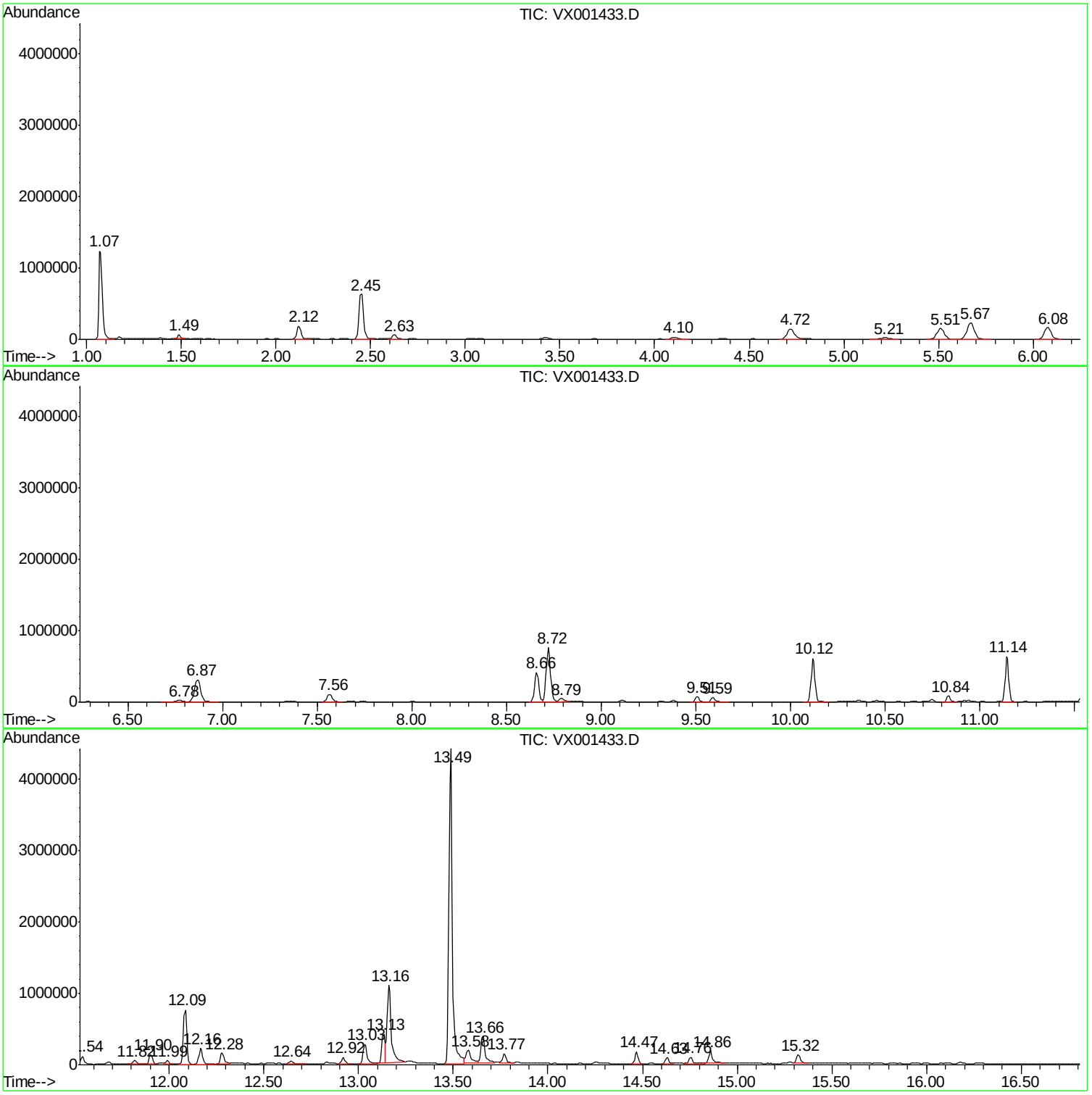
Sum of corrected areas: 22448674

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX050518\
Data File : VX001433.D
Acq On : 05 May 2018 21:55
Operator : JC/MD
Sample : J2695-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CS-DRUM-2

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X050518W.M
Quant Title : SW846 8260

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



Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX050518\
Data File : VX001433.D
Acq On : 05 May 2018 21:55
Operator : JC/MD
Sample : J2695-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CS-DRUM-2

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X050518W.M
Quant Title : SW846 8260

