

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN011620\
 Data File : VN059745.D
 Acq On : 16 Jan 2020 20:22
 Operator : JC/MD
 Sample : L1159-01
 Misc : 5.00mL/MSVOA N/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 4001157623

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_N\METHODS\82N011320W.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	3.776	605	623	660	rBV	354819	945650	14.12%	3.402%
2	4.008	678	695	724	rBV	65827	188520	2.81%	0.678%
3	4.725	887	918	962	rBV	1668782	5807883	86.71%	20.891%
4	6.783	1529	1558	1624	rBV2	2046887	6697947	100.00%	24.093%
5	7.175	1651	1680	1724	rBV2	682685	2127538	31.76%	7.653%
6	7.567	1783	1802	1813	rBV	123066	309793	4.63%	1.114%
7	7.641	1813	1825	1851	rVB	241402	570540	8.52%	2.052%
8	8.005	1915	1938	1958	rBV2	164408	471270	7.04%	1.695%
9	8.104	1959	1969	1987	rVB	46888	109184	1.63%	0.393%
10	8.419	2052	2067	2090	rBV	43307	97045	1.45%	0.349%
11	8.567	2095	2113	2131	rBV	329381	686571	10.25%	2.470%
12	9.021	2242	2254	2275	rVB	57387	122555	1.83%	0.441%
13	9.966	2531	2548	2563	rBV2	62988	132297	1.98%	0.476%
14	10.078	2569	2583	2595	rBV	499350	935287	13.96%	3.364%
15	10.143	2595	2603	2609	rVV	46620	85953	1.28%	0.309%
16	10.181	2609	2615	2630	rVB	50568	88249	1.32%	0.317%
17	10.709	2763	2779	2800	rVB	141590	265653	3.97%	0.956%
18	11.400	2981	2994	3012	rVB	461743	827671	12.36%	2.977%
19	11.503	3013	3026	3043	rBV2	110309	217229	3.24%	0.781%
20	11.609	3043	3059	3068	rBV	110138	212017	3.17%	0.763%
21	11.940	3152	3162	3175	rBV	84449	145732	2.18%	0.524%
22	12.397	3292	3304	3325	rVB	379626	649547	9.70%	2.336%
23	13.033	3491	3502	3517	rVB2	68834	114729	1.71%	0.413%
24	13.159	3528	3541	3552	rBV4	106087	202794	3.03%	0.729%
25	13.339	3586	3597	3610	rVV2	454062	864933	12.91%	3.111%
26	13.403	3610	3617	3624	rVV3	121932	214718	3.21%	0.772%
27	13.445	3625	3630	3641	rVB	73232	113305	1.69%	0.408%
28	13.538	3651	3659	3669	rBV	68842	103357	1.54%	0.372%
29	13.811	3728	3744	3757	rVV4	162234	416164	6.21%	1.497%
30	13.876	3757	3764	3778	rVB	69455	116972	1.75%	0.421%
31	14.216	3857	3870	3887	rBV	889826	1534560	22.91%	5.520%
32	14.477	3943	3951	3962	rBV5	70593	131491	1.96%	0.473%
33	14.570	3972	3980	3993	rBV5	38149	73659	1.10%	0.265%
34	14.641	3994	4002	4013	rBV3	79100	127744	1.91%	0.460%

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Integration Parameters: RTEINT.P

Integrator: RTE
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Title : SW846 8260

35	14.805	4040	4053	4056	rBV5	116082	225899	3.37%	0.813%
36	14.840	4057	4064	4072	rVV	383712	682652	10.19%	2.456%
37	14.888	4072	4079	4094	rVB5	301800	560648	8.37%	2.017%
38	15.030	4116	4123	4138	rVB2	79764	129757	1.94%	0.467%
39	15.126	4145	4153	4166	rVB	178978	307284	4.59%	1.105%
40	15.461	4249	4257	4271	rVB2	99217	185560	2.77%	0.667%

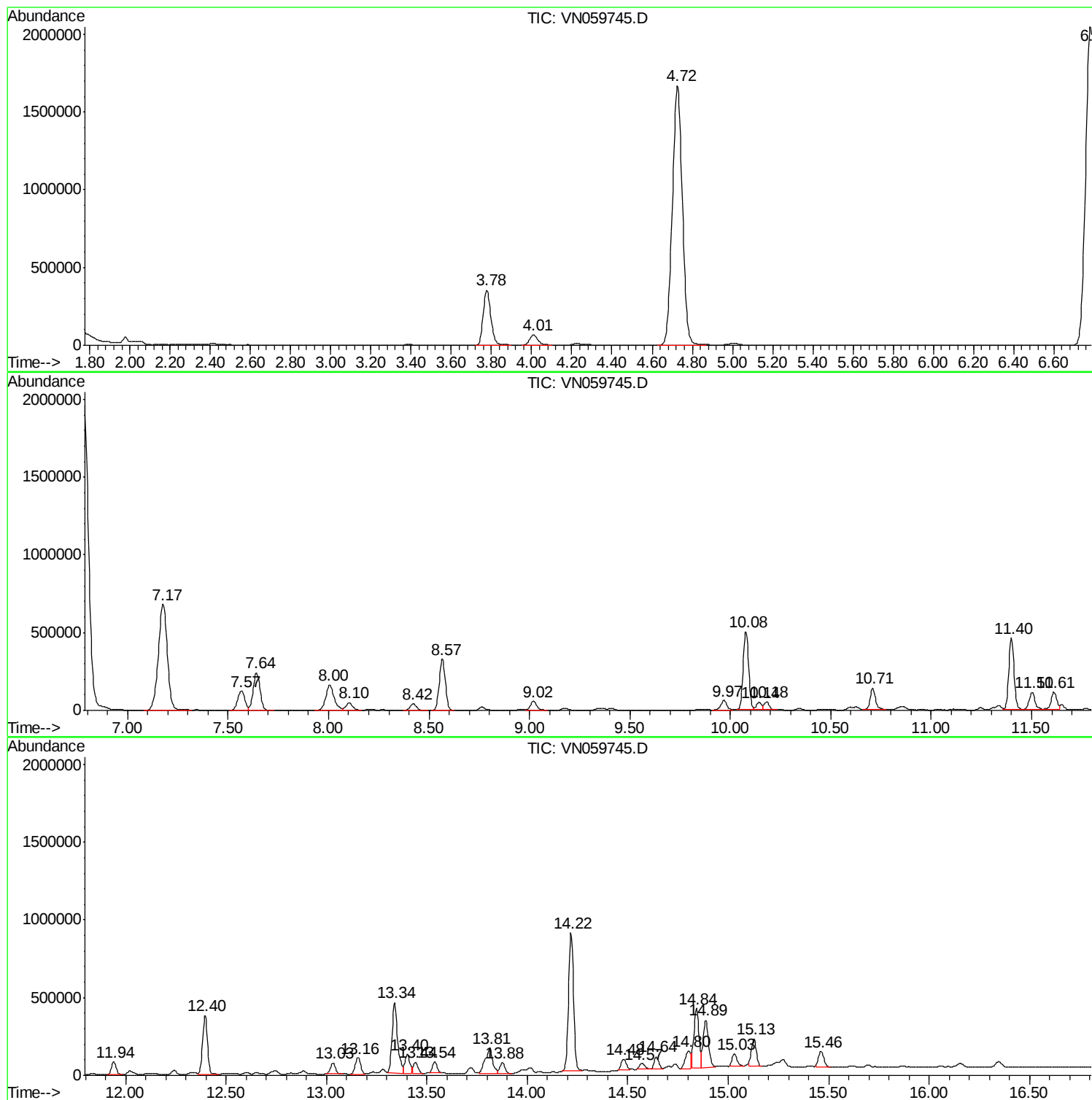
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

