

Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN062019\
 Data File : VN056408.D
 Acq On : 20 Jun 2019 17:23
 Operator : JC/SP
 Sample : K3465-01
 Misc : 5.00mL/MSVOA N/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 390619766-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_N\METHODS\82N061919W.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	1.992	61	68	88	rVB	112935	175452	2.48%	0.592%
2	3.818	615	636	659	rBV	249348	661935	9.34%	2.235%
3	4.793	896	939	991	rBV	1466267	5305715	74.87%	17.916%
4	5.047	1004	1018	1042	rVB2	22054	79233	1.12%	0.268%
5	6.831	1546	1573	1637	rBV	2292925	7087023	100.00%	23.931%
6	7.214	1672	1692	1734	rVB	822981	2291535	32.33%	7.738%
7	7.590	1791	1809	1820	rBV	230773	566321	7.99%	1.912%
8	7.664	1820	1832	1853	rVB	398177	949321	13.40%	3.206%
9	8.027	1927	1945	1966	rBV2	293218	744194	10.50%	2.513%
10	8.137	1968	1979	1994	rVB3	54113	127935	1.81%	0.432%
11	8.583	2103	2118	2145	rBV	628936	1337262	18.87%	4.516%
12	9.985	2538	2554	2564	rBV3	62237	127863	1.80%	0.432%
13	10.091	2573	2587	2600	rBV	1024410	1910494	26.96%	6.451%
14	10.156	2601	2607	2613	rVV	59656	106535	1.50%	0.360%
15	10.194	2613	2619	2634	rVB	64669	118591	1.67%	0.400%
16	10.718	2766	2782	2810	rVV	205805	403732	5.70%	1.363%
17	10.850	2811	2823	2846	rVB	26968	87655	1.24%	0.296%
18	11.406	2982	2996	3016	rVV	983785	1810422	25.55%	6.113%
19	11.506	3017	3027	3045	rVV2	65888	161264	2.28%	0.545%
20	11.615	3046	3061	3071	rVV	125693	252086	3.56%	0.851%
21	11.947	3153	3164	3178	rVB	118579	209572	2.96%	0.708%
22	12.400	3293	3305	3321	rVB	770955	1318454	18.60%	4.452%
23	12.754	3399	3415	3427	rBV4	27415	72387	1.02%	0.244%
24	13.037	3493	3503	3515	rVB	41195	71896	1.01%	0.243%
25	13.165	3528	3543	3553	rBV3	93773	162333	2.29%	0.548%
26	13.342	3585	3598	3616	rBV	779067	1427060	20.14%	4.819%
27	13.815	3733	3745	3755	rBV7	64935	136727	1.93%	0.462%
28	13.876	3756	3764	3778	rVB2	143511	238662	3.37%	0.806%
29	14.223	3857	3872	3888	rBV	510200	925339	13.06%	3.125%
30	14.808	4041	4054	4058	rBV5	83809	158684	2.24%	0.536%
31	14.847	4058	4066	4075	rVV	232739	417790	5.90%	1.411%
32	14.898	4075	4082	4096	rVB6	87718	171038	2.41%	0.578%

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ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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