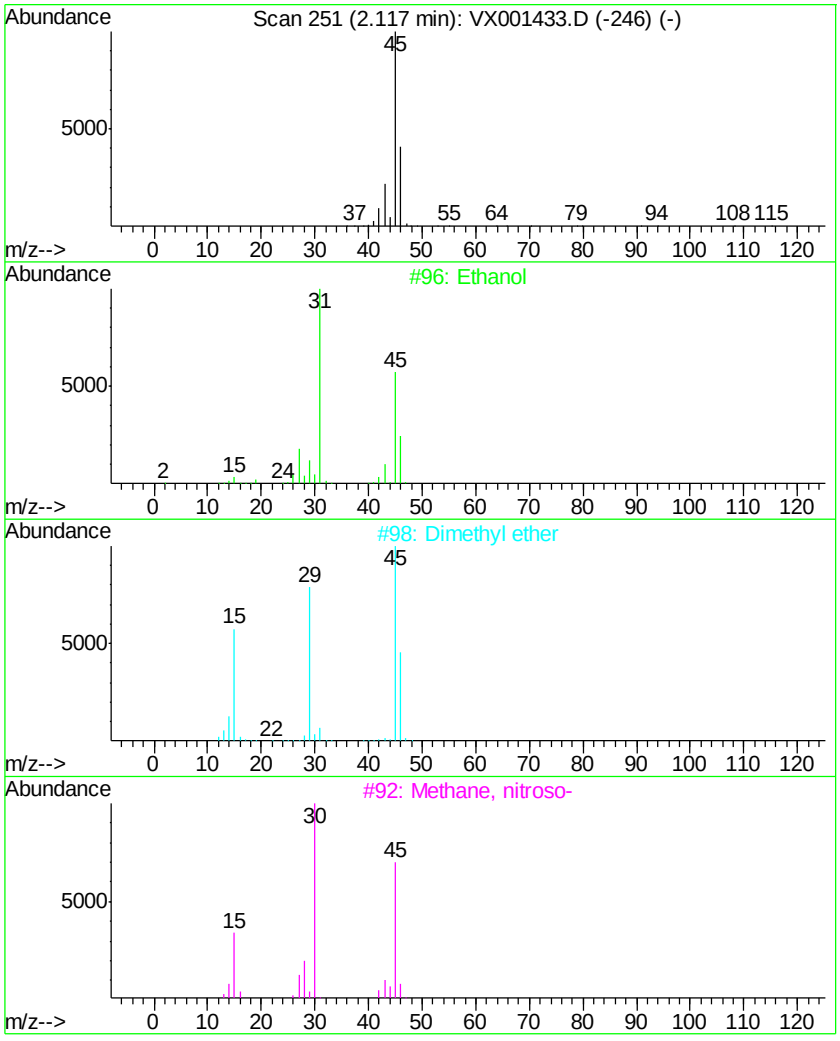
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

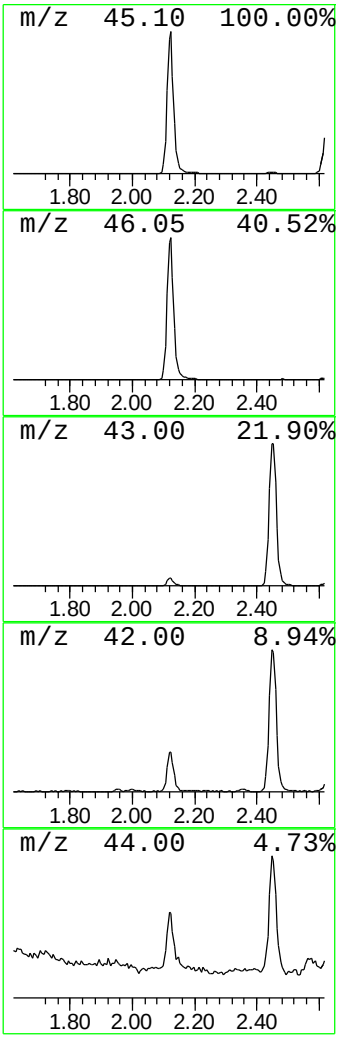
****

Peak Number 2 Ethanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	22.15 ug/l	284406	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





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX050518\
Data File : VX001433.D
Acq On : 05 May 2018 21:55
Operator : JC/MD
Sample : J2695-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CS-DRUM-2

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X050518W.M
Quant Title : SW846 8260

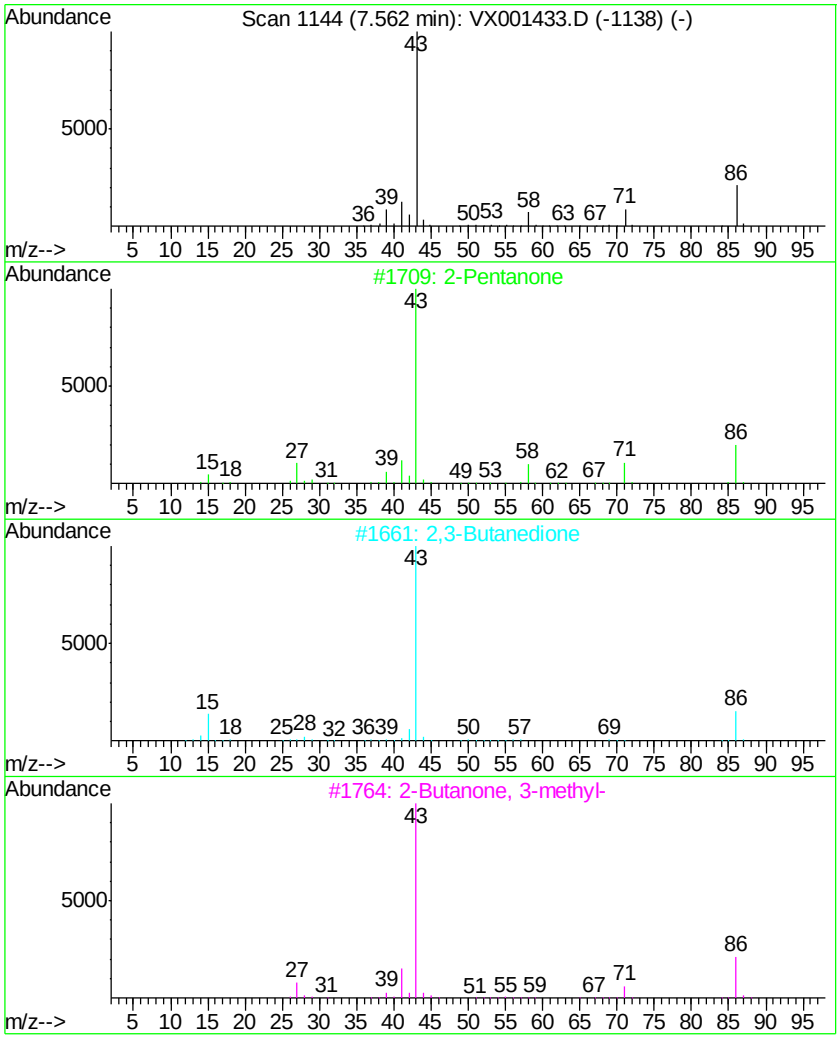
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