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



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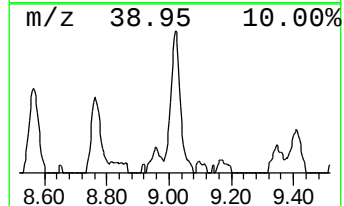
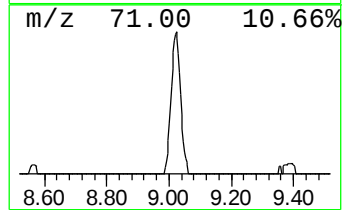
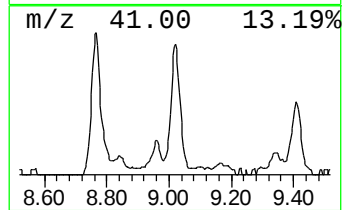
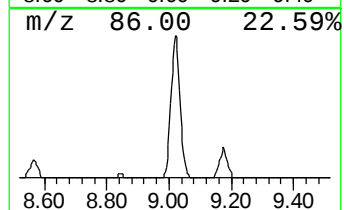
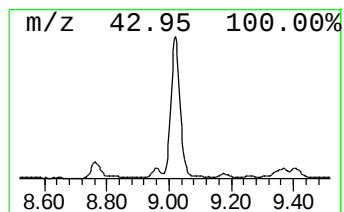
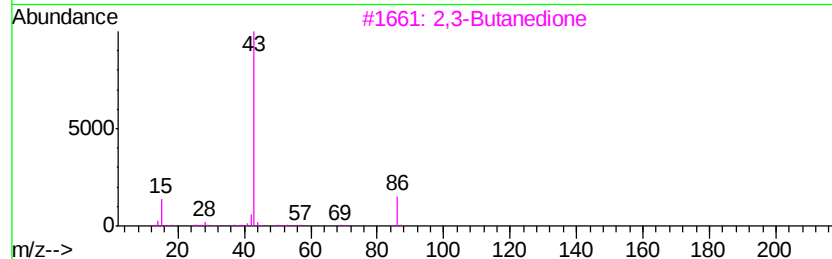
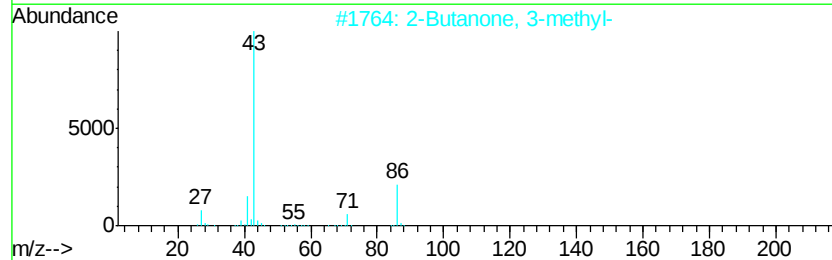
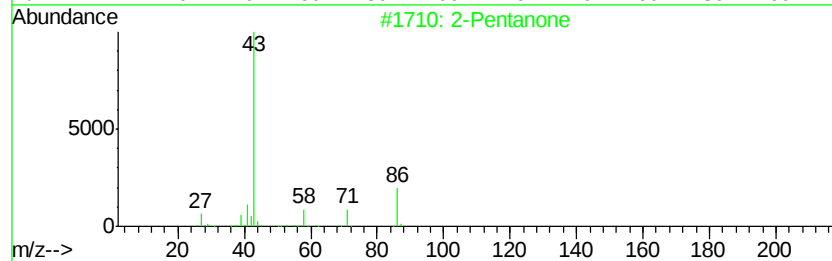
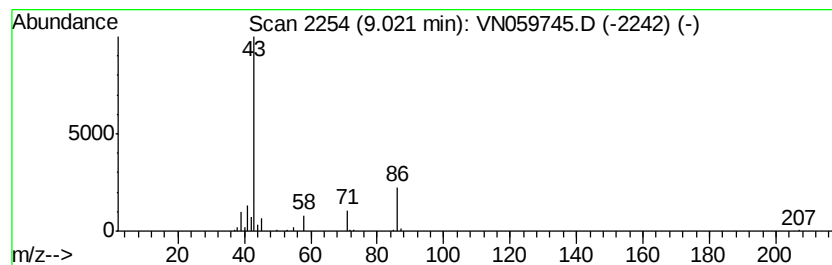
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

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

Peak Number 2 2-Pentanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.02	8.93 ug/l	122555	1,4-Difluorobenzene	8.57

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone	86	C5H10O	000107-87-9	80
2			2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	64
3			2,3-Butanedione	86	C4H6O2	000431-03-8	52
4			2,3-Pentanedione, 4-methyl-	114	C6H10O2	007493-58-5	25
5			Propane, 2-(ethenyl-oxo)-	86	C5H10O	000926-65-8	9



