

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX121919\
 Data File : VX014128.D
 Acq On : 19 Dec 2019 18:11
 Operator : JC/SP
 Sample : K6373-01
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 391218757.2

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.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	1.070	25	30	57	rBV	14280255	30621929	100.00%	33.169%
2	2.100	194	199	209	rBV	474405	717162	2.34%	0.777%
3	2.430	246	253	258	rBV	1538888	2495306	8.15%	2.703%
4	2.564	269	275	277	rVV	221469	352318	1.15%	0.382%
5	2.588	277	279	288	rVB	204455	327010	1.07%	0.354%
6	3.027	341	351	371	rBV	4101638	8881707	29.00%	9.620%
7	4.673	607	621	636	rBV2	3822436	13601194	44.42%	14.732%
8	5.112	681	693	712	rBV2	1318259	3960794	12.93%	4.290%
9	5.490	745	755	766	rBV2	288288	821099	2.68%	0.889%
10	5.655	770	782	795	rVB	516108	1456684	4.76%	1.578%
11	6.051	836	847	856	rBV	321244	853830	2.79%	0.925%
12	6.167	856	866	880	rVV8	129853	602901	1.97%	0.653%
13	6.850	969	978	989	rBV	808908	1855988	6.06%	2.010%
14	7.282	1042	1049	1058	rBV	407657	843948	2.76%	0.914%
15	7.532	1078	1090	1098	rBV	157251	368674	1.20%	0.399%
16	8.636	1262	1271	1277	rBV	248217	417447	1.36%	0.452%
17	8.709	1277	1283	1289	rVV	1727866	2625512	8.57%	2.844%
18	8.776	1289	1294	1300	rVV	424434	650882	2.13%	0.705%
19	9.434	1395	1402	1407	rBV	452111	657643	2.15%	0.712%
20	10.105	1503	1512	1524	rBV	1677243	2552465	8.34%	2.765%
21	10.245	1531	1535	1541	rBV2	218988	373170	1.22%	0.404%
22	10.355	1549	1553	1559	rVB	336876	488736	1.60%	0.529%
23	10.818	1621	1629	1634	rBV	257255	356129	1.16%	0.386%
24	11.135	1675	1681	1686	rBV	1310590	1799450	5.88%	1.949%
25	11.934	1806	1812	1820	rVB3	209589	362309	1.18%	0.392%
26	12.074	1829	1835	1843	rBV2	1750550	2630740	8.59%	2.850%
27	12.153	1843	1848	1852	rVV2	414060	573398	1.87%	0.621%
28	12.269	1862	1867	1869	rBV	352389	484244	1.58%	0.525%
29	12.574	1912	1917	1922	rVV2	418573	603947	1.97%	0.654%
30	12.629	1922	1926	1930	rVB	270182	340181	1.11%	0.368%
31	12.812	1949	1956	1960	rBV	328392	479795	1.57%	0.520%
32	12.958	1968	1980	1985	rBV	2797323	3649557	11.92%	3.953%
33	13.525	2068	2073	2076	rBV2	322754	492031	1.61%	0.533%
34	13.562	2076	2079	2086	rVB	1483308	1887021	6.16%	2.044%

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Integrator: RTE
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Start Thrs: 0.2 Max Peaks: 100
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35	13.641	2086	2092	2100	rBV3	966107	1422365	4.64%	1.541%
36	13.781	2111	2115	2119	rBV2	369386	461202	1.51%	0.500%
37	13.830	2119	2123	2129	rVB	660905	874203	2.85%	0.947%
38	14.153	2169	2176	2188	rBV2	216398	378320	1.24%	0.410%