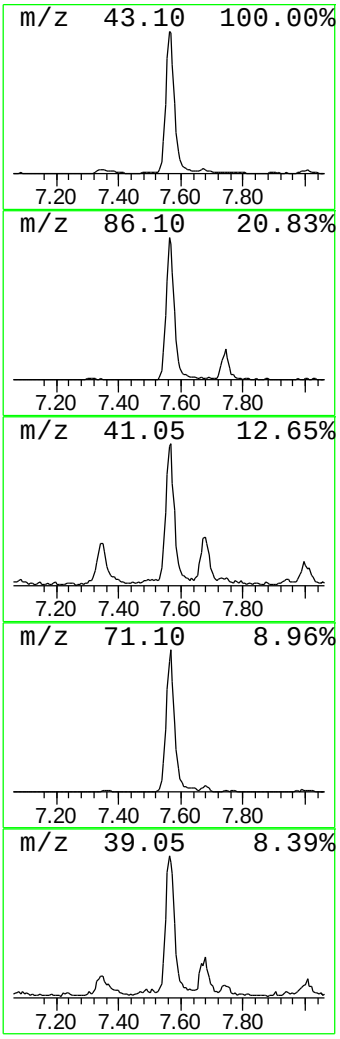
****

Peak Number 3 2-Pentanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	14.48 ug/l	216283	1,4-Difluorobenzene	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	86
2	2,3-Butanedione	86	C4H6O2	000431-03-8	64
3	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	59
4	2,3-Hexanedione	114	C6H10O2	003848-24-6	9
5	2-Pentanone, 3-ethyl-	114	C7H14O	006137-03-7	9





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX050518\
Data File : VX001433.D
Acq On : 05 May 2018 21:55
Operator : JC/MD
Sample : J2695-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CS-DRUM-2

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X050518W.M
Quant Title : SW846 8260

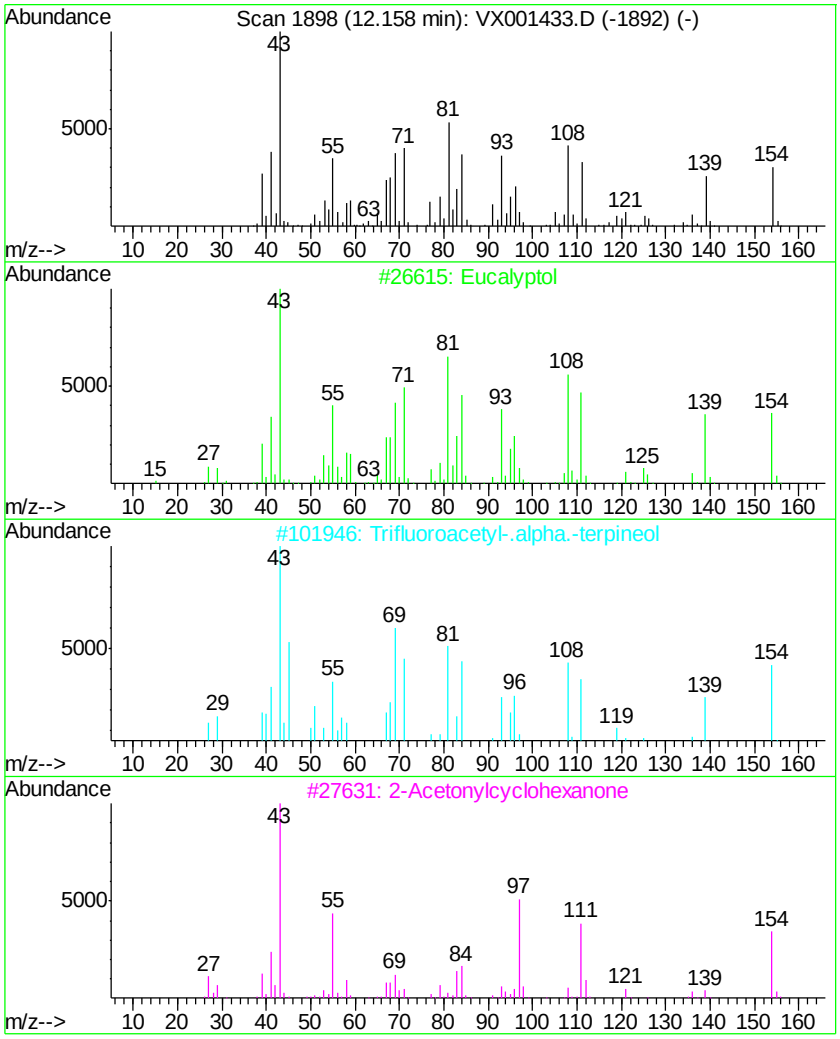
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