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Title : SW846 8260

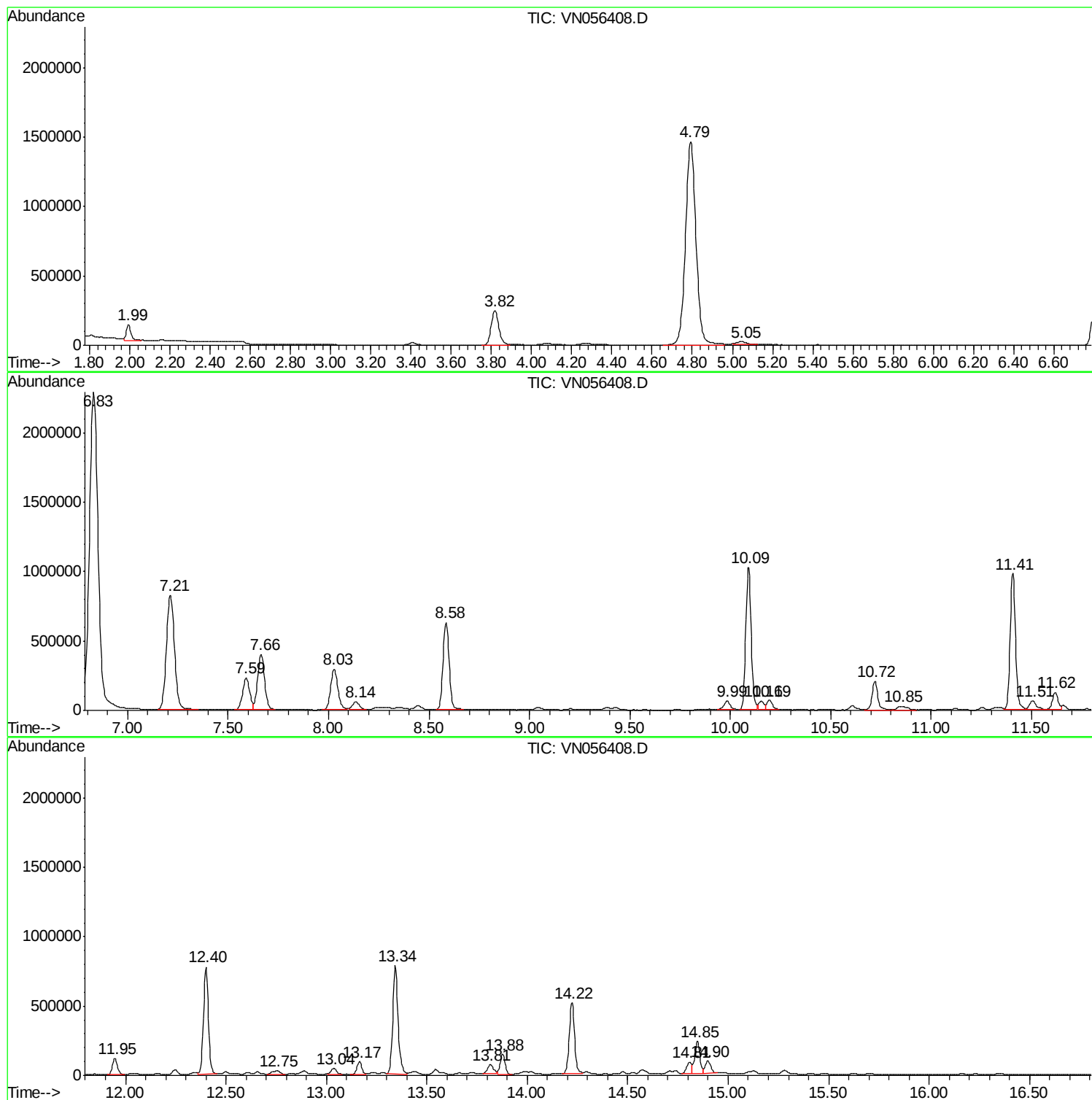
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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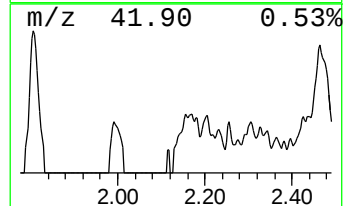
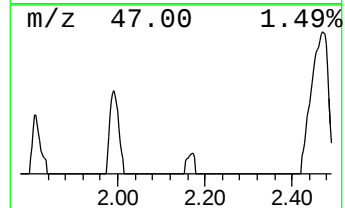
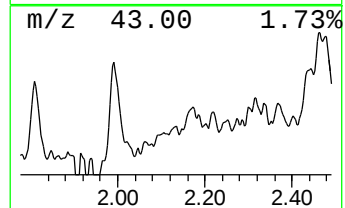
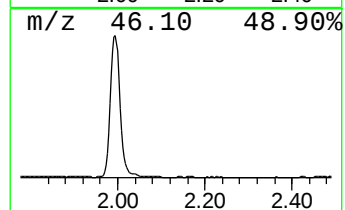
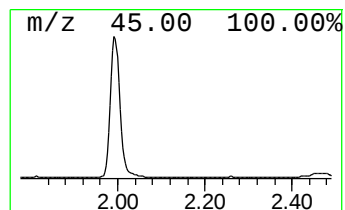
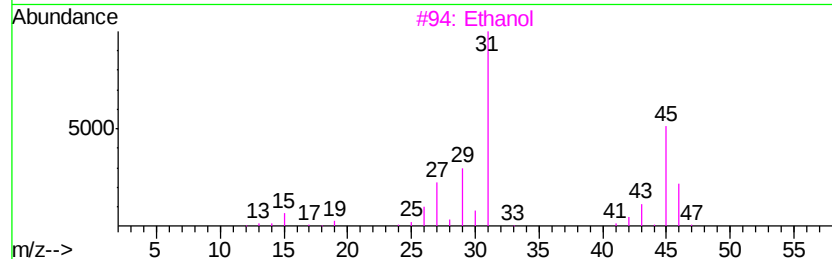
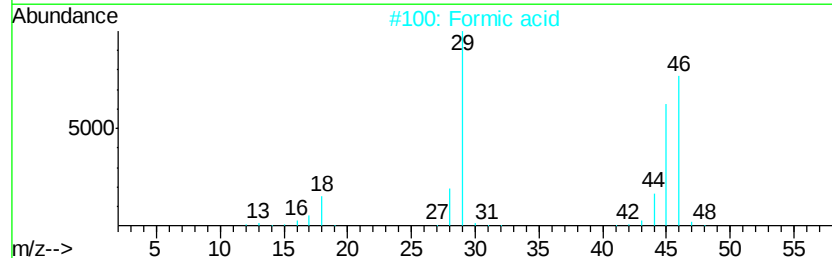
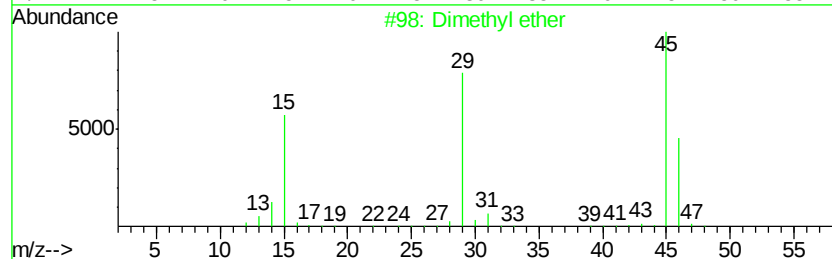
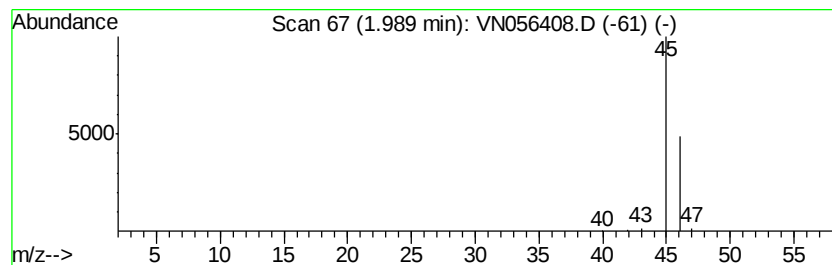
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ClientSampleId :
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N061919W.M
Quant Title : SW846 8260

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

Peak Number 1 Dimethyl ether Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.99	9.24 ug/l	175452	Pentafluorobenzene	7.66	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl ether	46	C2H6O	000115-10-6	74
2	Formic acid	46	CH2O2	000064-18-6	7
3	Ethanol	46	C2H6O	000064-17-5	7
4	Oxalic acid	90	C2H2O4	000144-62-7	4
5	Methane, nitroso-	45	CH3NO	000865-40-7	3