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Instrument :
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ClientSampleId :
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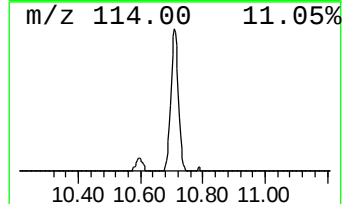
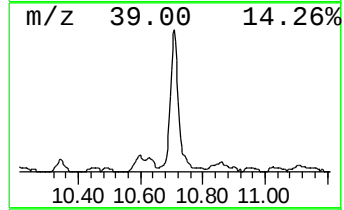
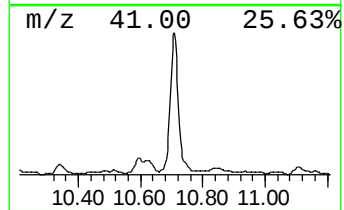
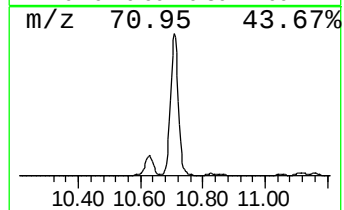
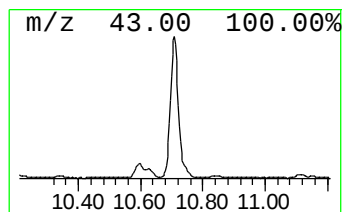
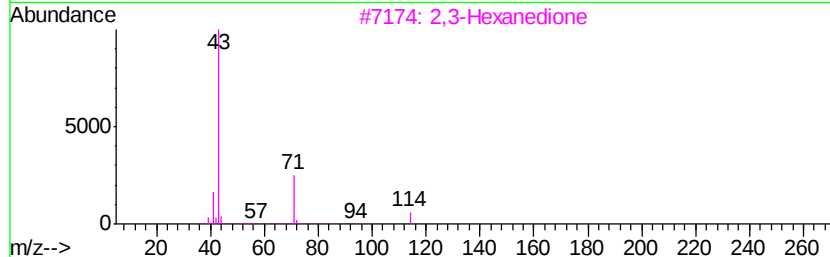
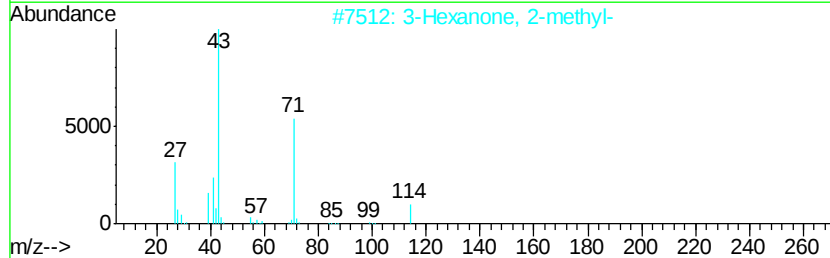
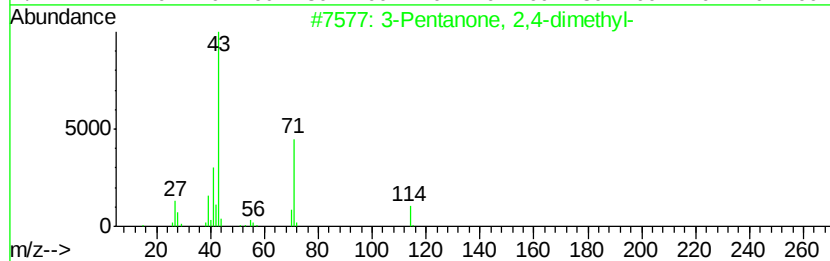
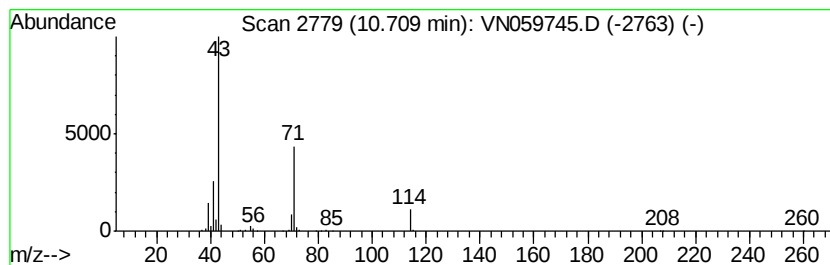
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 3-Pentanone, 2,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.71	16.05 ug/l	265653	Chlorobenzene-d5	11.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	86
2		3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	86
3		2,3-Hexanedione	114	C6H10O2	003848-24-6	80
4		4-Heptanone	114	C7H14O	000123-19-3	59
5		Pyrrolidine	71	C4H9N	000123-75-1	42



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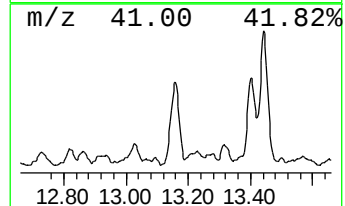
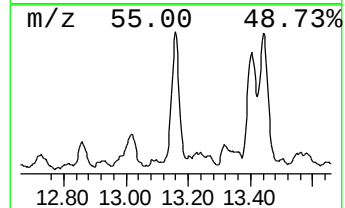
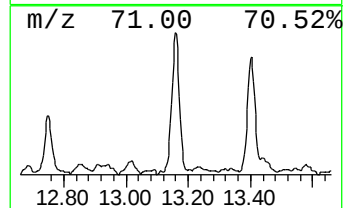
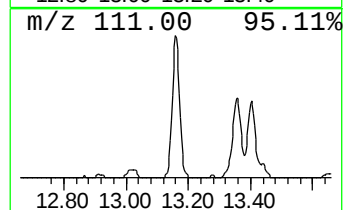
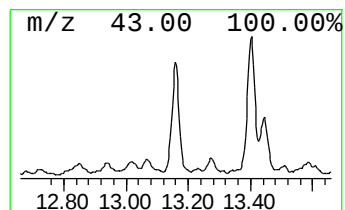
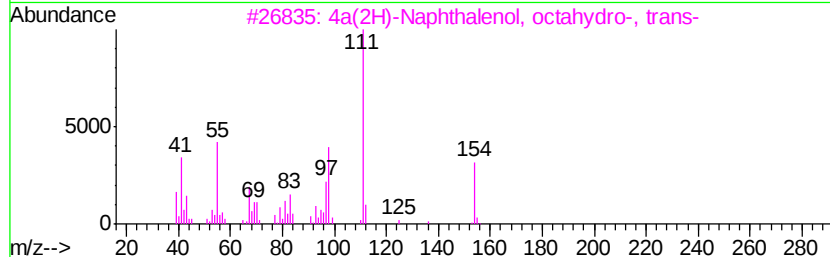
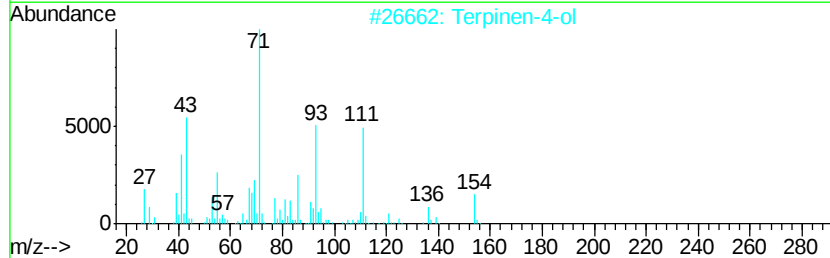
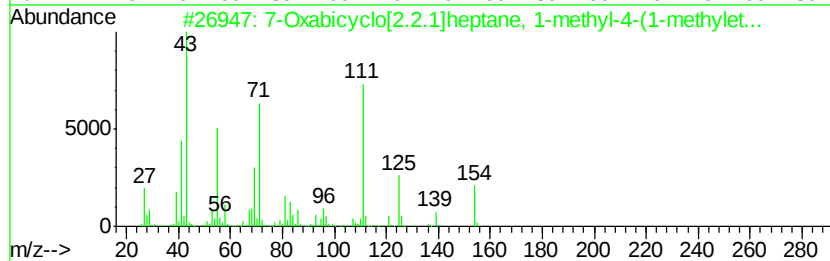
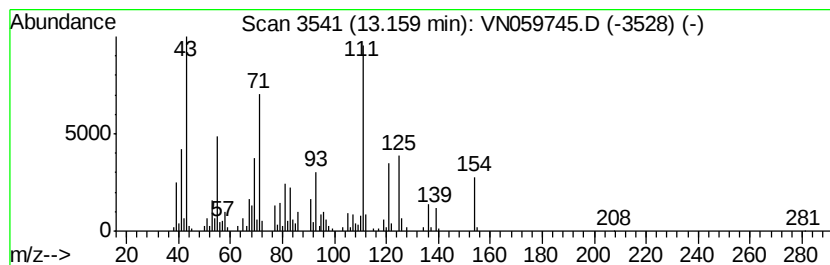
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 7-Oxabicyclo[2.2.1]heptane,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.16	11.72 ug/l	202794	1,4-Dichlorobenzene-d4	13.34