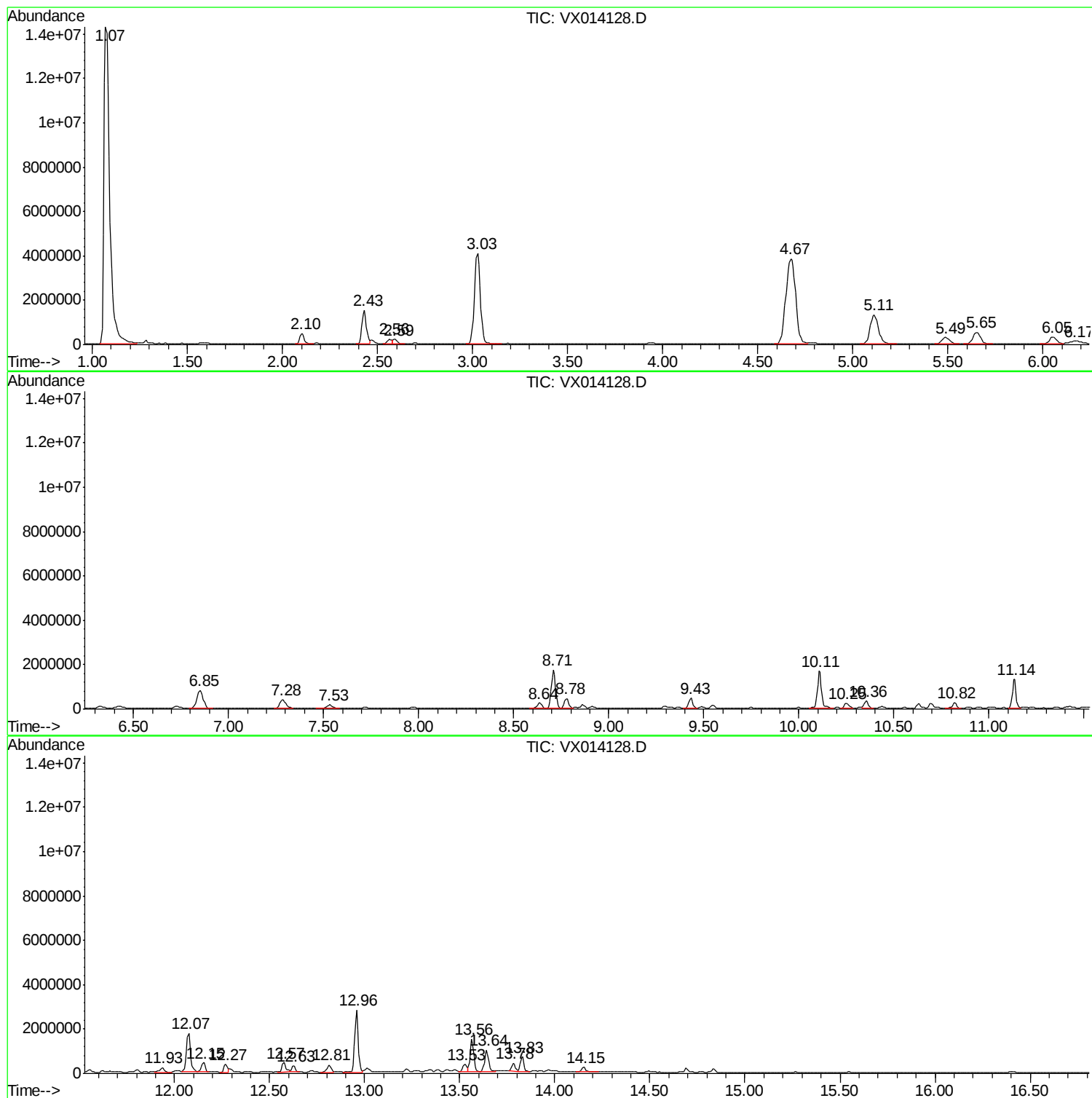
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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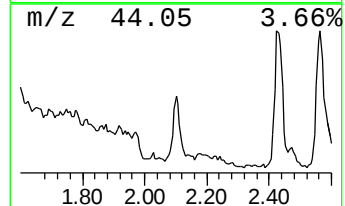
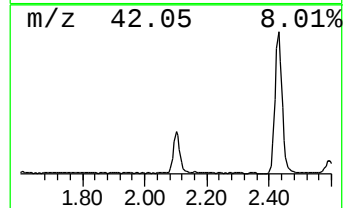
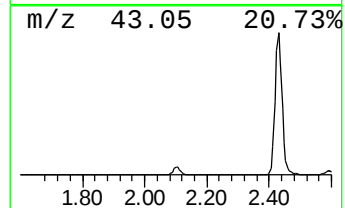
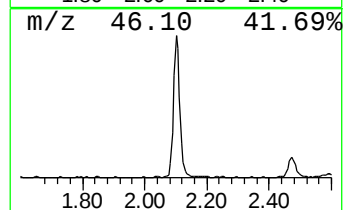
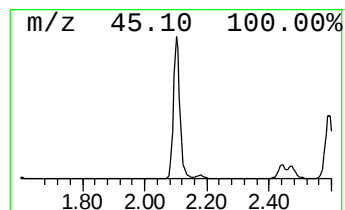
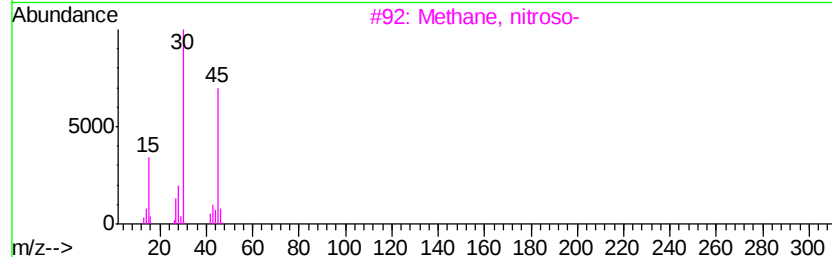
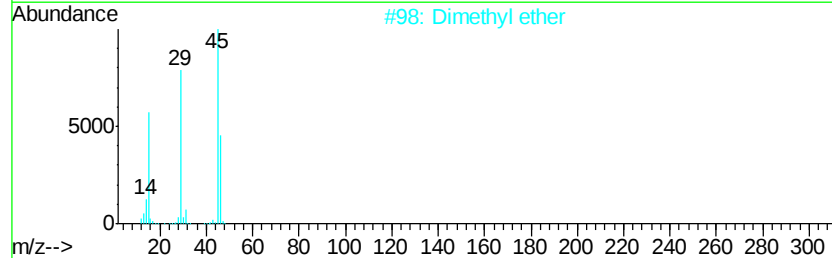
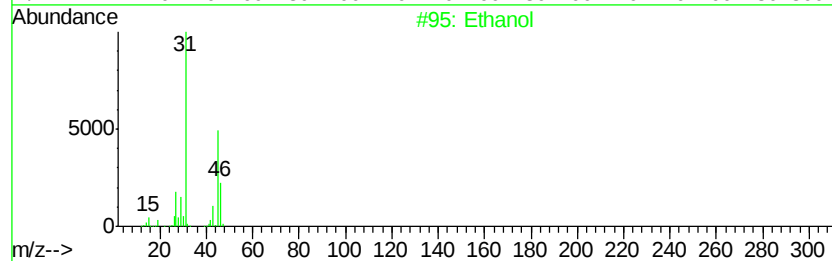
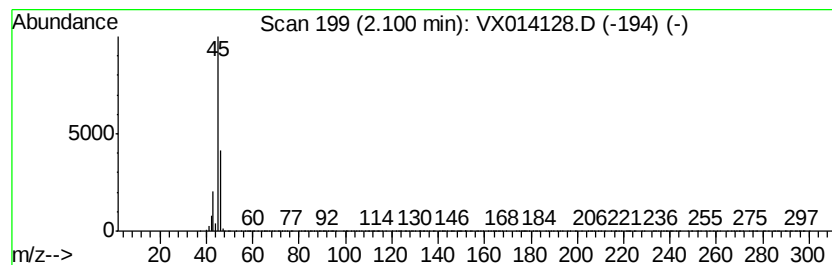
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Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.10	24.62 ug/l	717162	Pentafluorobenzene	5.65