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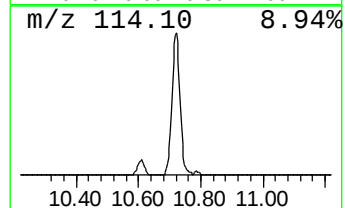
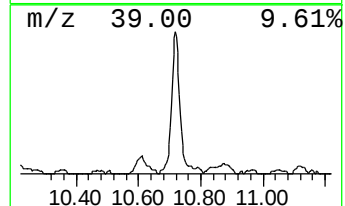
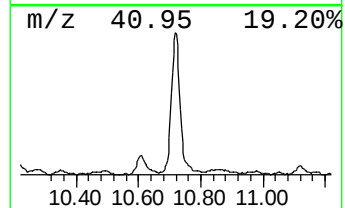
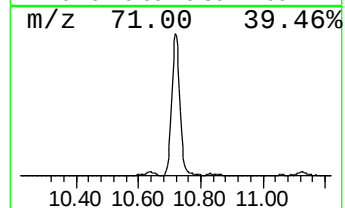
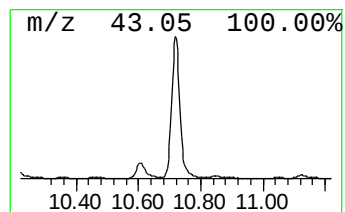
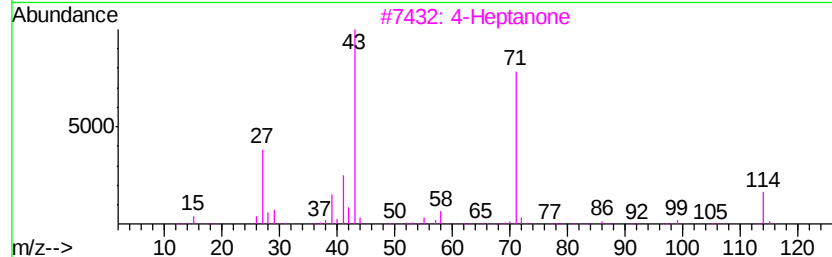
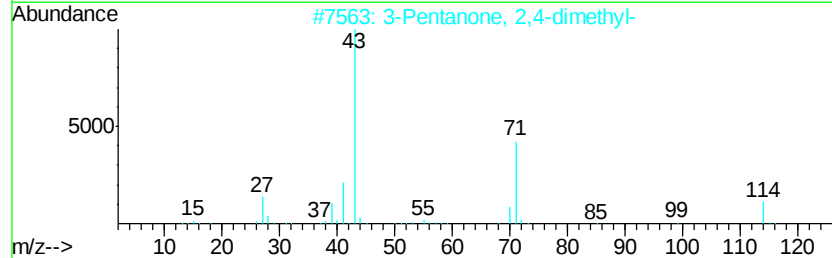
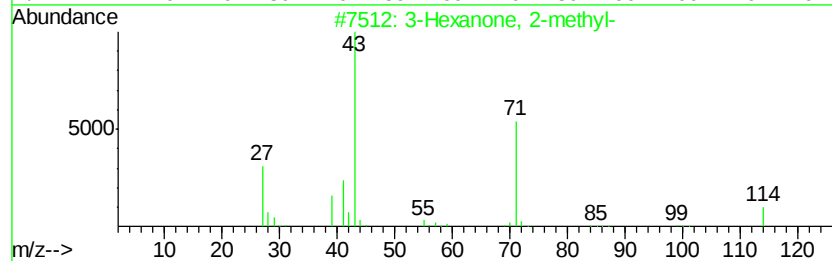
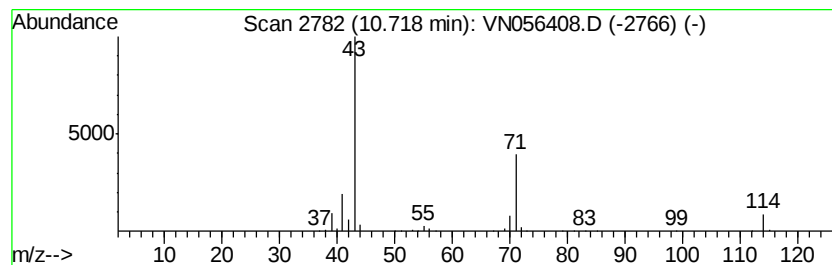
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N061919W.M
Quant Title : SW846 8260

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

Peak Number 2 3-Hexanone, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	11.15 ug/l	403732	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	80
2		3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	64
3		4-Heptanone	114	C7H14O	000123-19-3	59
4		Pyrrolidine	71	C4H9N	000123-75-1	59
5		n-Caproic acid vinyl ester	142	C8H14O2	003050-69-9	39



