

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX020620\
 Data File : VX014856.D
 Acq On : 06 Feb 2020 18:30
 Operator : JC/SP
 Sample : L1420-01
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 400205799-VOA

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\82X012220W.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	62	rBV	17598383	41176586	100.00%	43.062%
2	3.027	339	351	369	rBV	6262995	13629770	33.10%	14.254%
3	4.685	607	623	635	rBV	4331659	14012189	34.03%	14.654%
4	5.106	681	692	711	rBV	1425969	4273757	10.38%	4.469%
5	5.490	743	755	767	rBV	245192	702531	1.71%	0.735%
6	5.649	767	781	794	rVB	438385	1225370	2.98%	1.281%
7	6.051	836	847	856	rBV2	264198	707776	1.72%	0.740%
8	6.850	969	978	991	rVB	673753	1557488	3.78%	1.629%
9	8.709	1276	1283	1289	rBV	1444427	2191664	5.32%	2.292%
10	9.428	1392	1401	1407	rBV	581551	883736	2.15%	0.924%
11	10.105	1502	1512	1524	rBV	1462571	2205628	5.36%	2.307%
12	10.355	1548	1553	1558	rVB	295503	420874	1.02%	0.440%
13	11.129	1674	1680	1686	rBV	1191287	1606212	3.90%	1.680%
14	12.074	1828	1835	1842	rBV	1586925	2175099	5.28%	2.275%
15	12.153	1842	1848	1852	rBV2	345699	535927	1.30%	0.560%
16	12.812	1949	1956	1961	rBV	651088	916535	2.23%	0.958%
17	12.958	1968	1980	1985	rBV	3448264	4464018	10.84%	4.668%
18	13.525	2068	2073	2077	rBV3	595909	856440	2.08%	0.896%
19	13.641	2087	2092	2101	rBV2	1141199	1528097	3.71%	1.598%
20	14.153	2168	2176	2187	rBV2	330837	552723	1.34%	0.578%

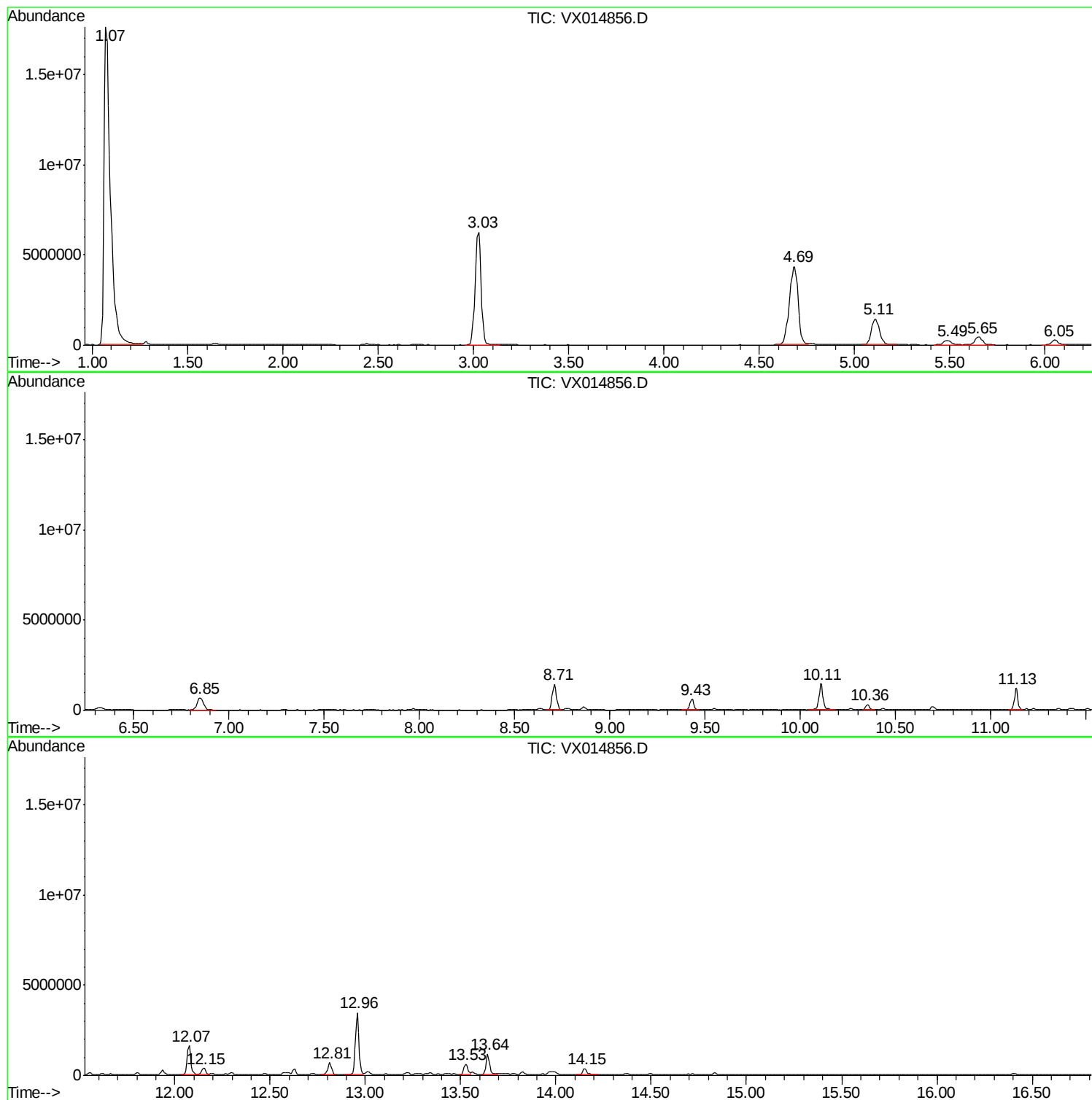
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Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX020620\
Data File : VX014856.D
Acq On : 06 Feb 2020 18:30
Operator : JC/SP
Sample : L1420-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
400205799-VOA