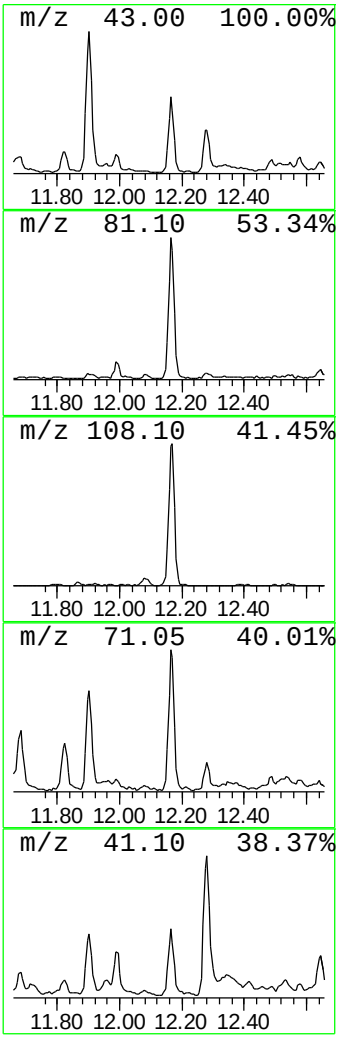
****

Peak Number 4 Eucalyptol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.16	16.35 ug/l	317335	1,4-Dichlorobenzene-d4	12.09

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	38
3	2-Acetonylcyclohexanone	154	C9H14O2	006126-53-0	25
4	Cyclopentanol, 1,2-dimethyl-3-(1...	154	C10H18O	004099-07-4	22
5	Sulfurous acid, 2-pentyl propyl ...	194	C8H18O3S	1000309-15-1	22





Library Search Compound Report

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX050518\
Data File : VX001433.D
Acq On : 05 May 2018 21:55
Operator : JC/MD
Sample : J2695-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CS-DRUM-2

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X050518W.M
Quant Title : SW846 8260

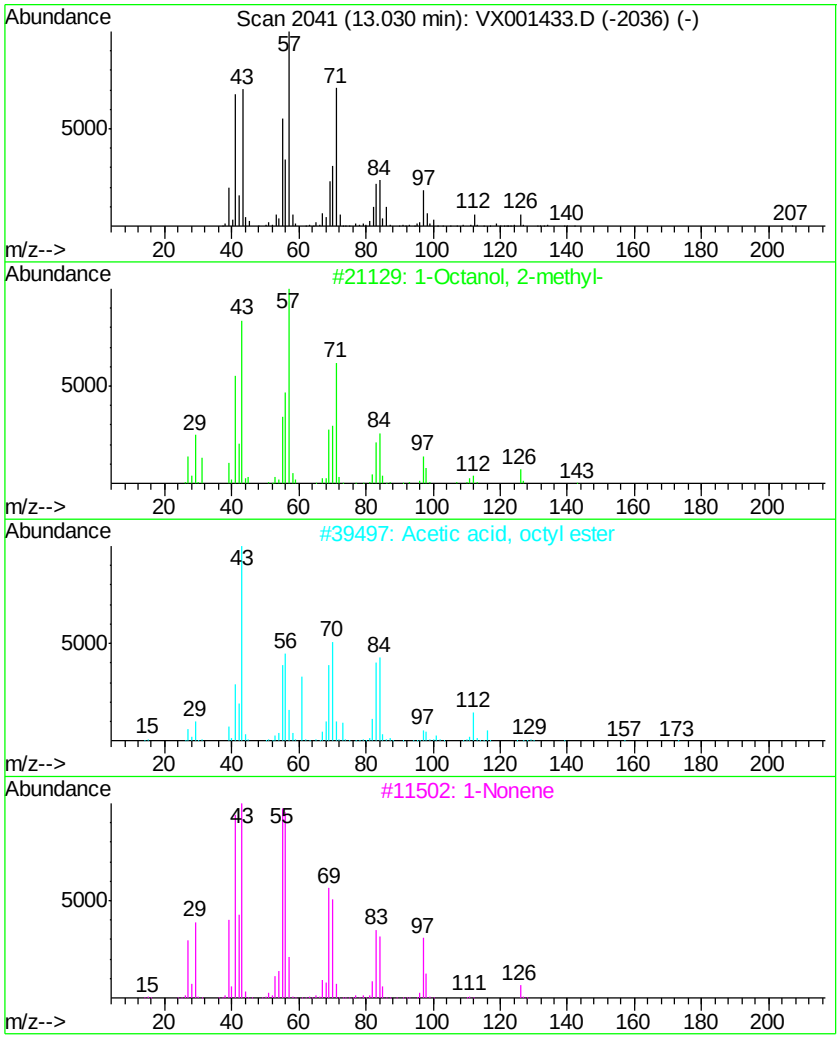
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