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



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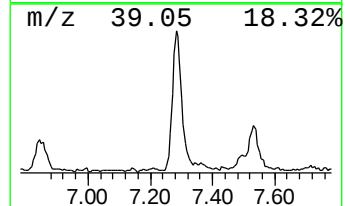
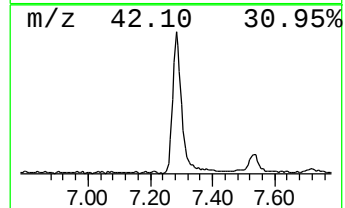
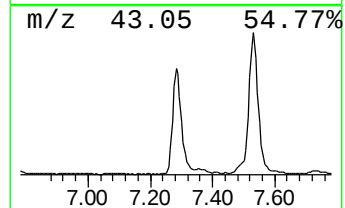
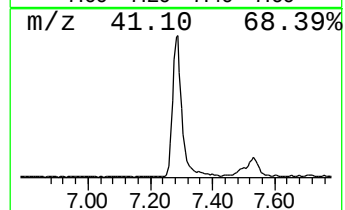
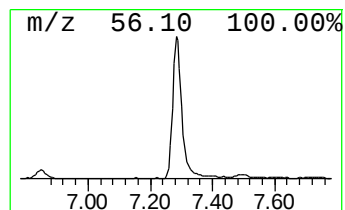
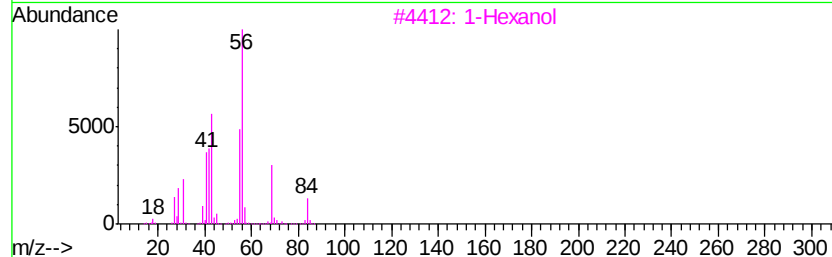
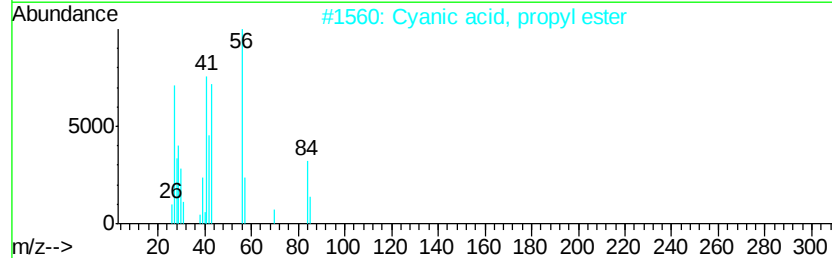
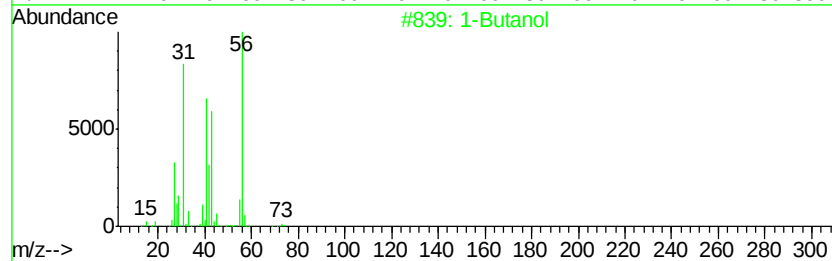
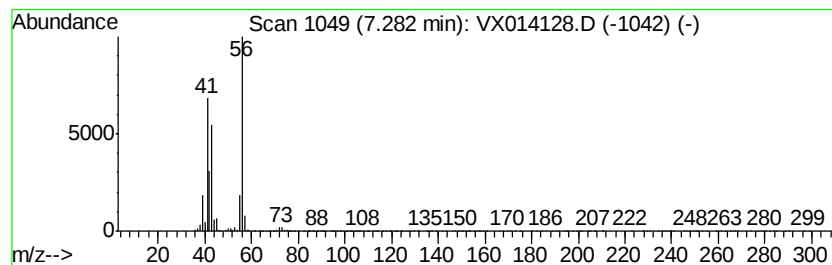
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 1-Butanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.28	22.74 ug/l	843948	1,4-Difluorobenzene	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Butanol	74	C4H10O	000071-36-3	91
2		Cyanoic acid, propyl ester	85	C4H7NO	001768-36-1	50
3		1-Hexanol	102	C6H14O	000111-27-3	43
4		2,3-Dimethylsuccinic acid	146	C6H10O4	013545-04-5	42
5		1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	38