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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



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Sample : L1420-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
400205799-VOA

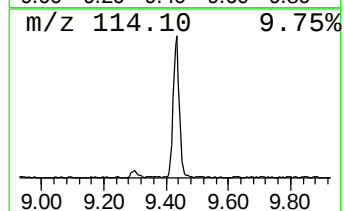
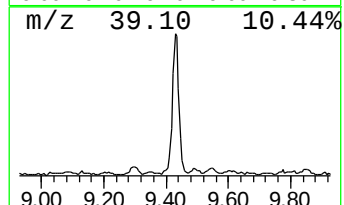
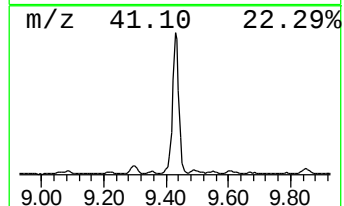
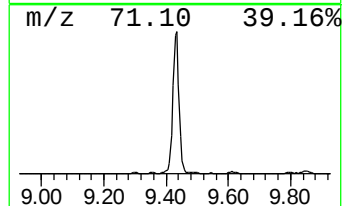
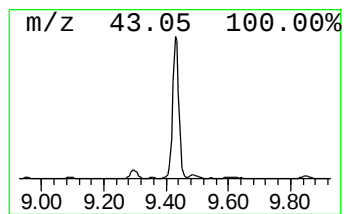
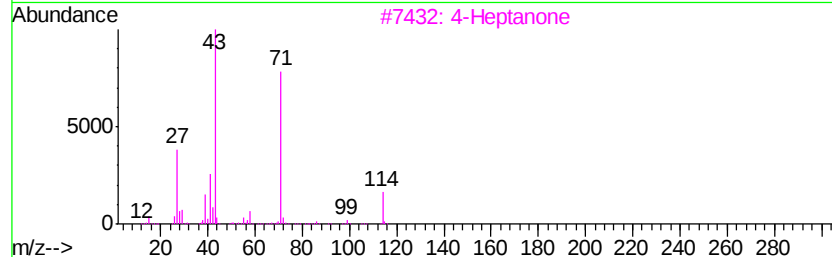
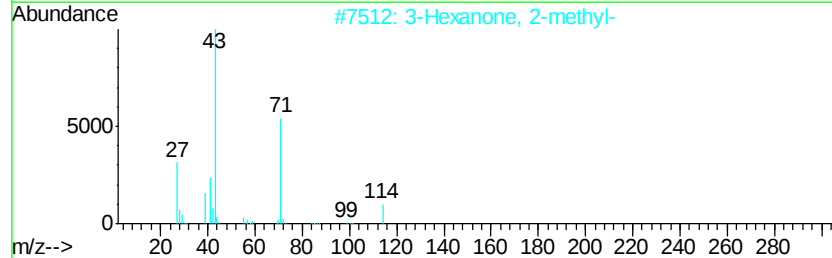
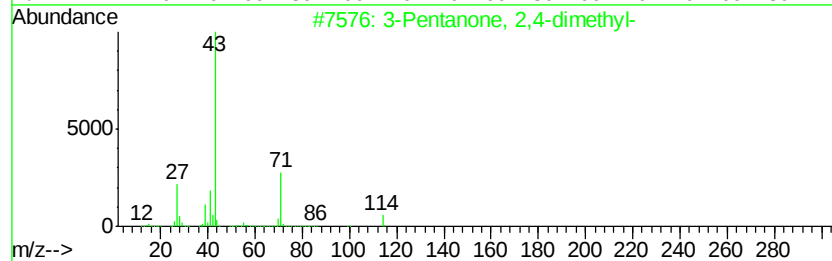
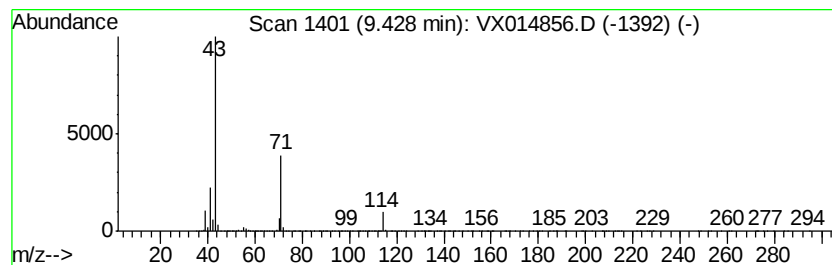
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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