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		7-Oxabicyclo[2.2.1]heptane, 1-me...	154	C10H18O	000470-67-7	94
2		Terpinen-4-ol	154	C10H18O	000562-74-3	43
3		4a(2H)-Naphthalenol, octahydro-,...	154	C10H18O	001654-87-1	38
4		cis-1-Hydroxybicyclo[4.4.0]decane	154	C10H18O	003574-58-1	38
5		2(5H)-Furanone, 3,5,5-trimethyl-	126	C7H10O2	050598-50-0	30



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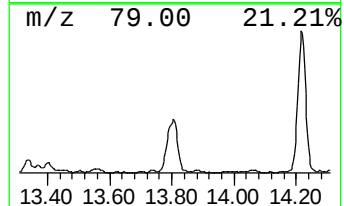
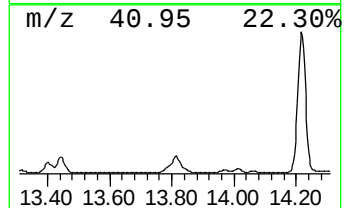
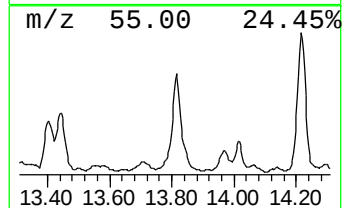
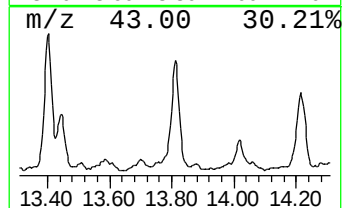
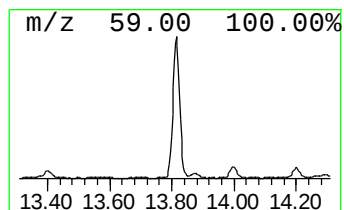
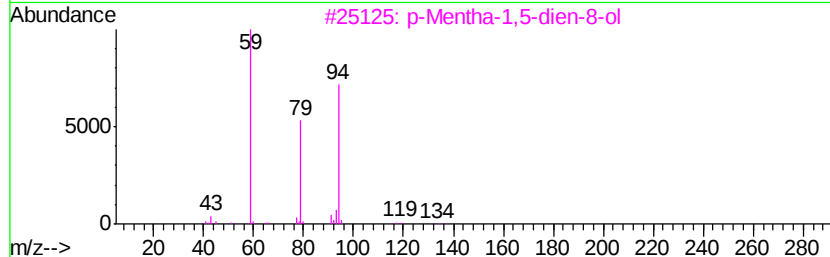
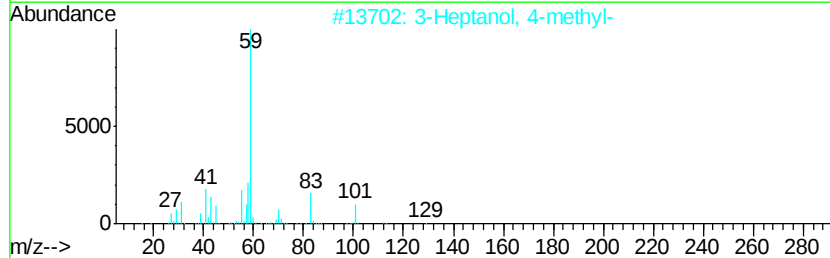
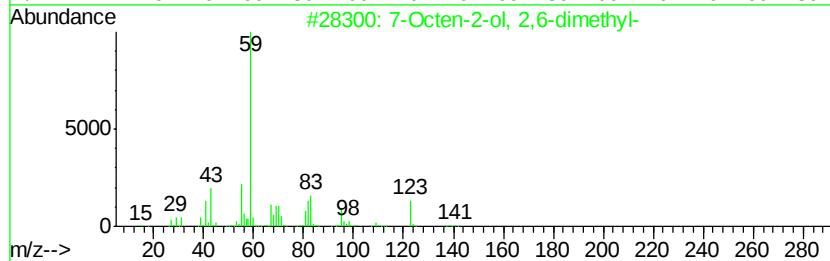
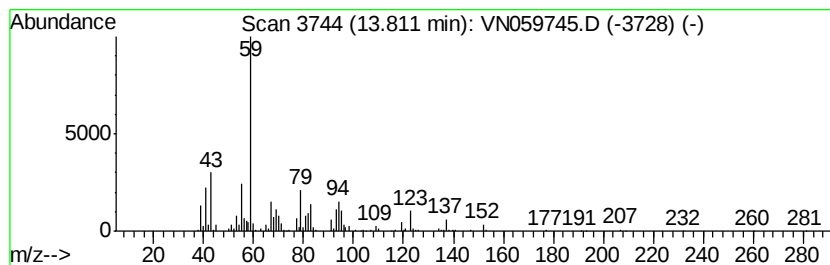
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Peak Number 5 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	24.06 ug/l	416164	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	52
2		3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	43
3		p-Mentha-1,5-dien-8-ol	152	C10H16O	001686-20-0	40
4		2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	40
5		2-(3,4-Dibromo-4-methylcyclohexy...	312	C10H18Br2O	110202-13-6	40