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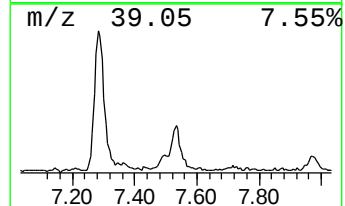
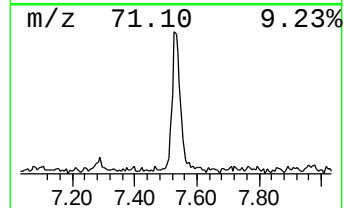
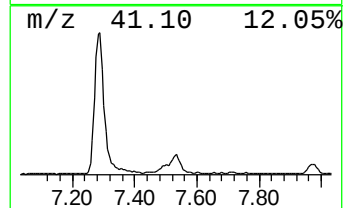
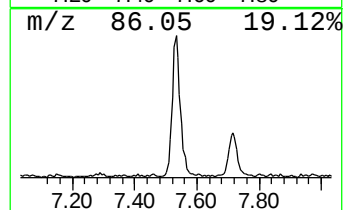
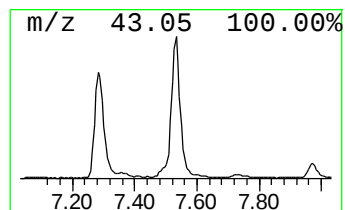
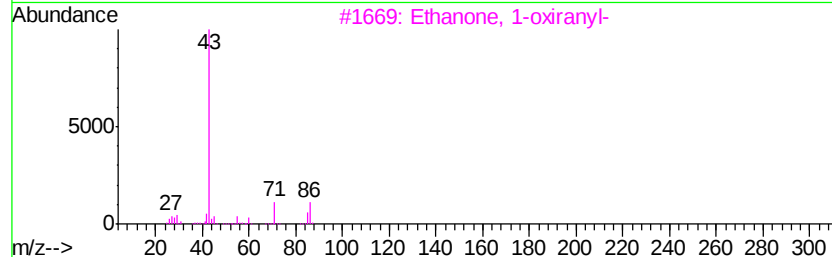
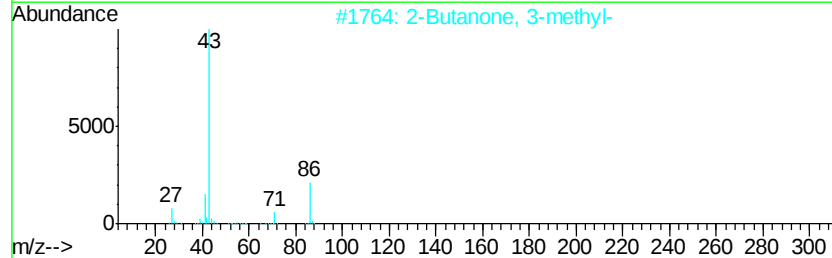
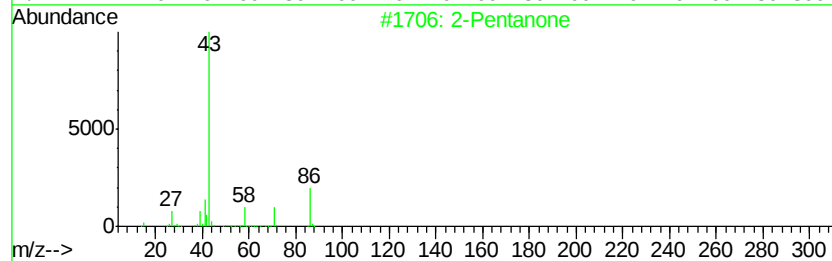
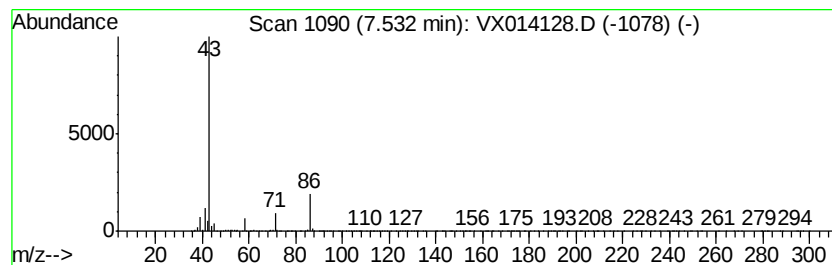
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 2-Pentanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.53	9.93 ug/l	368674	1,4-Difluorobenzene	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone	86	C5H10O	000107-87-9	74
2		2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	64
3		Ethanone, 1-oxiran-2-yl-	86	C4H6O2	004401-11-0	39
4		2,3-Butanedione	86	C4H6O2	000431-03-8	9
5		dl-Mevalonic acid lactone	130	C6H10O3	000674-26-0	9