Peak Number 3 3-Pentanone, 2,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.43	20.03 ug/l	883736	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	90
3		4-Heptanone	114	C7H14O	000123-19-3	59
4		2,3-Hexanedione	114	C6H10O2	003848-24-6	50
5		Pentane, 3-ethyl-	100	C7H16	000617-78-7	39



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Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

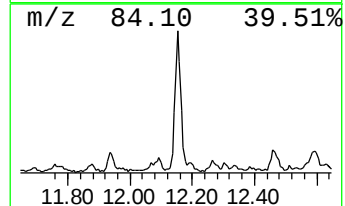
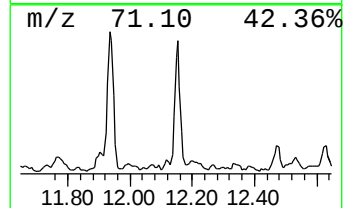
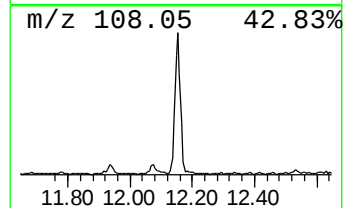
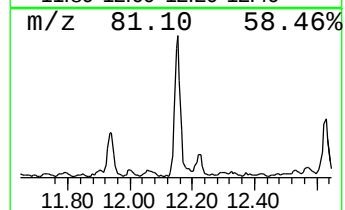
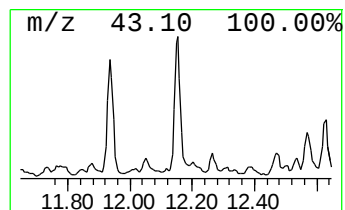
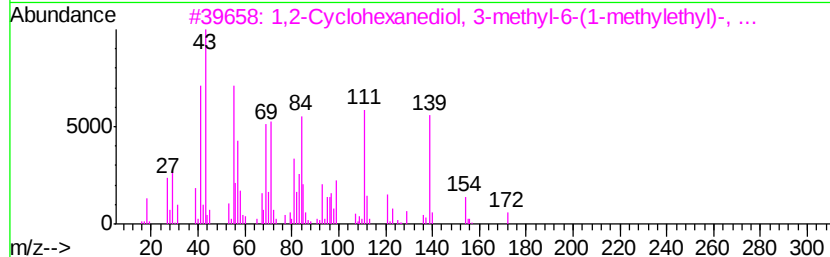
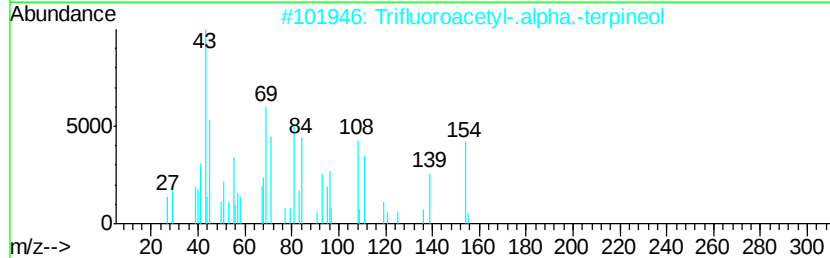
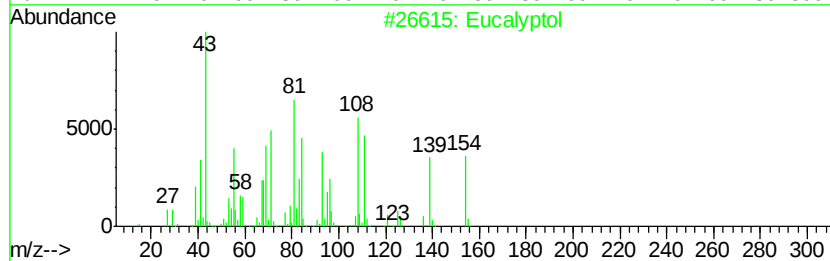
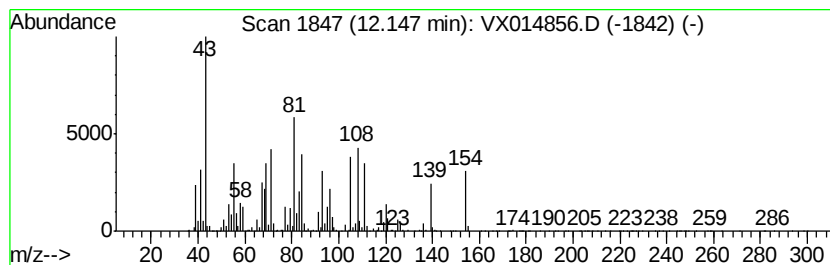
Instrument :
MSVOA_X
ClientSampleId :
400205799-VOA