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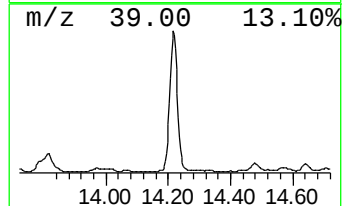
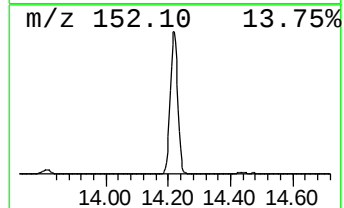
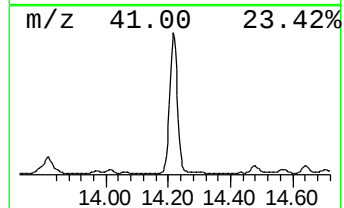
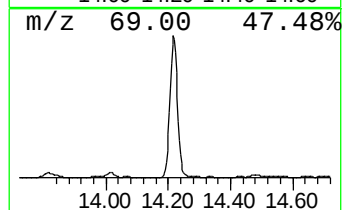
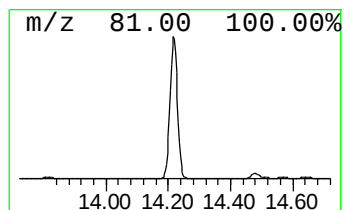
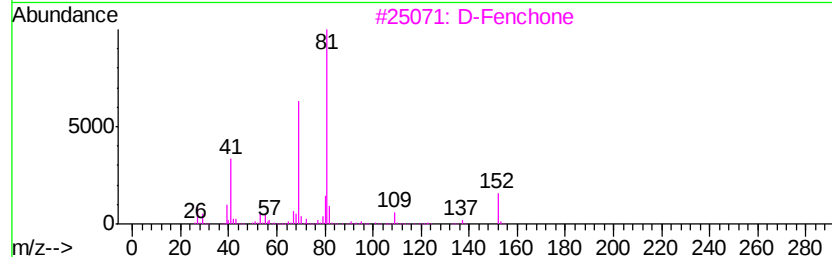
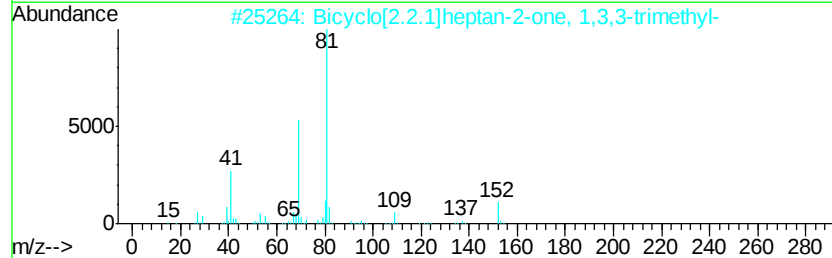
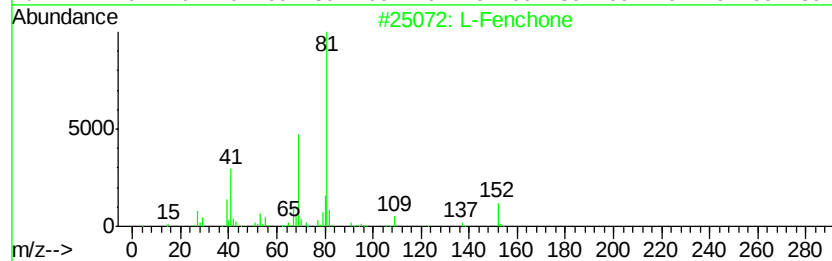
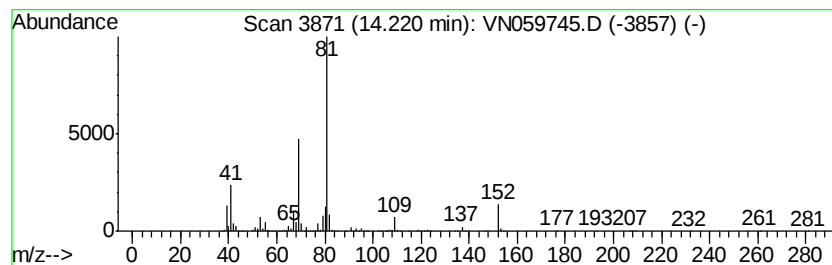
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Quant Title : SW846 8260

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

Peak Number 6 L-Fenchone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.22	88.71 ug/l	1534560	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	L-Fenchone	152	C10H16O	007787-20-4	95
2		Bicyclo[2.2.1]heptan-2-one, 1,3,...	152	C10H16O	001195-79-5	95
3		D-Fenchone	152	C10H16O	004695-62-9	94
4		Ethanone, 1-(2-methyl-2-cyclopent...	124	C8H12O	001767-84-6	45
5		2-Cyclopentene-1-carboxylic acid...	140	C8H12O2	068317-73-7	42



Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN011620\
Data File : VN059745.D
Acq On : 16 Jan 2020 20:22
Operator : JC/MD
Sample : L1159-01
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 26 Sample Multiplier: 1