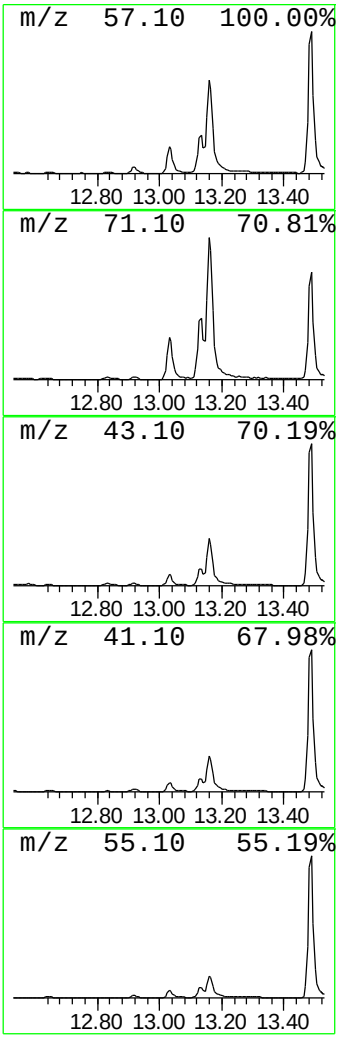
****

Peak Number 5 1-Octanol, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.03	22.82 ug/l	442827	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol, 2-methyl-	144	C9H20O	000818-81-5	78
2	Acetic acid, octyl ester	172	C10H20O2	000112-14-1	43
3	1-Nonene	126	C9H18	000124-11-8	38
4	Cyclopentane, 1-methyl-2-propyl-	126	C9H18	003728-57-2	38
5	1-Dodecene	168	C12H24	000112-41-4	38





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX050518\
Data File : VX001433.D
Acq On : 05 May 2018 21:55
Operator : JC/MD
Sample : J2695-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CS-DRUM-2

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X050518W.M
Quant Title : SW846 8260

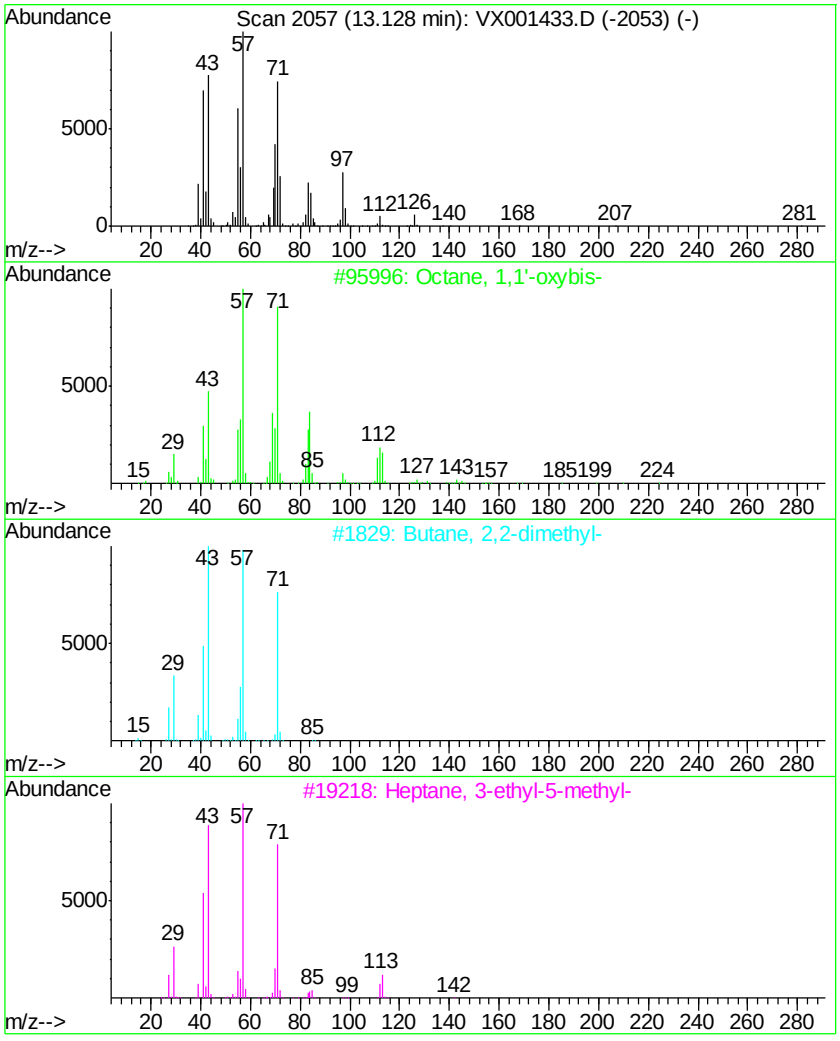
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