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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.
12.15	12.32 ug/l	535927	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	83
3	1,2-Cyclohexanediol, 3-methyl-6-...	172 C10H20O2	042962-93-6	45
4	2-Oxabicyclo[2.2.2]octan-6-ol, 1...	170 C10H18O2	018679-48-6	35
5	exo-2-Hydroxycineole	170 C10H18O2	092999-78-5	25



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Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
400205799-VOA

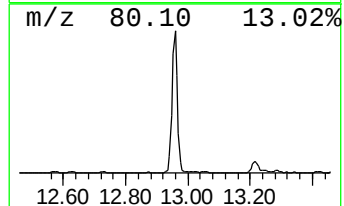
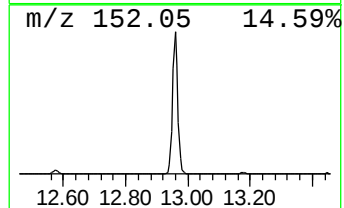
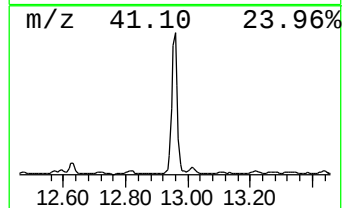
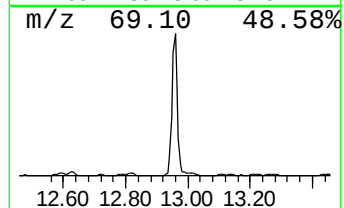
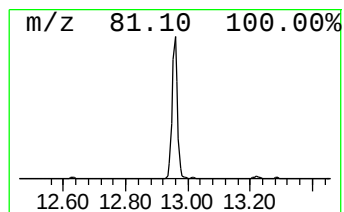
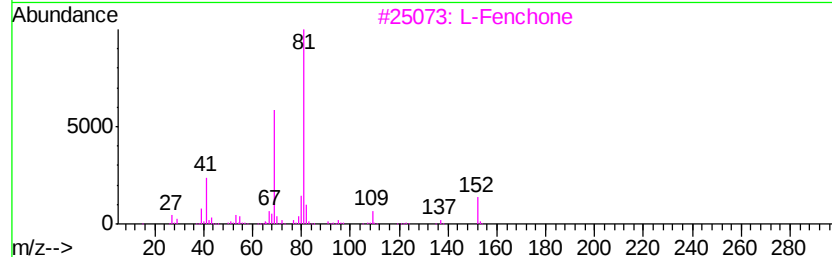
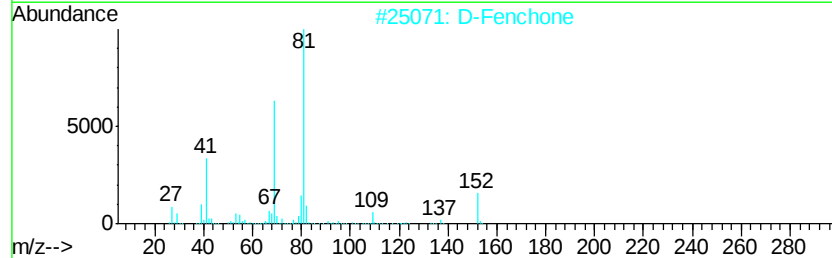
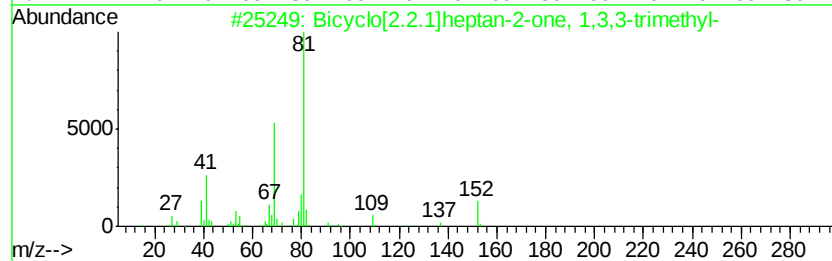
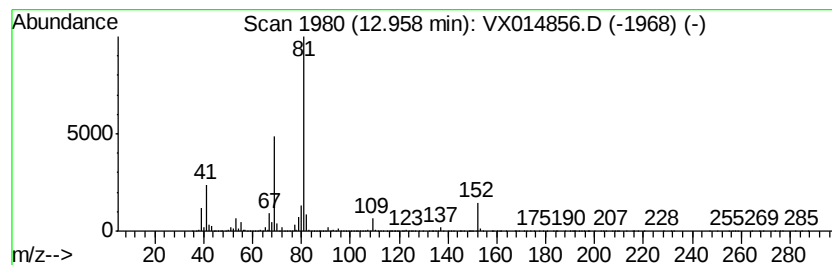
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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