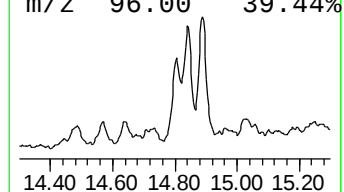
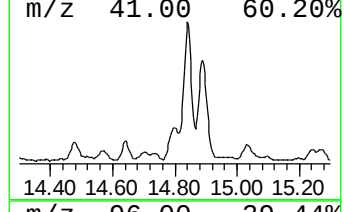
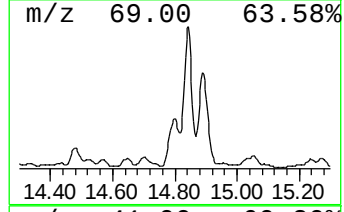
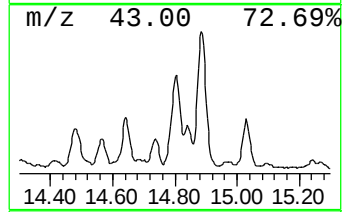
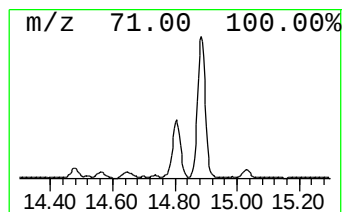
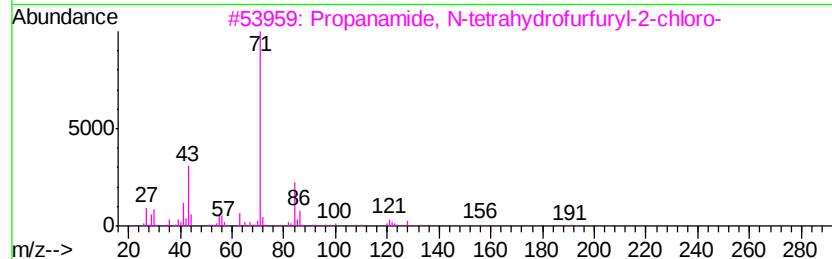
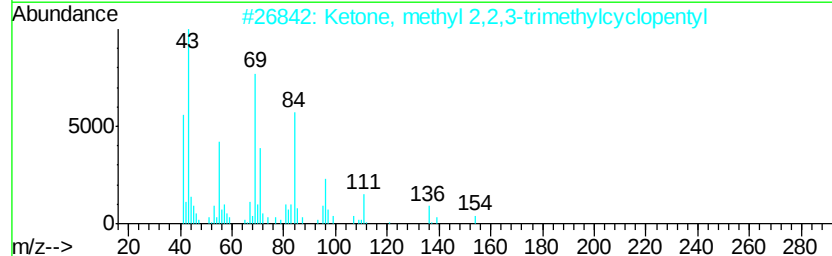
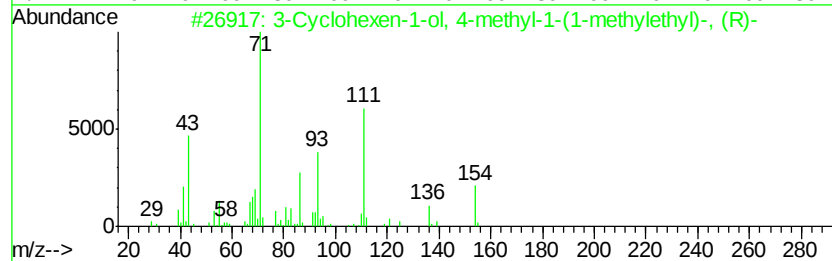
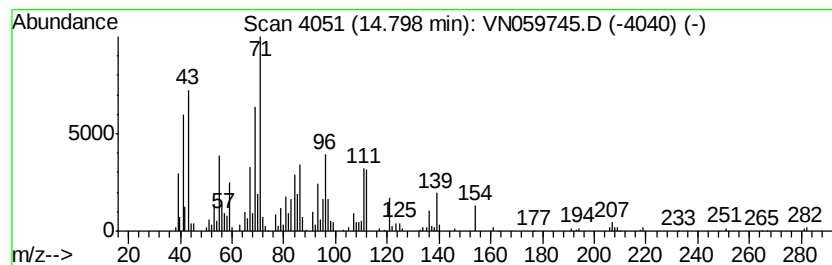
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ClientSampleId :
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

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

Peak Number 7 3-Cyclohexen-1-ol, 4-methyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	13.06 ug/l	225899	1,4-Dichlorobenzene-d4	13.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	3-Cyclohexen-1-ol, 4-methyl-1-(1...	154 C10H18O	020126-76-5	43
2	Ketone, methyl 2,2,3-trimethylcy...	154 C10H18O	017983-22-1	38
3	Propanamide, N-tetrahydrofurfurv...	191 C8H14ClN02	1000307-48-2	35
4	1,3-Diacetyl-cyclopentane	154 C9H14O2	1000143-37-1	35
5	1-Propene, 3-methoxy-2-methyl-	86 C5H10O	022418-49-1	30



Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN011620\
Data File : VN059745.D
Acq On : 16 Jan 2020 20:22
Operator : JC/MD
Sample : L1159-01
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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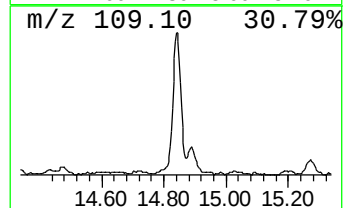
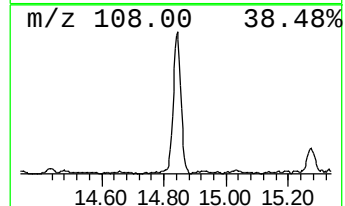
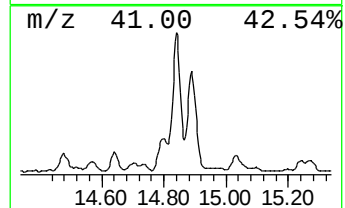
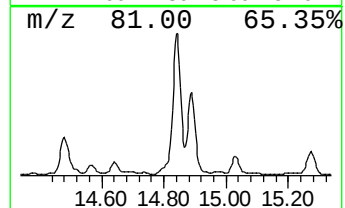
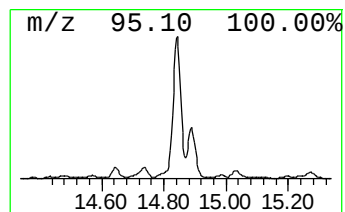
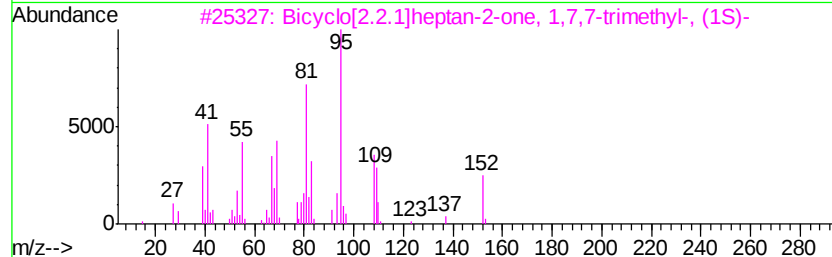
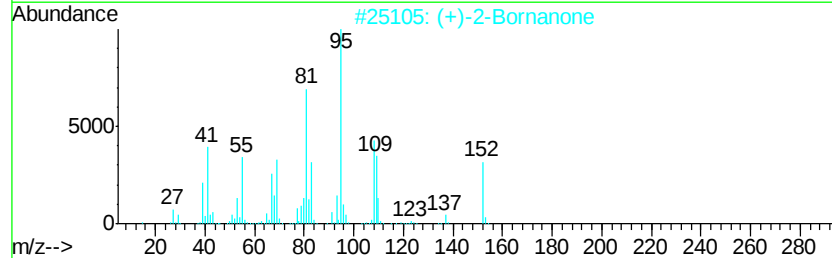
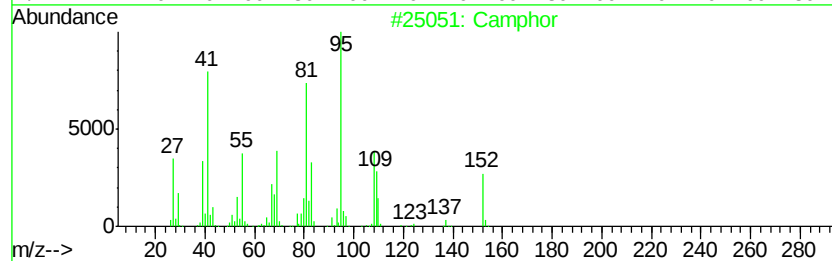
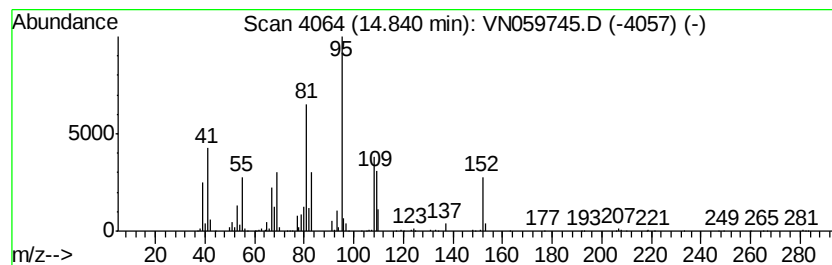
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Quant Title : SW846 8260