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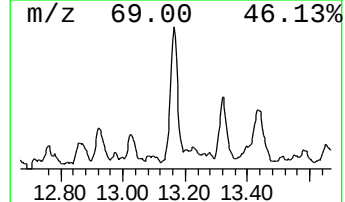
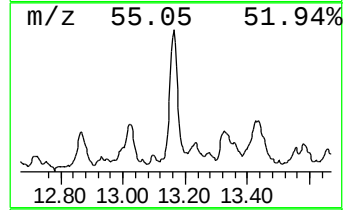
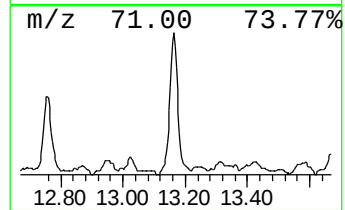
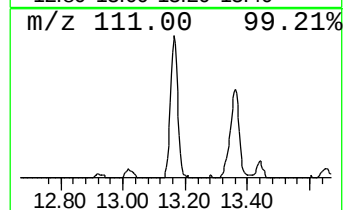
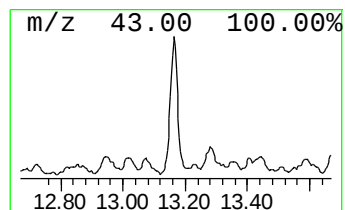
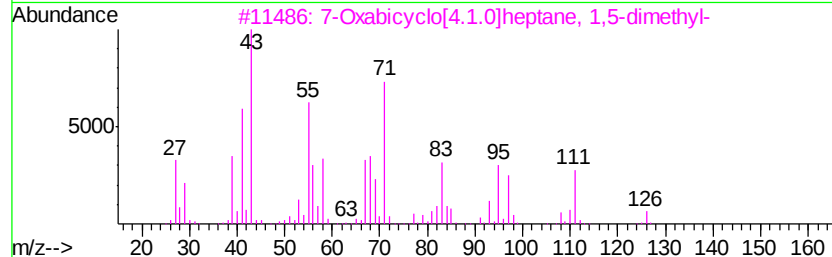
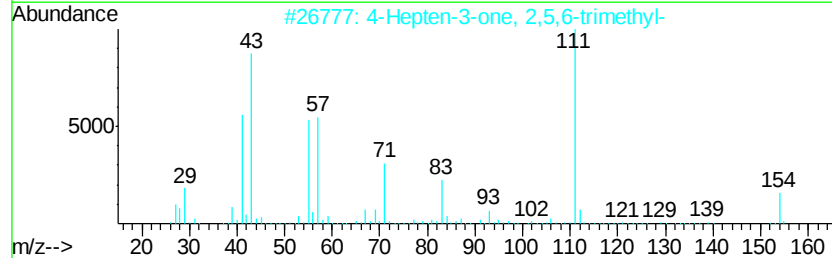
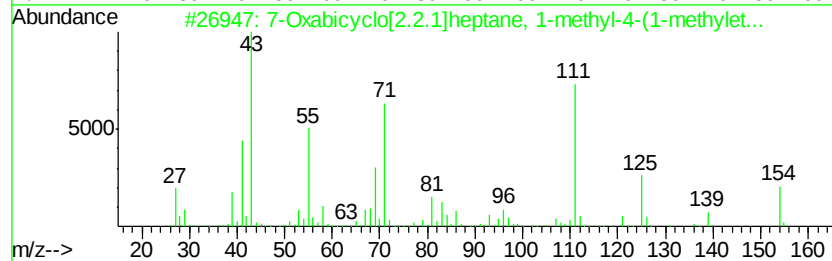
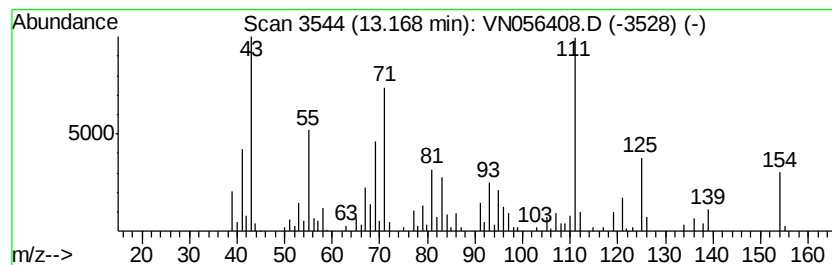
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 7-Oxabicyclo[2.2.1]heptane,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.17	5.69 ug/l	162333	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 91
2		4-Hepten-3-one, 2,5,6-trimethyl-	154 C10H18O	016466-21-0 27
3		7-Oxabicyclo[4.1.0]heptane, 1,5-...	126 C8H14O	162239-52-3 25
4		2-Aminopyrimidine-1-oxide	111 C4H5N3O	035034-15-2 25
5		2(1H)-Pyridinone, 5-hydroxy-	111 C5H5NO2	005154-01-8 14