Peak Number 6 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.96	102.62 ug/l	4464020	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[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		Formic acid, cis-4-methylcyclohe...	142	C8H14O2	1000368-24-7	36
5		Cyclohexane, 1,3-dichloro-, trans-	152	C6H10Cl2	024955-62-2	36



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Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
400205799-VOA

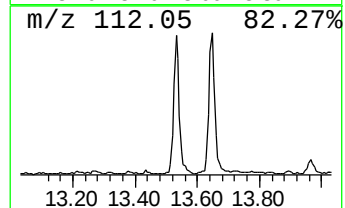
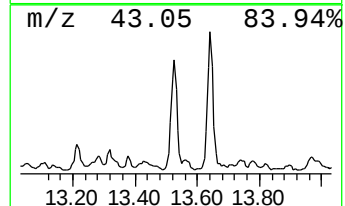
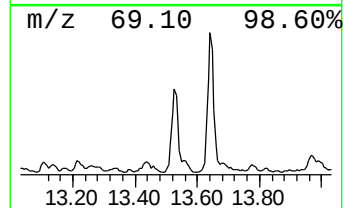
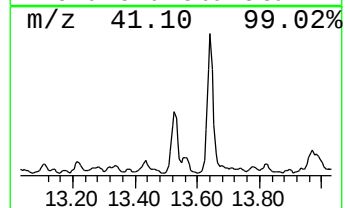
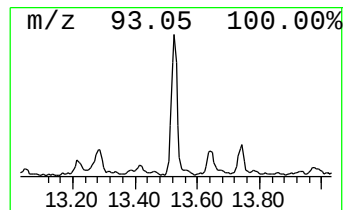
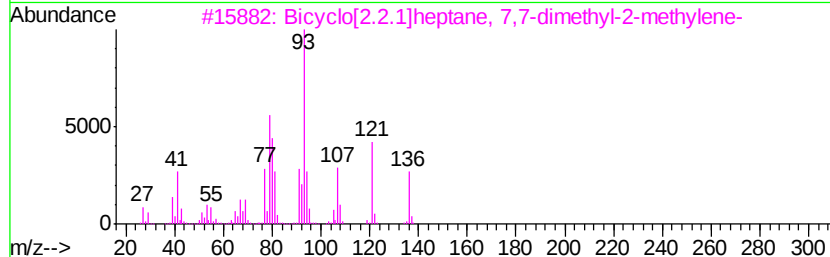
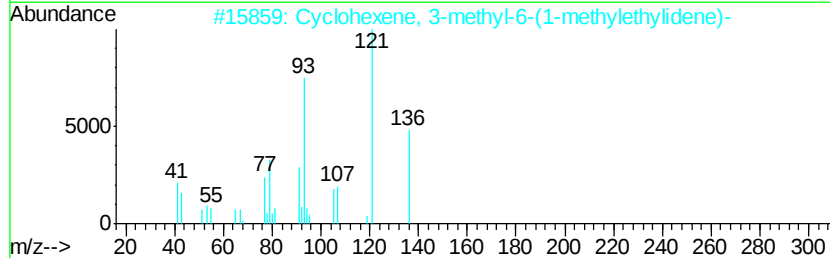
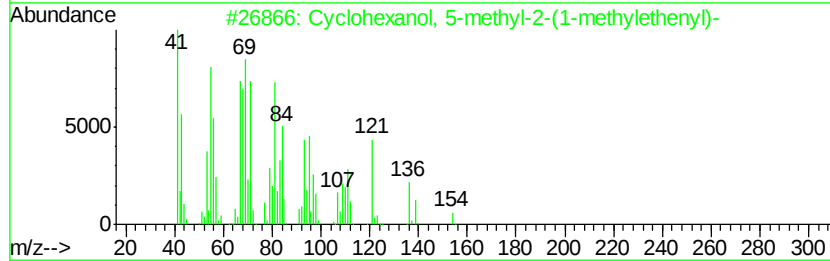
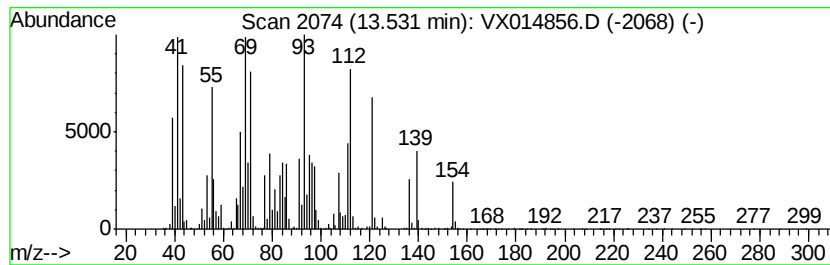
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Quant Title : SW846 8260

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

Peak Number 7 unknown13.53 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.53	19.69 ug/l	856440	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexanol, 5-methyl-2-(1-meth...	154	C10H18O	007786-67-6	41
2		Cyclohexene, 3-methyl-6-(1-methv...	136	C10H16	000586-63-0	25
3		Bicyclo[2.2.1]heptane, 7,7-dimet...	136	C10H16	000471-84-1	20
4		Cyclohexene, 1-methyl-3-(1-methv...	136	C10H16	000499-03-6	18
5		Camphene	136	C10H16	000079-92-5	15



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ALS Vial : 21 Sample Multiplier: 1