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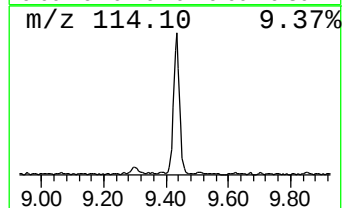
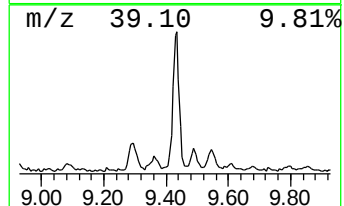
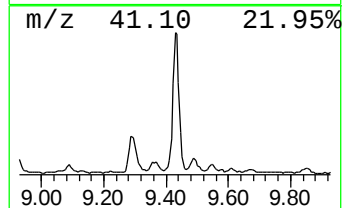
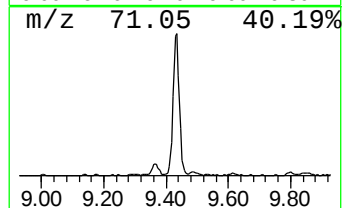
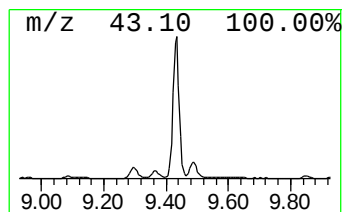
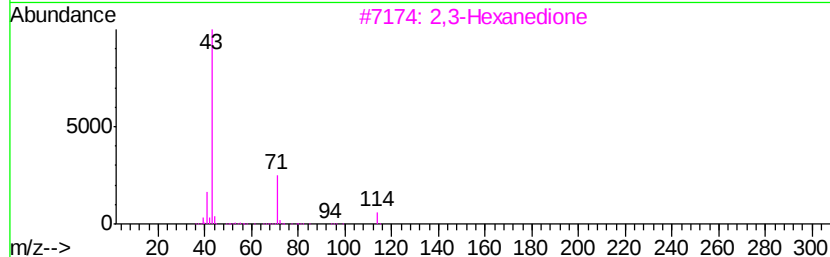
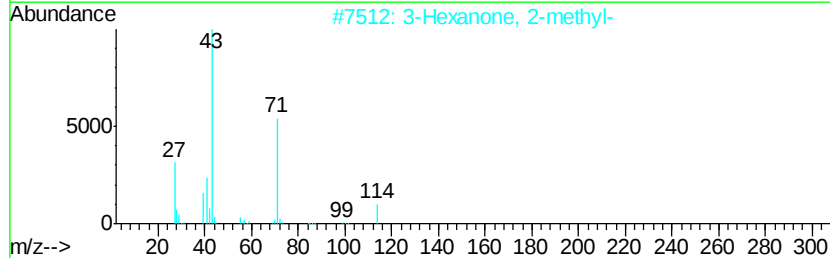
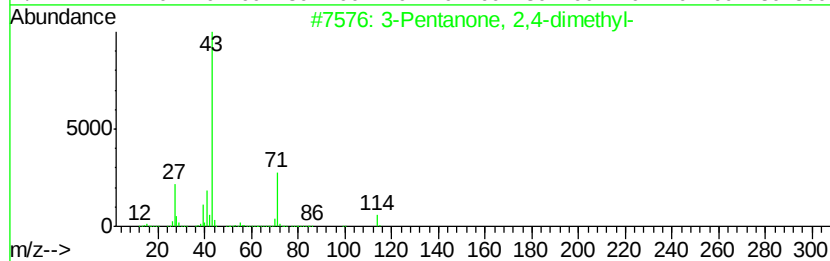
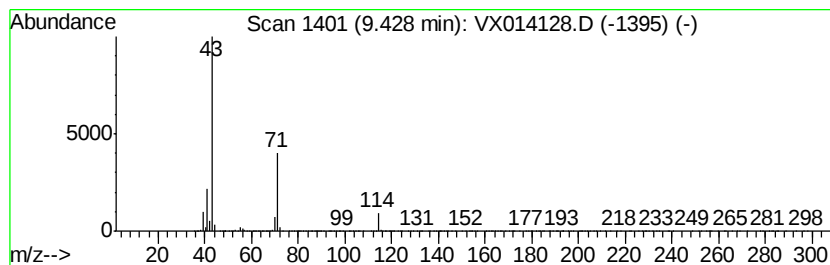
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 3-Pentanone, 2,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.43	12.88 ug/l	657643	Chlorobenzene-d5	10.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	90
2		3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	72
3		2,3-Hexanedione	114	C6H10O2	003848-24-6	72
4		4-Heptanone	114	C7H14O	000123-19-3	59
5		Pentane, 3-ethyl-	100	C7H16	000617-78-7	38



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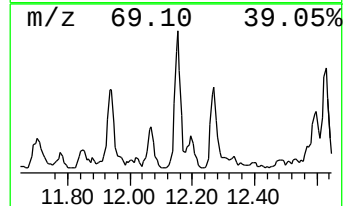
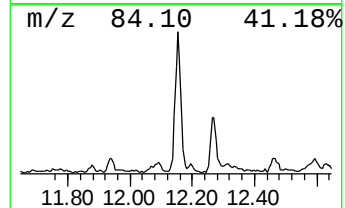
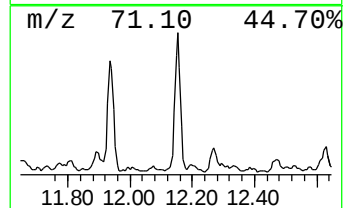
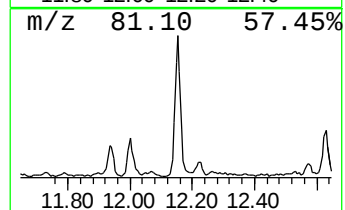
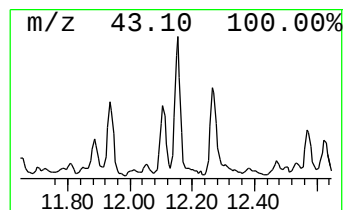
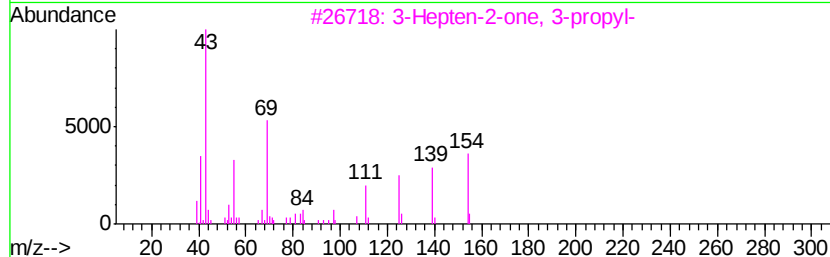
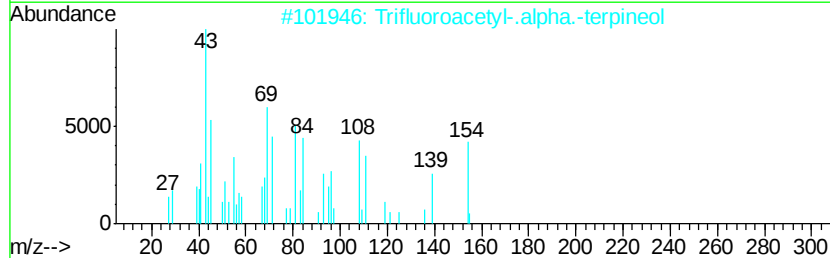
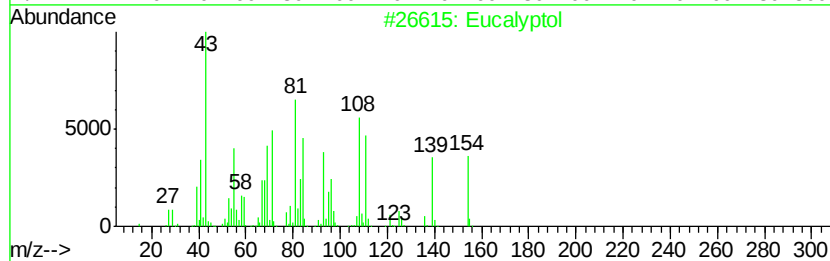
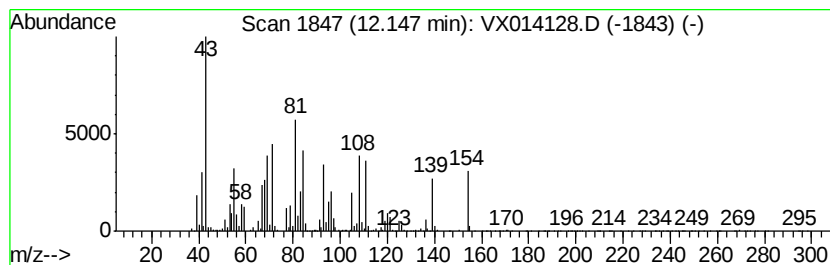
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Peak Number 6 Eucalyptol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.15	10.90 ug/l	573398	1,4-Dichlorobenzene-d4	12.07
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	53
3	3-Hepten-2-one, 3-propyl-	154 C10H18O	032064-69-0	25
4	2-Isopropyl-5-methylhex-2-enal	154 C10H18O	035158-25-9	22
5	Sulfurous acid, 2-pentyl propyl ...	194 C8H18O3S	1000309-15-1	22