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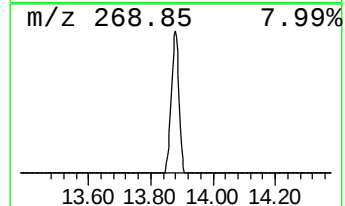
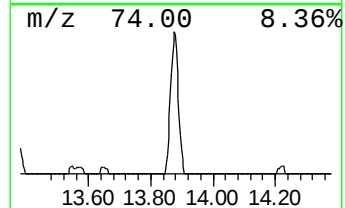
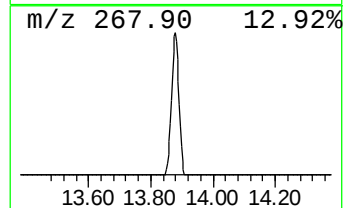
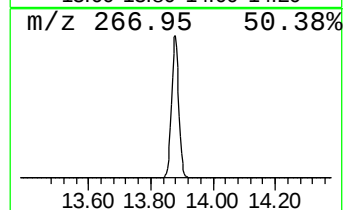
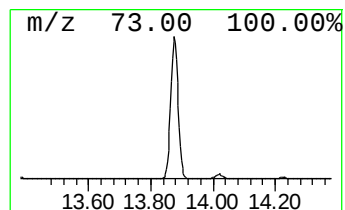
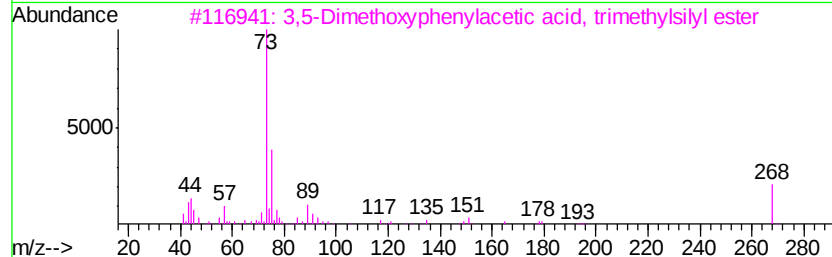
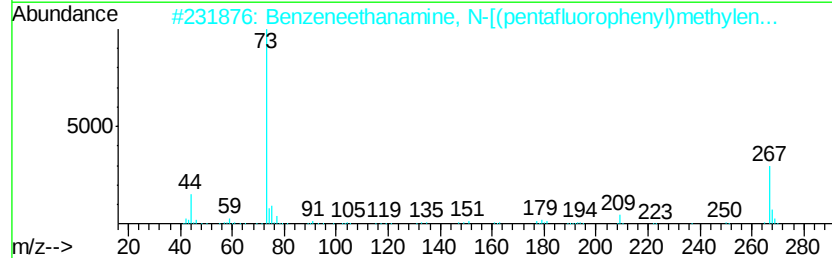
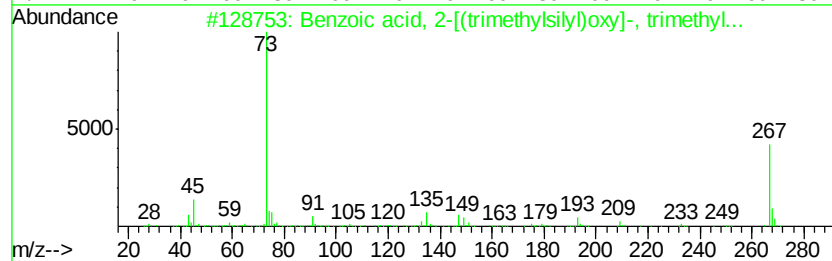
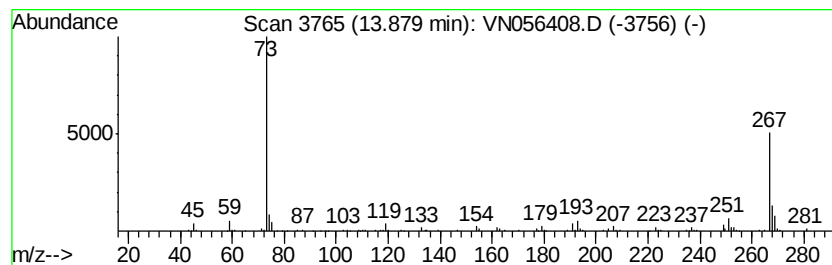
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzoic acid, 2-[(trimethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.88	8.36 ug/l	238662	1,4-Dichlorobenzene-d4	13.34		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzoic acid, 2-[(trimethylsilyl)oxy]-, trimethylsilyl ester	282	C13H22O3Si2	003789-85-3	64
2		Benzenethanamine, N-[(pentafluorophenyl)methyl]-, trimethylsilyl ether	475	C21H26F5N2Si2	055429-85-1	38
3		3,5-Dimethoxyphenylacetic acid, trimethylsilyl ester	268	C13H20O4Si	1000071-82-4	22
4		1-Boraindane, 3-methyl-1-[1-(trimethylsilyl)oxy]-	266	C17H23BSi	190316-36-0	14
5		4-Methylcatechol, bis(trimethylsilyl) ether	268	C13H24O2Si2	1000332-79-9	12



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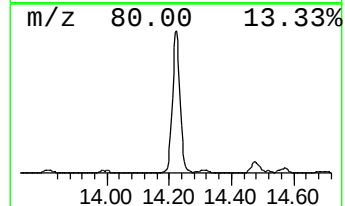
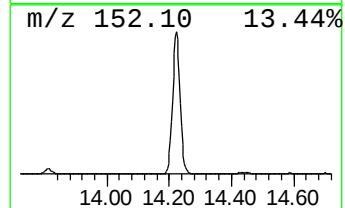
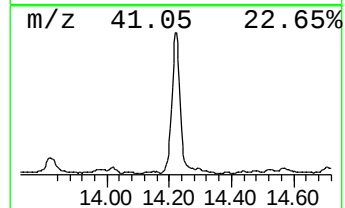
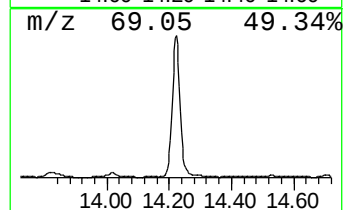
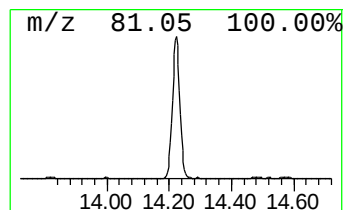
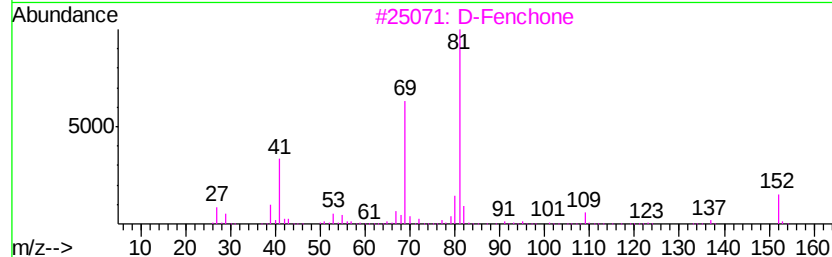
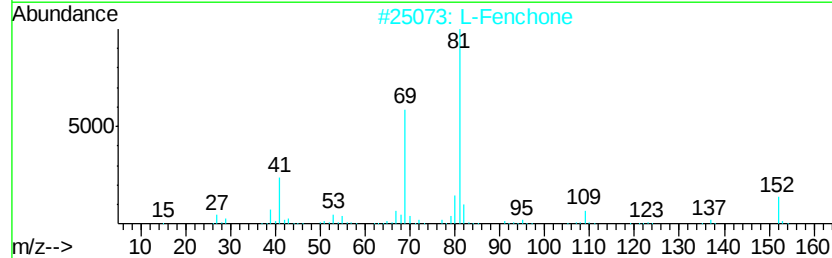
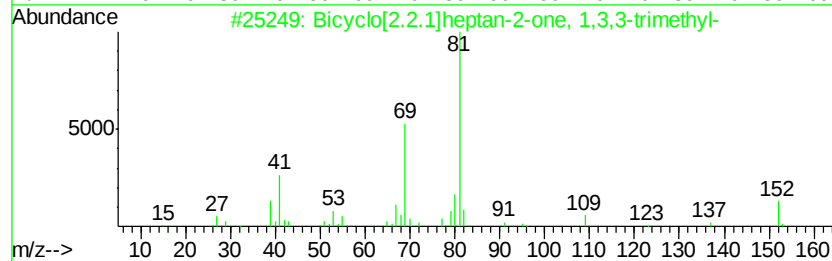
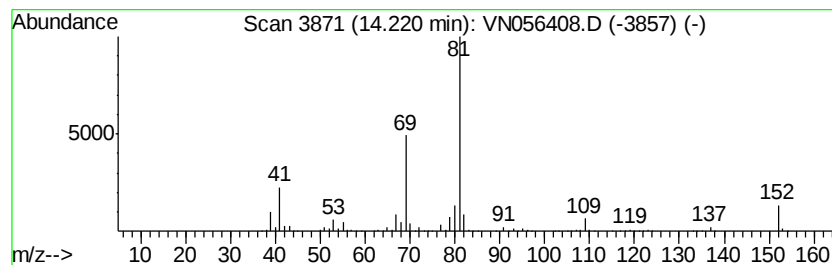
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.22	32.42 ug/l	925339	1,4-Dichlorobenzene-d4	13.34