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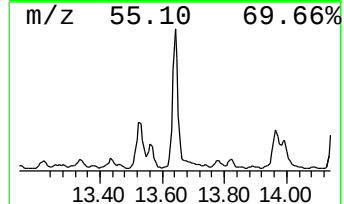
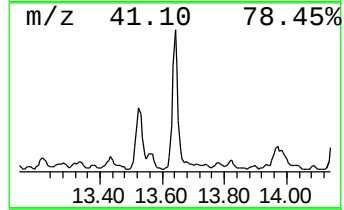
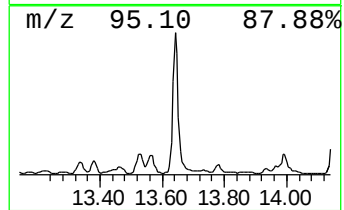
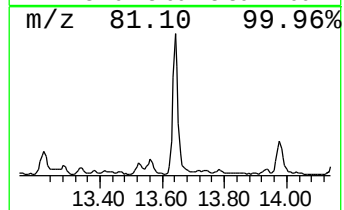
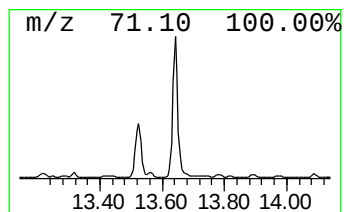
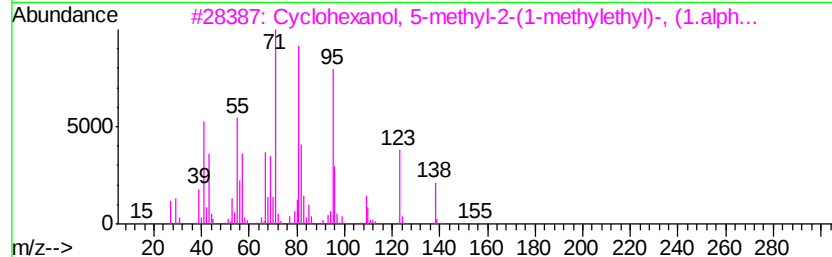
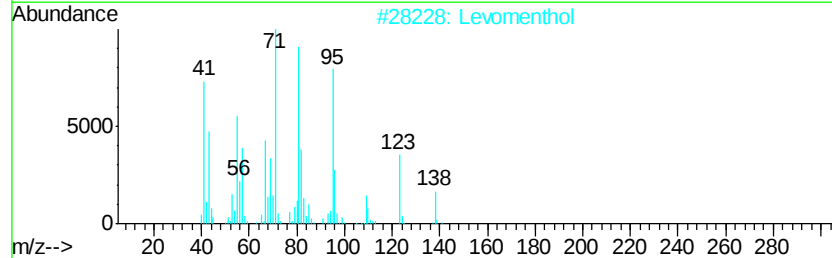
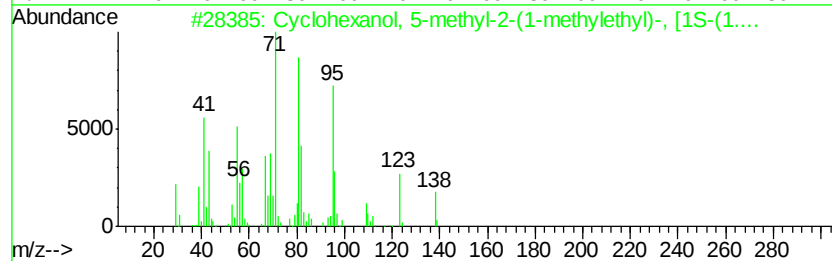
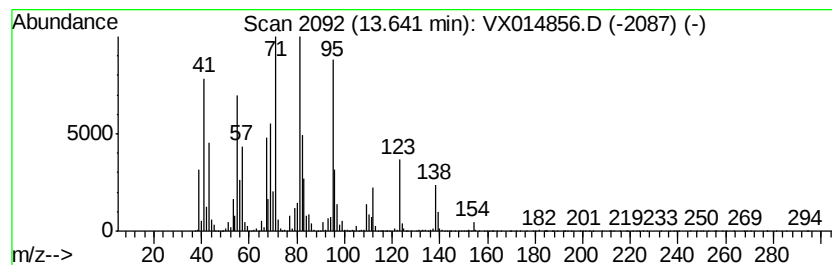
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Cyclohexanol, 5-methyl-2-(1... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.64	35.13 ug/l	1528100	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	002216-52-6	91
2		Levomenthol	156	C10H20O	002216-51-5	90
3		Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	015356-70-4	90
4		dl-Menthol	156	C10H20O	000089-78-1	87
5		Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	001490-04-6	87