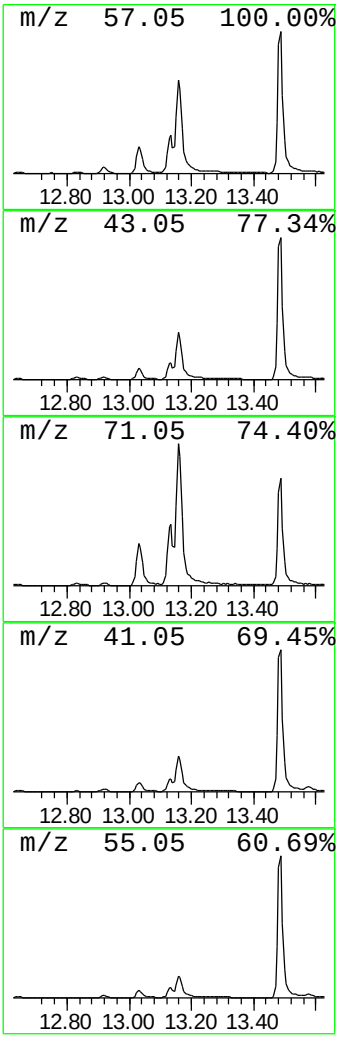
****

Peak Number 6 Octane, 1,1'-oxybis- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.13	25.26 ug/l	490110	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	50
2	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	38
3	Heptane, 3-ethyl-5-methyl-	142	C10H22	052896-90-9	38
4	Cyclopropane, 1-(2-methylbutyl)-...	168	C12H24	064723-36-0	35
5	Cyclodecane	140	C10H20	000293-96-9	35





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX050518\
Data File : VX001433.D
Acq On : 05 May 2018 21:55
Operator : JC/MD
Sample : J2695-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CS-DRUM-2

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X050518W.M
Quant Title : SW846 8260

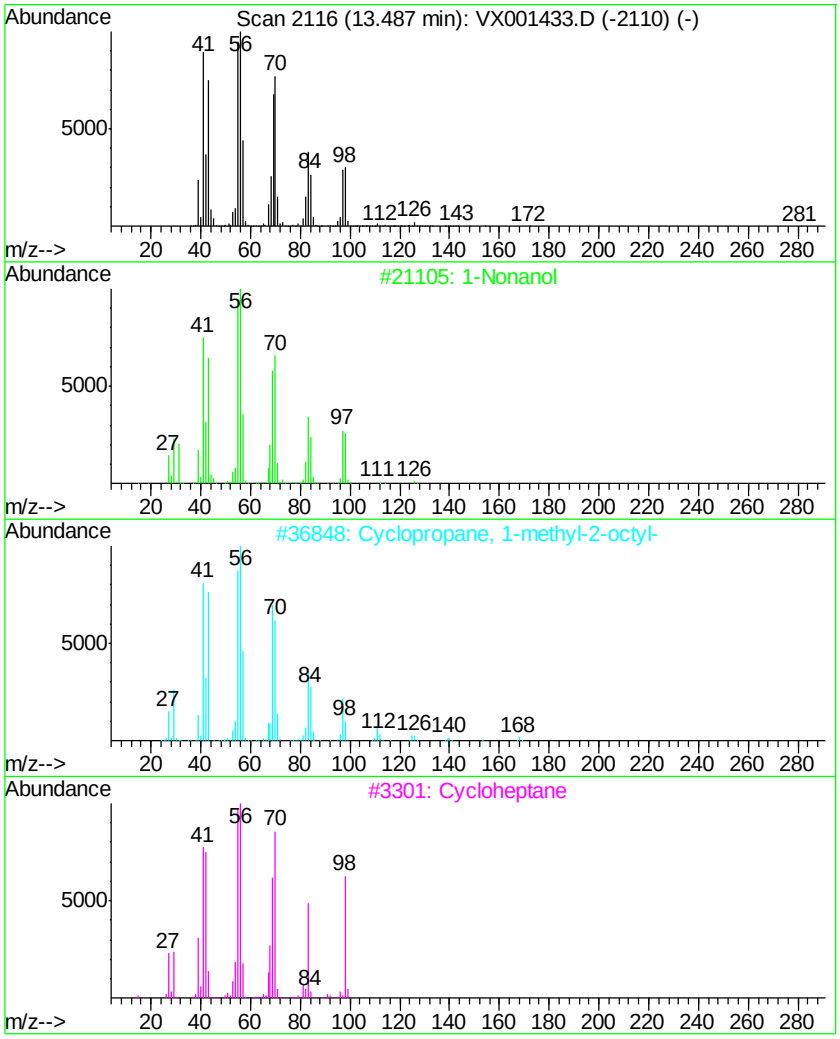
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

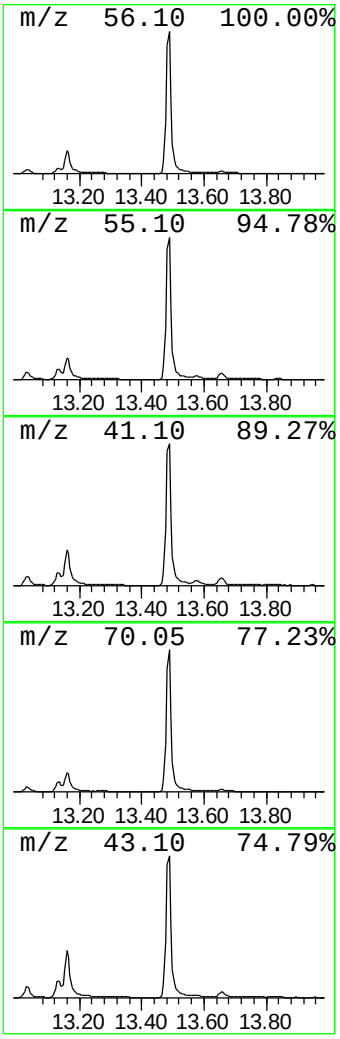
****

Peak Number 8 1-Nonanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	284.98 ug/l	5529960	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonanol	144	C9H20O	000143-08-8	91
2	Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	86
3	Cycloheptane	98	C7H14	000291-64-5	74
4	Cyclopropane, 1-ethyl-2-heptyl-	168	C12H24	074663-86-8	72
5	1-Heptene	98	C7H14	000592-76-7	62