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX121919\
Data File : VX014128.D
Acq On : 19 Dec 2019 18:11
Operator : JC/SP
Sample : K6373-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 19 Sample Multiplier: 1

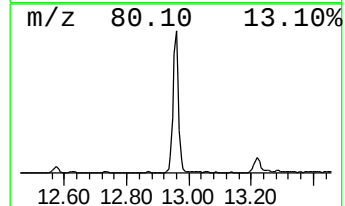
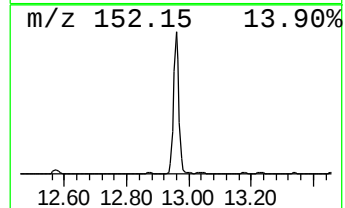
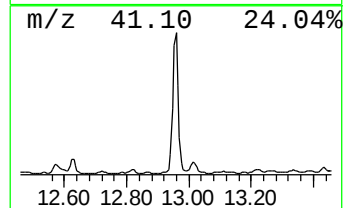
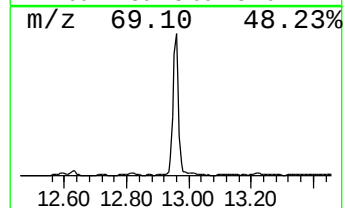
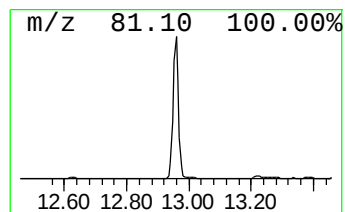
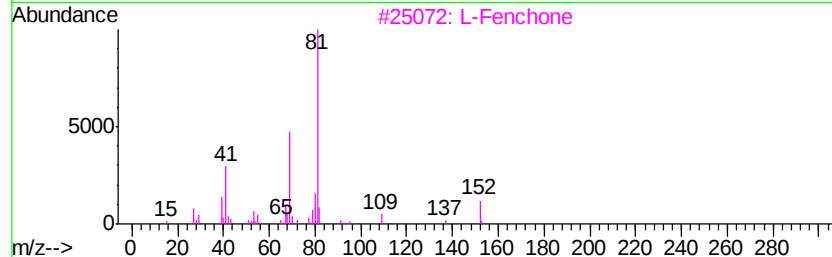
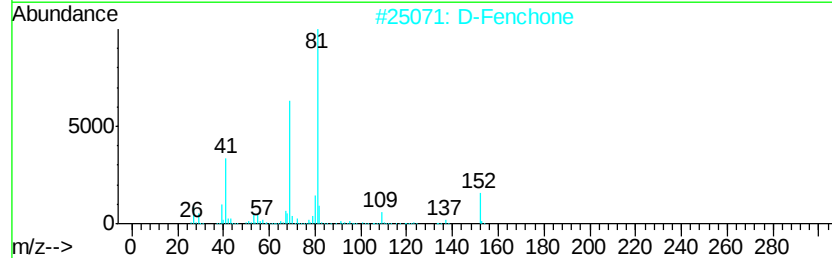
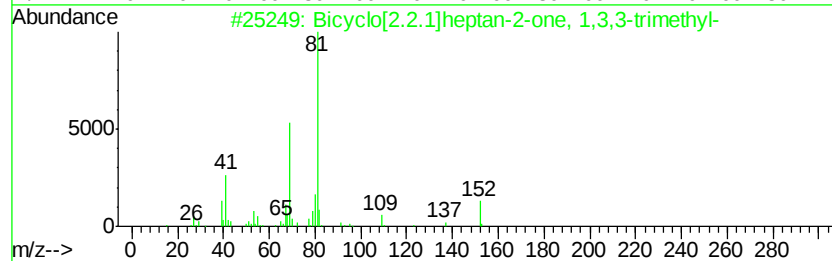
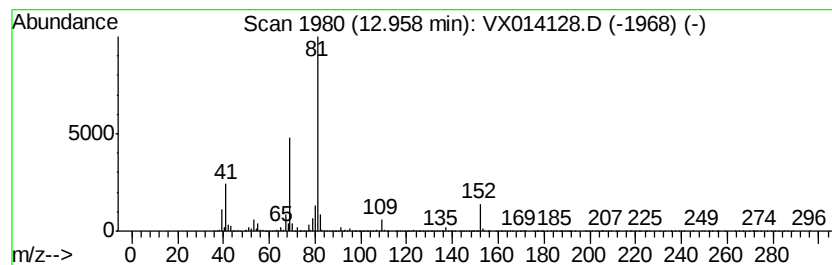
Instrument :
MSVOA_X
ClientSampleId :
391218757.2