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

Peak Number 8 Camphor Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	39.46 ug/l	682652	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Camphor	152	C10H16O	000076-22-2	98
2		(+)-2-Bornanone	152	C10H16O	000464-49-3	98
3		Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	95
4		2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	46
5		1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	38



Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN011620\
Data File : VN059745.D
Acq On : 16 Jan 2020 20:22
Operator : JC/MD
Sample : L1159-01
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 26 Sample Multiplier: 1

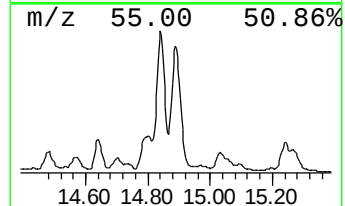
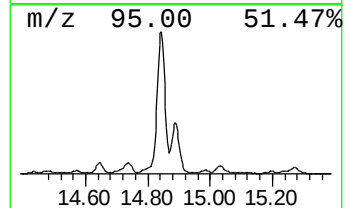
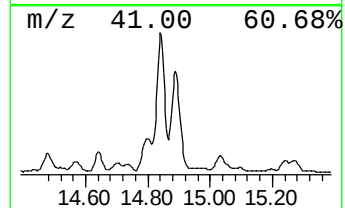
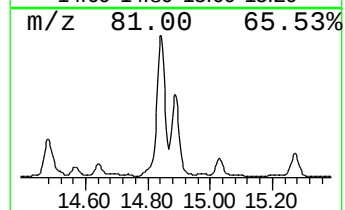
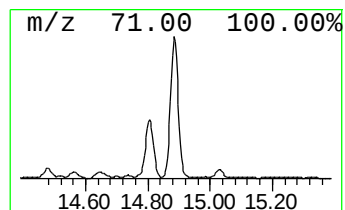
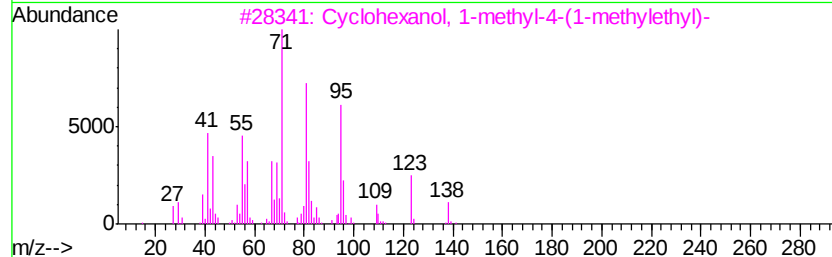
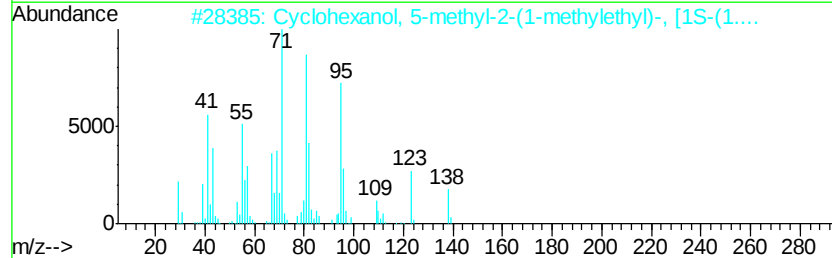
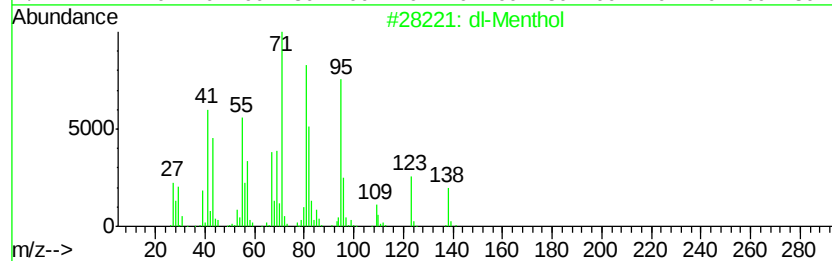
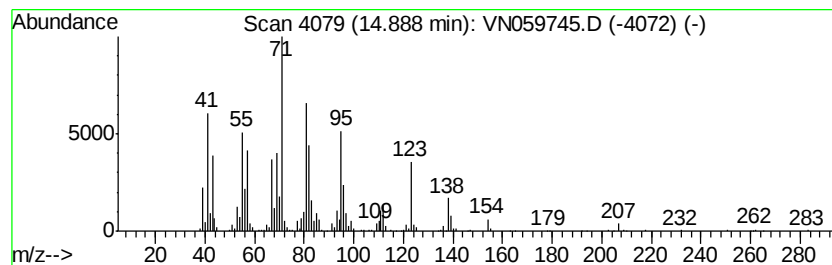
Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