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX050518\
Data File : VX001433.D
Acq On : 05 May 2018 21:55
Operator : JC/MD
Sample : J2695-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CS-DRUM-2

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X050518W.M
Quant Title : SW846 8260

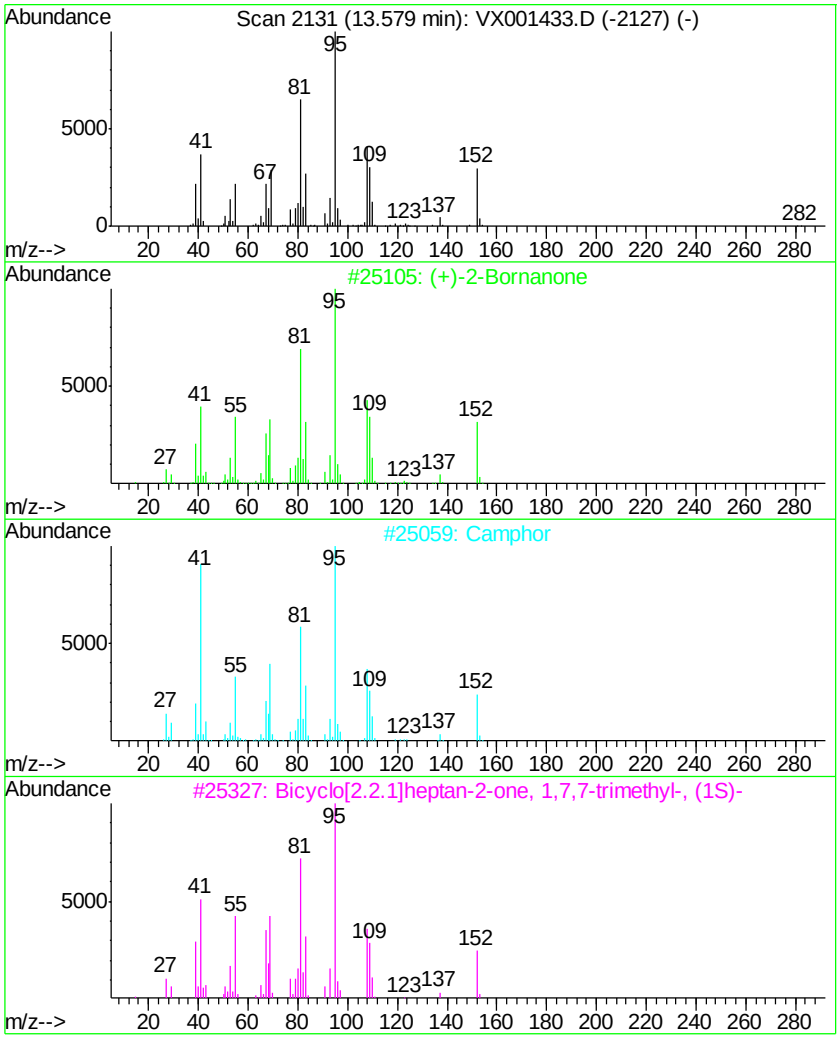
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

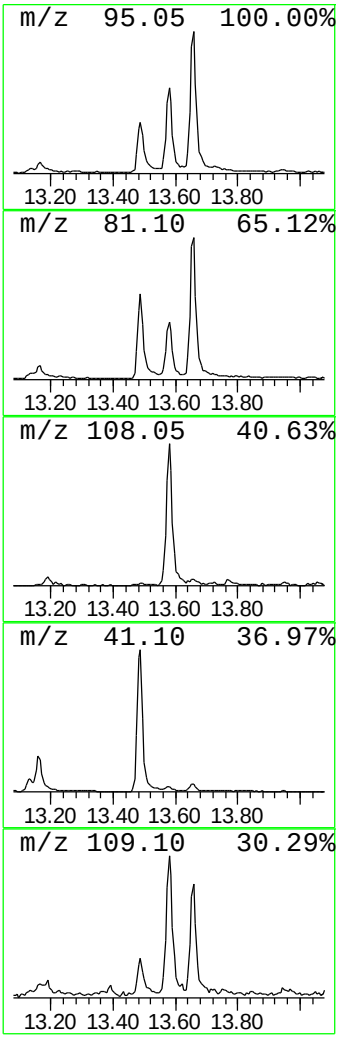
****

Peak Number 9 (+)-2-Bornanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.58	18.93 ug/l	367422	1,4-Dichlorobenzene-d4	12.09

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	95
3	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	94
4	Spirobicyclo[2.2.1]heptane-2,2'-...	236	C14H20O3	1000155-15-2	59
5	1,4-Cyclohexanedimethanol, trans-	144	C8H16O2	003236-48-4	50





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX050518\
Data File : VX001433.D
Acq On : 05 May 2018 21:55
Operator : JC/MD
Sample : J2695-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CS-DRUM-2

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X050518W.M
Quant Title : SW846 8260