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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

Peak Number 8 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.96	69.36 ug/l	3649560	1,4-Dichlorobenzene-d4	12.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicvclo[2.2.1]heptan-2-one, 1,3,...	152	C10H16O	001195-79-5	95
2	D-Fenchone	152	C10H16O	004695-62-9	94
3	L-Fenchone	152	C10H16O	007787-20-4	94
4	Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	000529-00-0	38
5	Formic acid, trans-4-methylcyclo...	142	C8H14O2	1000368-24-5	36



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX121919\
Data File : VX014128.D
Acq On : 19 Dec 2019 18:11
Operator : JC/SP
Sample : K6373-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 19 Sample Multiplier: 1

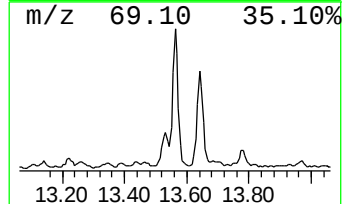
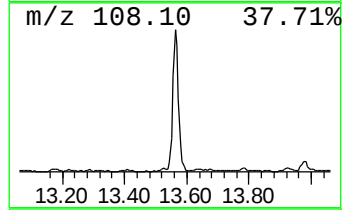
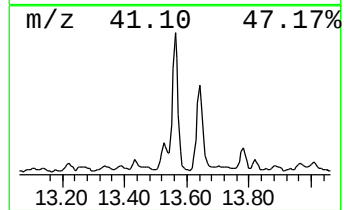
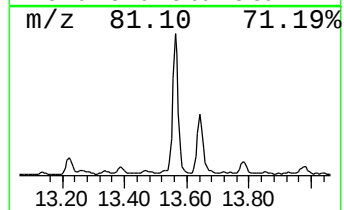
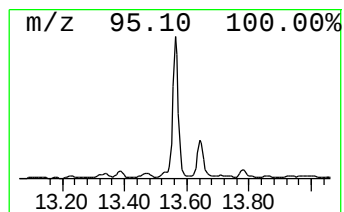
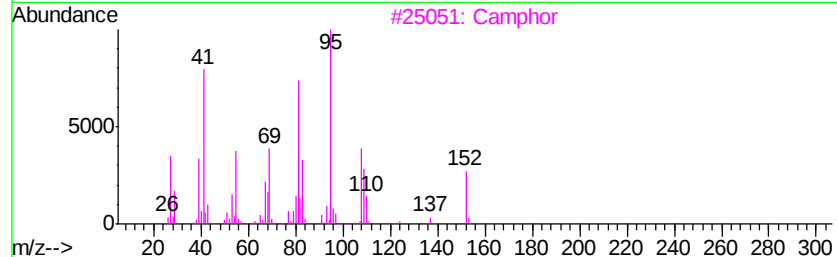
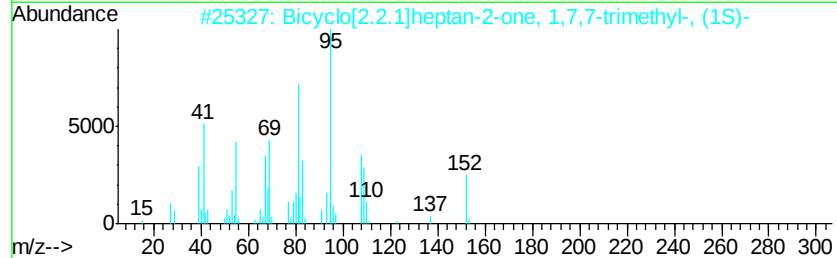
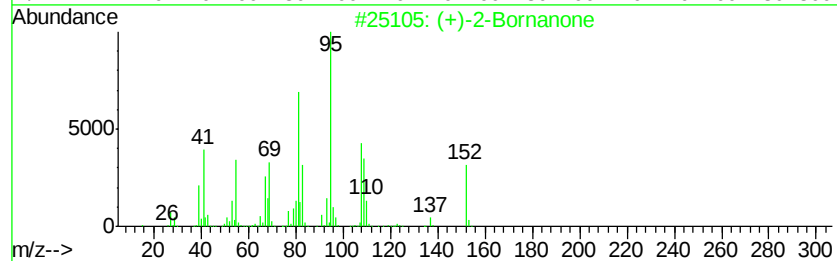
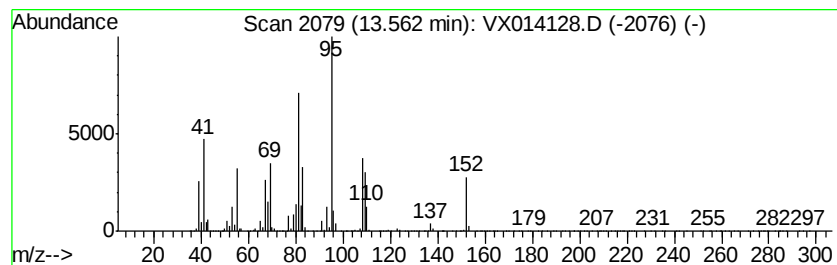
Instrument :
MSVOA_X
ClientSampleId :
391218757.2

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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

Peak Number 9 (+)-2-Bornanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.56	35.86 ug/l	1887020	1,4-Dichlorobenzene-d4	12.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-2-Bornanone	152	C10H16O	000464-49-3	98
2	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	98
3	Camphor	152	C10H16O	000076-22-2	96
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	49