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

Peak Number 9 dl-Menthol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	32.41 ug/l	560648	1,4-Dichlorobenzene-d4	13.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	dl-Menthol	156 C10H20O	000089-78-1	72
2	Cyclohexanol, 5-methyl-2-(1-meth...	156 C10H20O	002216-52-6	72
3	Cyclohexanol, 1-methyl-4-(1-meth...	156 C10H20O	021129-27-1	64
4	Cyclohexanol, 5-methyl-2-(1-meth...	156 C10H20O	023283-97-8	59
5	Cyclohexene,1-(2-methylpropyl)-	138 C10H18	003983-03-7	46



Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN011620\
Data File : VN059745.D
Acq On : 16 Jan 2020 20:22
Operator : JC/MD
Sample : L1159-01
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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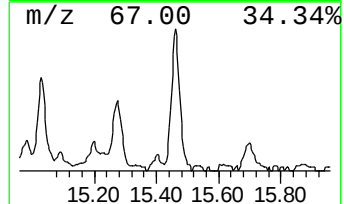
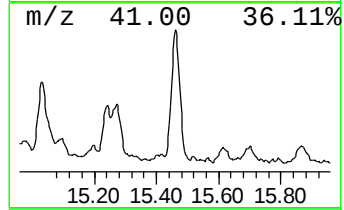
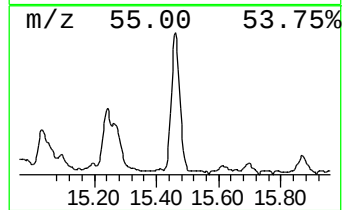
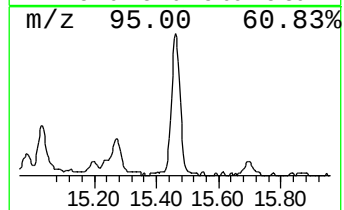
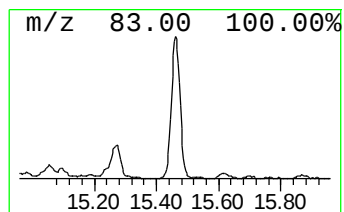
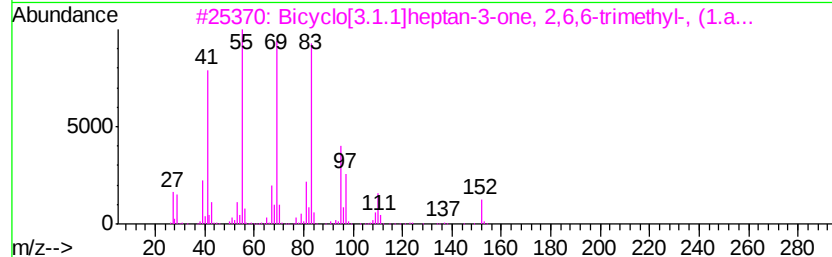
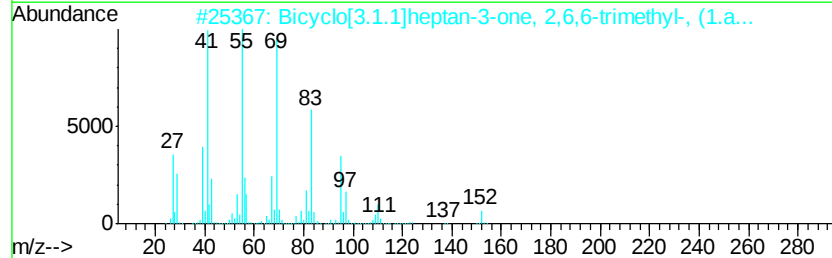
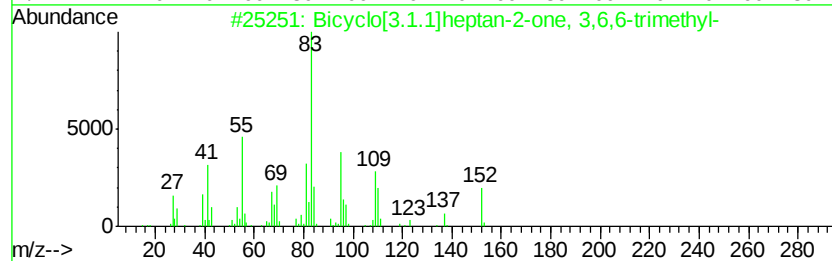
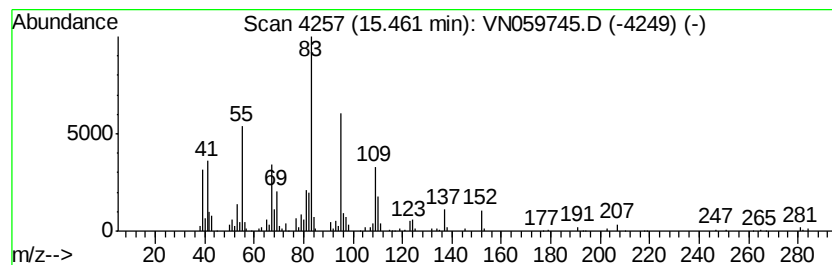
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

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

Peak Number 10 Bicyclo[3.1.1]heptan-2-one,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.46	10.73 ug/l	185560	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[3.1.1]heptan-2-one, 3,6,...	152	C10H16O	016022-08-5	64
2		Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	64
3		Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	000547-60-4	52
4		Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	43
5		1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	38



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN011620\
Data File : VN059745.D
Acq On : 16 Jan 2020 20:22
Operator : JC/MD
Sample : L1159-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
4001157623

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.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
2-Pentanone	9.02	8.9	ug/l	122555	2	8.57	686571	50.0
3-Pentanone, 2,4-...	10.71	16.1	ug/l	265653	3	11.40	827671	50.0
7-Oxabicyclo[2.2...	13.16	11.7	ug/l	202794	4	13.34	864933	50.0
7-Octen-2-ol, 2,6...	13.81	24.1	ug/l	416164	4	13.34	864933	50.0
L-Fenchone	14.22	88.7	ug/l	1534560	4	13.34	864933	50.0
3-Cyclohexen-1-ol...	14.80	13.1	ug/l	225899	4	13.34	864933	50.0
Camphor	14.84	39.5	ug/l	682652	4	13.34	864933	50.0
d1-Menthol	14.89	32.4	ug/l	560648	4	13.34	864933	50.0
Bicyclo[3.1.1]hep...	15.46	10.7	ug/l	185560	4	13.34	864933	50.0