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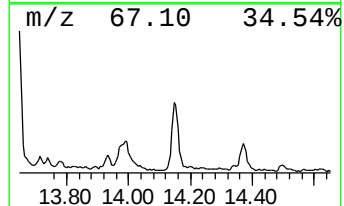
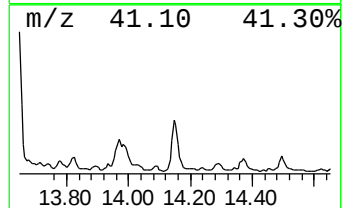
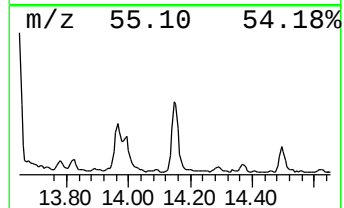
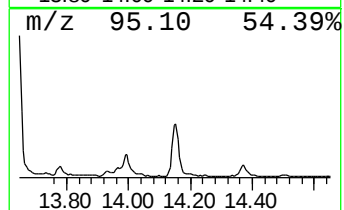
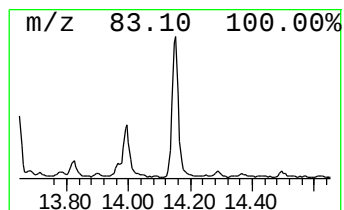
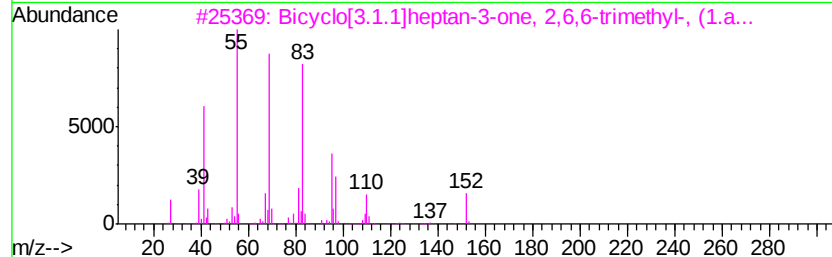
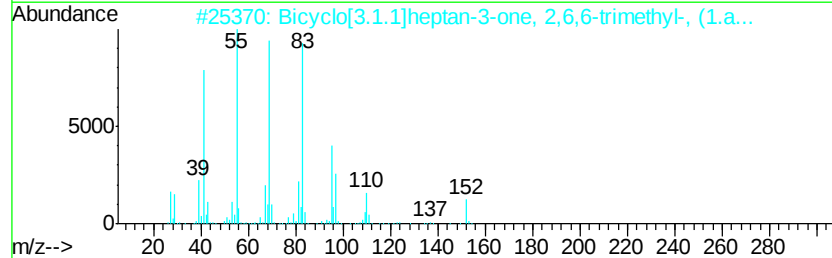
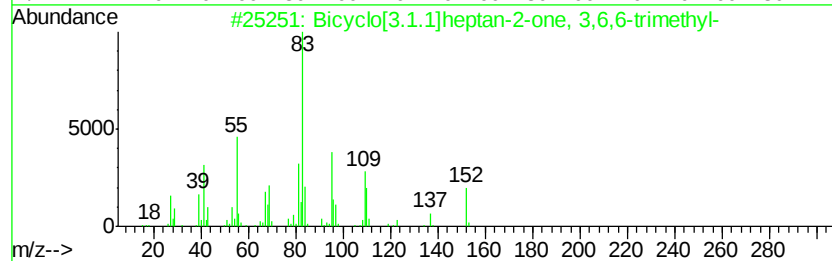
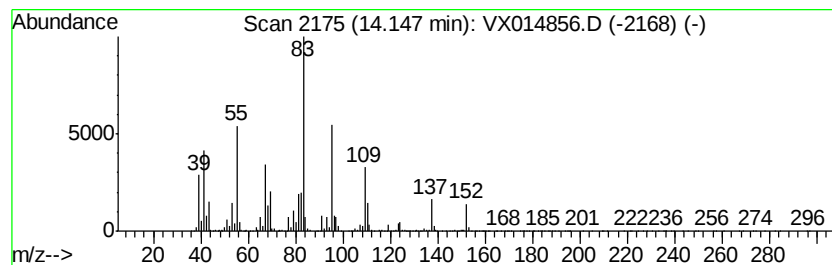
Instrument :
MSVOA_X
ClientSampleId :
400205799-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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

Peak Number 9 Bicyclo[3.1.1]heptan-2-one,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.15	12.71 ug/l	552723	1,4-Dichlorobenzene-d4	12.07
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Bicyclo[3.1.1]heptan-2-one, 3,6,...	152 C10H16O	016022-08-5 68
2		Bicyclo[3.1.1]heptan-3-one, 2,6,...	152 C10H16O	000547-60-4 64
3		Bicyclo[3.1.1]heptan-3-one, 2,6,...	152 C10H16O	015358-88-0 49
4		Bicyclo[3.1.0]hexan-2-one, 4-met...	152 C10H16O	002506-61-8 46
5		2,4-Hexadiene, 2,5-dimethyl-	110 C8H14	000764-13-6 38



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX020620\
Data File : VX014856.D
Acq On : 06 Feb 2020 18:30
Operator : JC/SP
Sample : L1420-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
400205799-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.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
3-Pentanone, 2,4-...	9.43	20.0	ug/l	883736	3	10.11	2205630	50.0
Eucalyptol	12.15	12.3	ug/l	535927	4	12.07	2175100	50.0
Bicyclo[2.2.1]hep...	12.96	102.6	ug/l	4464020	4	12.07	2175100	50.0
unknown13.53	13.53	19.7	ug/l	856440	4	12.07	2175100	50.0
Cyclohexanol, 5-m...	13.64	35.1	ug/l	1528100	4	12.07	2175100	50.0
Bicyclo[3.1.1]hep...	14.15	12.7	ug/l	552723	4	12.07	2175100	50.0