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		L-Fenchone	152	C10H16O	007787-20-4	94
3		D-Fenchone	152	C10H16O	004695-62-9	94
4		Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	000529-00-0	45
5		Ethanone, 1-(2-methyl-2-cyclopen...	124	C8H12O	001767-84-6	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN062019\
Data File : VN056408.D
Acq On : 20 Jun 2019 17:23
Operator : JC/SP
Sample : K3465-01
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 22 Sample Multiplier: 1

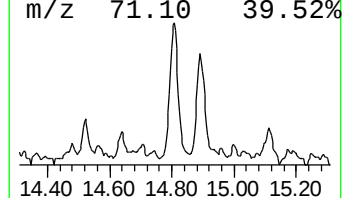
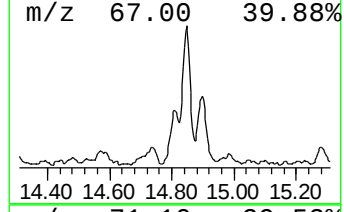
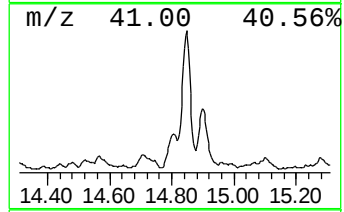
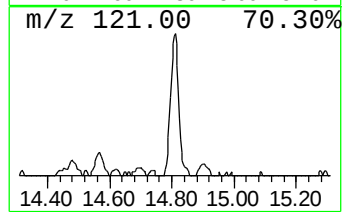
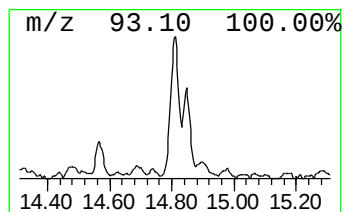
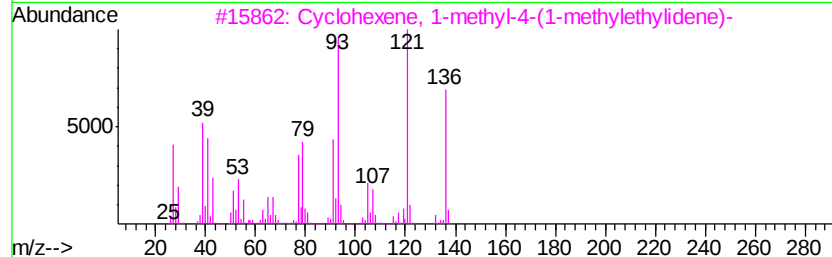
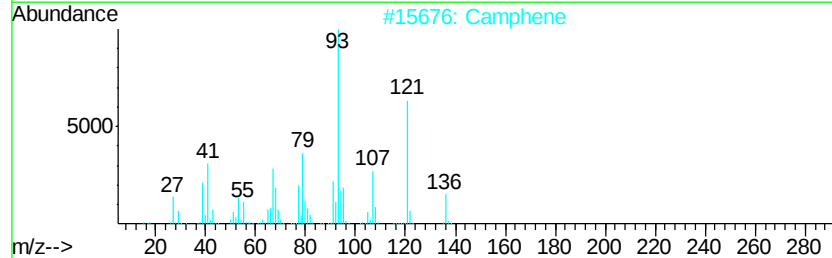
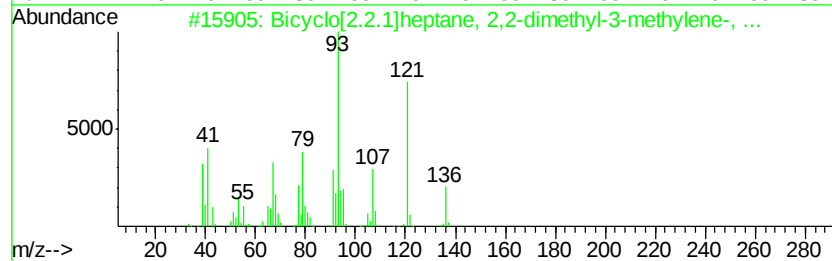
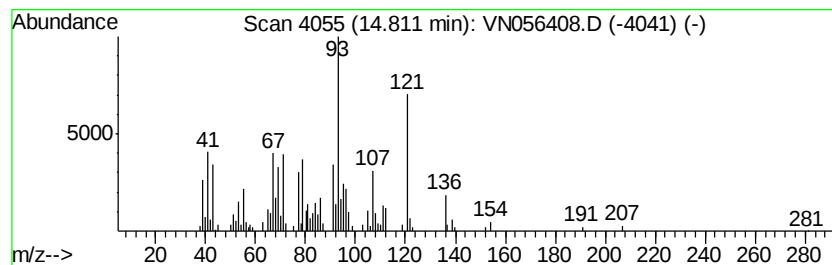
Instrument :
MSVOA_N
ClientSampleId :
390619766-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N061919W.M
Quant Title : SW846 8260