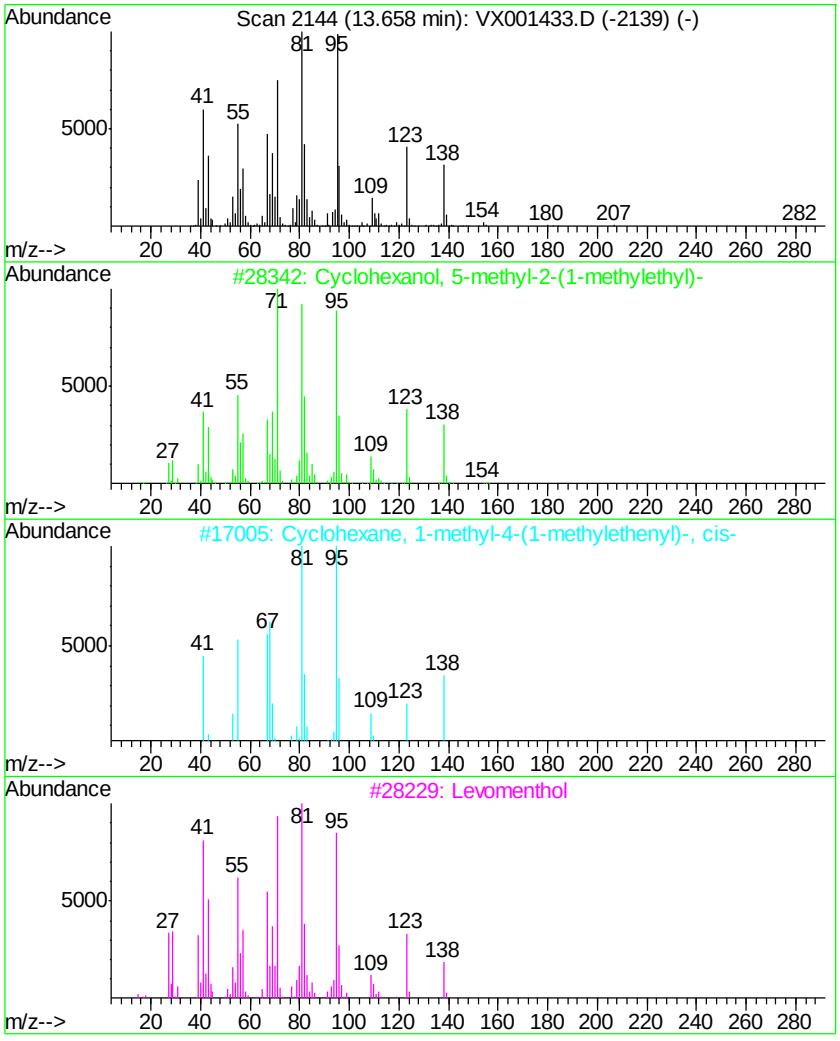
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

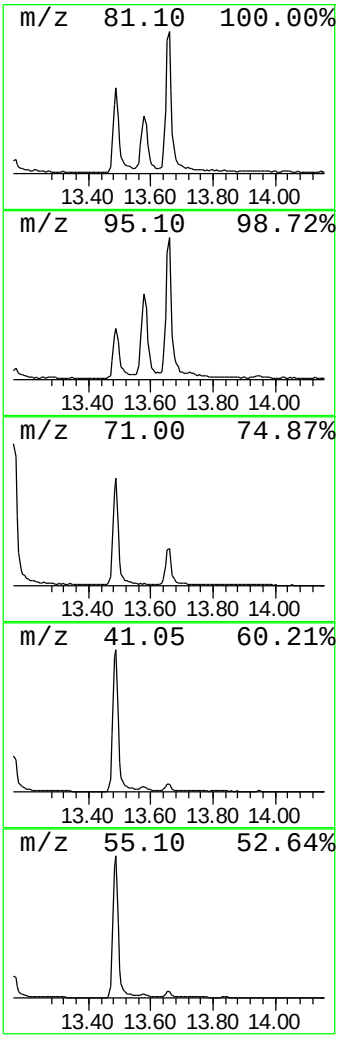
****

Peak Number 10 Cyclohexanol, 5-methyl-2-(1... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	31.05 ug/l	602463	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	001490-04-6	91
2	Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001879-07-8	86
3	Levomenthol	156	C10H20O	002216-51-5	86
4	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	015356-70-4	74
5	L-Menthyl chloroformate	218	C11H19ClO2	014602-86-9	68





Tentatively Identified Compound (LSC) summary

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX050518\
Data File : VX001433.D
Acq On : 05 May 2018 21:55
Operator : JC/MD
Sample : J2695-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CS-DRUM-2

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X050518W.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	22.1	ug/l	284406	1	5.67	641918	50.0
2-Pentanone	7.56	14.5	ug/l	216283	2	6.87	746849	50.0
Eucalyptol	12.16	16.4	ug/l	317335	4	12.09	970233	50.0
1-Octanol, 2-methyl-	13.03	22.8	ug/l	442827	4	12.09	970233	50.0
Octane, 1,1'-oxybis-	13.13	25.3	ug/l	490110	4	12.09	970233	50.0
1-Nonanol	13.49	285.0	ug/l	5529960	4	12.09	970233	50.0
(+)-2-Bornanone	13.58	18.9	ug/l	367422	4	12.09	970233	50.0
Cyclohexanol, 5-m...	13.66	31.1	ug/l	602463	4	12.09	970233	50.0