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX121919\
Data File : VX014128.D
Acq On : 19 Dec 2019 18:11
Operator : JC/SP
Sample : K6373-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
391218757.2

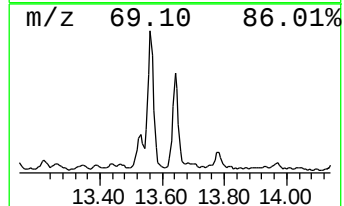
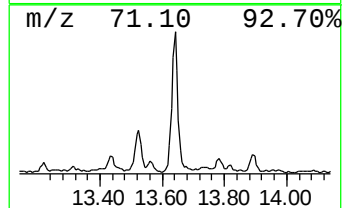
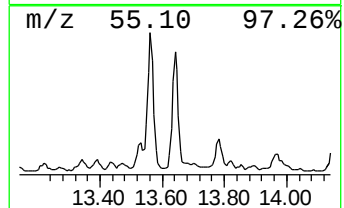
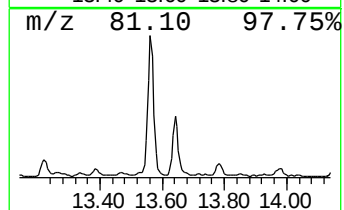
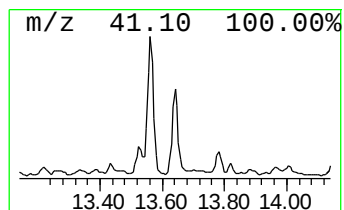
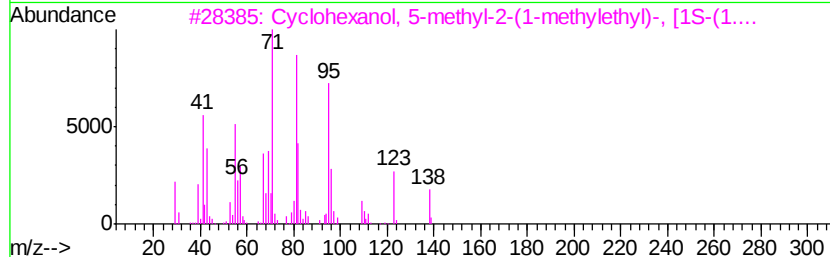
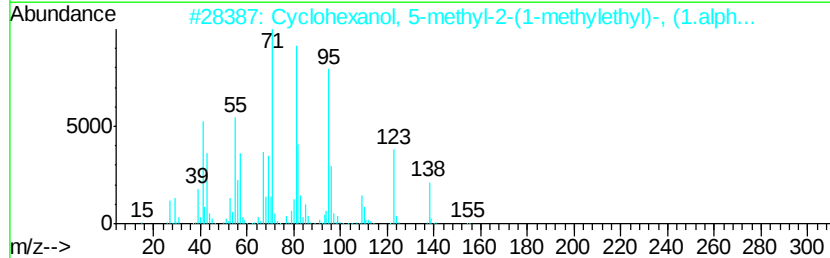
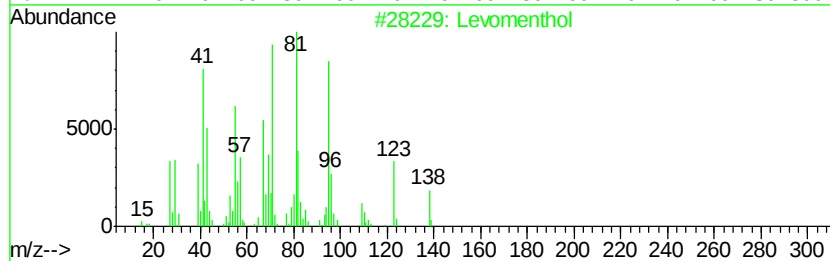
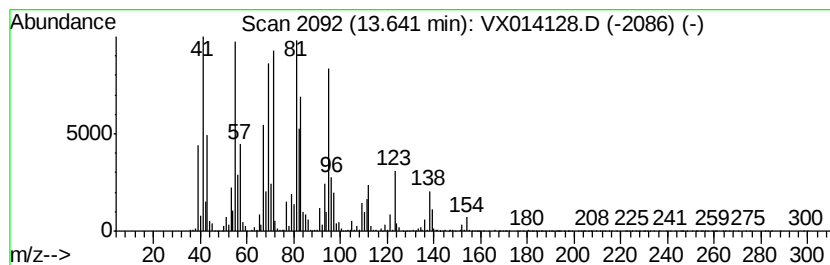
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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

Peak Number 10 Levomenthol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.64	27.03 ug/l	1422370	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Levomenthol	156	C10H20O	002216-51-5	58
2		Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	015356-70-4	58
3		Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	002216-52-6	52
4		Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	001490-04-6	49
5		Bicyclo[3.1.0]hexan-2-one, 5-(1-...	138	C9H14O	000513-20-2	46



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX121919\
Data File : VX014128.D
Acq On : 19 Dec 2019 18:11
Operator : JC/SP
Sample : K6373-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
391218757.2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol	2.10	24.6	ug/l	717162	1	5.65	1456680	50.0
1-Butanol	7.28	22.7	ug/l	843948	2	6.85	1855990	50.0
2-Pentanone	7.53	9.9	ug/l	368674	2	6.85	1855990	50.0
3-Pentanone, 2,4-...	9.43	12.9	ug/l	657643	3	10.11	2552470	50.0
Eucalyptol	12.15	10.9	ug/l	573398	4	12.07	2630740	50.0
Cyclohexene, 1-me...	12.57	11.5	ug/l	603947	4	12.07	2630740	50.0
Bicyclo[2.2.1]hep...	12.96	69.4	ug/l	3649560	4	12.07	2630740	50.0
(+)-2-Bornanone	13.56	35.9	ug/l	1887020	4	12.07	2630740	50.0
Levomenthol	13.64	27.0	ug/l	1422370	4	12.07	2630740	50.0