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

Peak Number 6 Bicyclo[2.2.1]heptane, 2,2-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.81	5.56 ug/l	158684	1,4-Dichlorobenzene-d4	13.34	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-04-7	96
2	Camphene	136	C10H16	000079-92-5	96
3	Cyclohexene, 1-methyl-4-(1-methyl...	136	C10H16	000586-62-9	50
4	1,3,6-Heptatriene, 2,5,5-trimethyl-	136	C10H16	029548-02-5	49
5	p-Menth-2-en-7-ol, cis-	154	C10H18O	019898-86-3	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN062019\
Data File : VN056408.D
Acq On : 20 Jun 2019 17:23
Operator : JC/SP
Sample : K3465-01
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 22 Sample Multiplier: 1

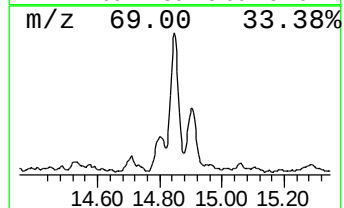
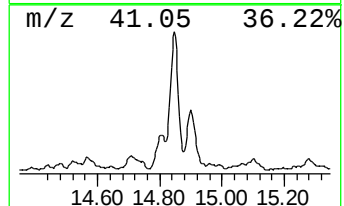
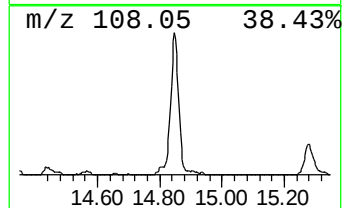
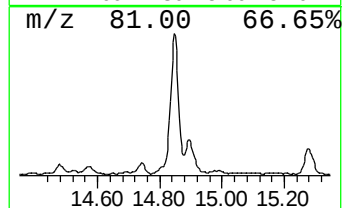
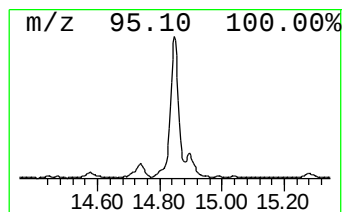
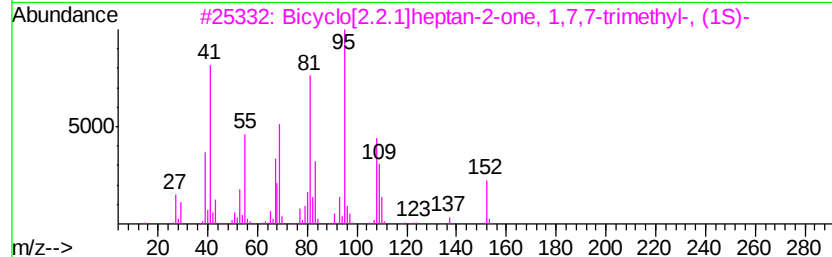
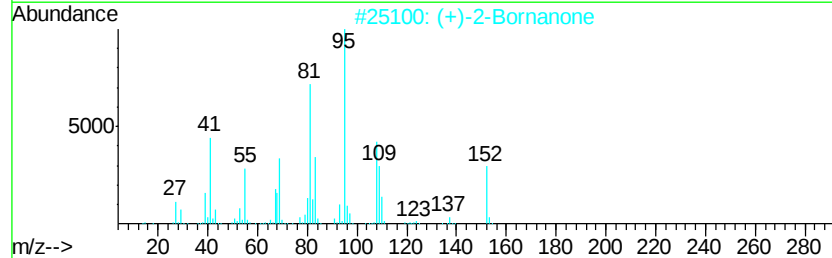
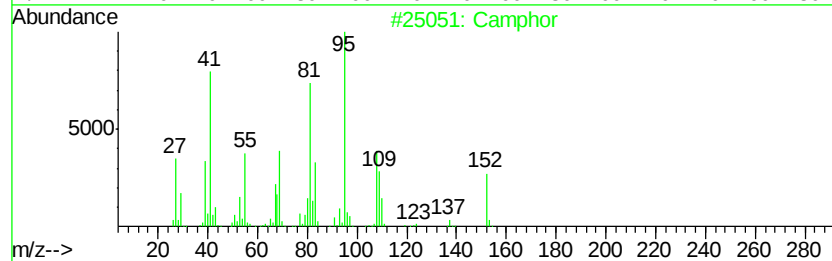
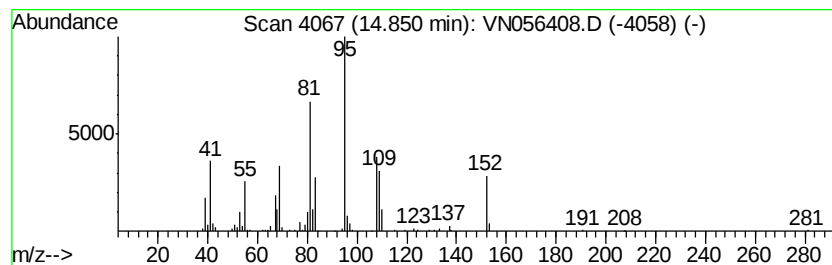
Instrument :
MSVOA_N
ClientSampleId :
390619766-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N061919W.M
Quant Title : SW846 8260

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

Peak Number 7 Camphor Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.85	14.64 ug/l	417790	1,4-Dichlorobenzene-d4	13.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Camphor	152 C10H16O	000076-22-2	97
2	(+)-2-Bornanone	152 C10H16O	000464-49-3	97
3	Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-, (1S)-	152 C10H16O	000464-48-2	94
4	Spirobicyclo[2.2.1]heptane-2,2'-diol	236 C14H20O3	1000155-15-2	59
5	2-Butanone, 4-(5-methyl-2-furanyl)-	152 C9H12O2	013679-56-6	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN062019\
Data File : VN056408.D
Acq On : 20 Jun 2019 17:23
Operator : JC/SP
Sample : K3465-01
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
390619766-VOA

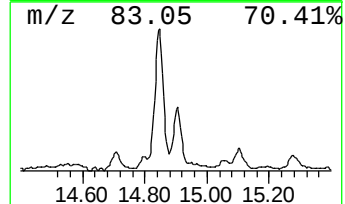
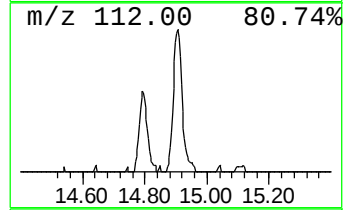
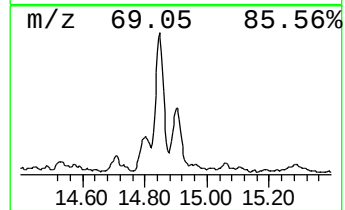
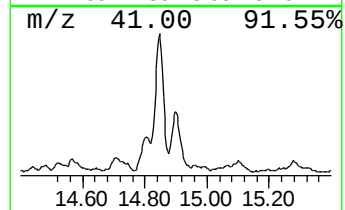
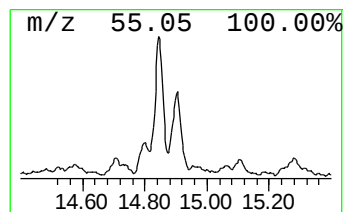
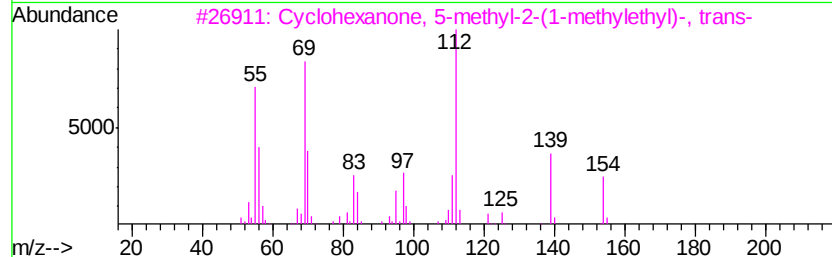
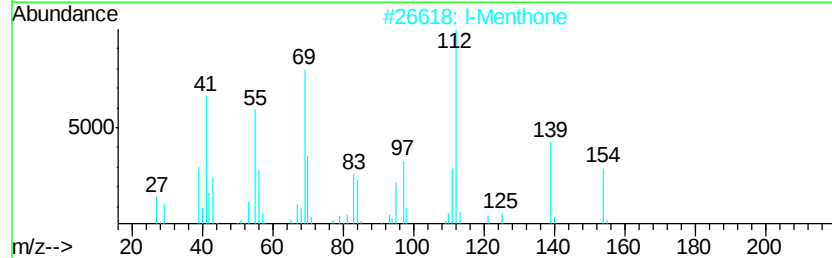
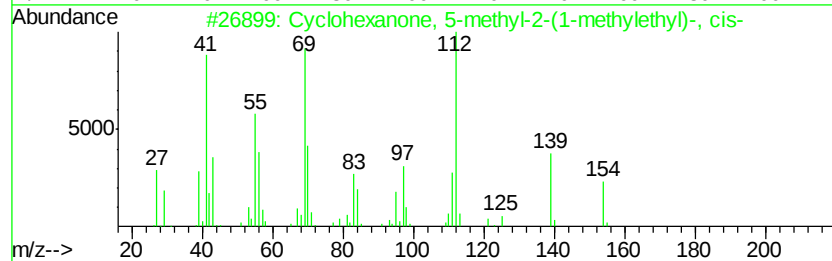
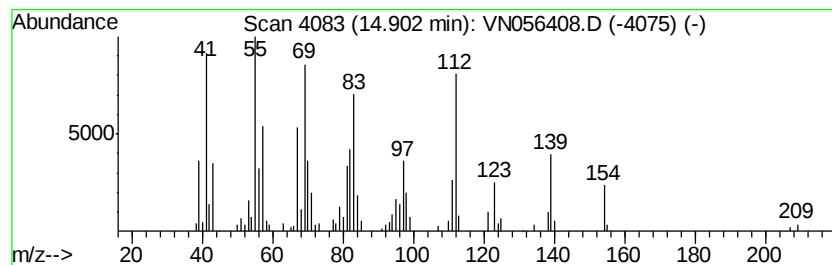
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N061919W.M
Quant Title : SW846 8260

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

Peak Number 8 Cyclohexanone, 5-methyl-2-(... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.90	5.99 ug/l	171038	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	000491-07-6	94
2		l-Menthone	154	C10H18O	014073-97-3	94
3		Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	000089-80-5	93
4		Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	001196-31-2	76
5		Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	010458-14-7	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062019\
Data File : VN056408.D
Acq On : 20 Jun 2019 17:23
Operator : JC/SP
Sample : K3465-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
390619766-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N061919W.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
Dimethyl ether	1.99	9.2	ug/l	175452	1	7.66	949321	50.0
3-Hexanone, 2-met...	10.72	11.2	ug/l	403732	3	11.41	1810420	50.0
7-Oxabicyclo[2.2...	13.17	5.7	ug/l	162333	4	13.34	1427060	50.0
Benzoic acid, 2-[...	13.88	8.4	ug/l	238662	4	13.34	1427060	50.0
Bicyclo[2.2.1]hep...	14.22	32.4	ug/l	925339	4	13.34	1427060	50.0
Bicyclo[2.2.1]hep...	14.81	5.6	ug/l	158684	4	13.34	1427060	50.0
Camphor	14.85	14.6	ug/l	417790	4	13.34	1427060	50.0
Cyclohexanone, 5-...	14.90	6.0	ug/l	171038	4	13.34	1427060	50.0