

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN091919\
 Data File : VN058213.D
 Acq On : 19 Sep 2019 18:54
 Operator : JC/SP
 Sample : K4949-03
 Misc : 5.00mL/MSVOA N/WATER
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 390918737.1-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\82N091819W.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	1.979	56	64	77	rVB	352176	469474	5.14%	1.078%
2	3.802	613	631	656	rBV3	92544	251732	2.75%	0.578%
3	4.239	748	767	788	rBV3	37090	115120	1.26%	0.264%
4	4.754	892	927	979	rBV	1940846	6848861	74.95%	15.732%
5	6.799	1536	1563	1619	rBV	2816430	9137462	100.00%	20.990%
6	7.191	1660	1685	1718	rBV	1935186	5280084	57.79%	12.129%
7	7.574	1783	1804	1815	rBV	330297	820060	8.97%	1.884%
8	7.651	1815	1828	1857	rVB	690930	1656891	18.13%	3.806%
9	8.014	1921	1941	1963	rBV2	467084	1194394	13.07%	2.744%
10	8.117	1963	1973	1987	rVB3	69982	155455	1.70%	0.357%
11	8.226	1987	2007	2020	rBV4	112115	523720	5.73%	1.203%
12	8.432	2063	2071	2089	rVB2	44657	108573	1.19%	0.249%
13	8.574	2100	2115	2141	rVB	1027310	2119669	23.20%	4.869%
14	9.377	2353	2365	2372	rBV3	50336	95874	1.05%	0.220%
15	9.966	2534	2548	2563	rBV8	47526	140705	1.54%	0.323%
16	10.085	2571	2585	2598	rBV	1503856	2777580	30.40%	6.380%
17	10.149	2598	2605	2611	rVV	96045	171954	1.88%	0.395%
18	10.191	2611	2618	2631	rVB	137028	245637	2.69%	0.564%
19	10.718	2765	2782	2802	rBV	352237	644877	7.06%	1.481%
20	10.844	2810	2821	2848	rVB	41644	122826	1.34%	0.282%
21	11.406	2983	2996	3016	rVV	1400719	2471291	27.05%	5.677%
22	11.503	3017	3026	3035	rBV3	54180	97770	1.07%	0.225%
23	11.619	3049	3062	3071	rBV	283597	532394	5.83%	1.223%
24	11.950	3153	3165	3181	rVB	202597	348375	3.81%	0.800%
25	12.249	3248	3258	3270	rVB2	61274	112562	1.23%	0.259%
26	12.406	3295	3307	3327	rVB	1049984	1779577	19.48%	4.088%
27	13.046	3495	3506	3521	rVB	104260	180859	1.98%	0.415%
28	13.172	3533	3545	3555	rBV2	134278	237709	2.60%	0.546%
29	13.348	3588	3600	3618	rVB	1304010	2336392	25.57%	5.367%
30	13.551	3648	3663	3671	rBV	63012	125505	1.37%	0.288%
31	13.824	3738	3748	3759	rVV7	121659	264424	2.89%	0.607%
32	13.885	3759	3767	3778	rVB2	214318	359994	3.94%	0.827%
33	14.229	3859	3874	3890	rBV	404137	797447	8.73%	1.832%
34	14.583	3976	3984	4013	rVB	48343	137522	1.51%	0.316%

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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

35	14.818	4045	4057	4062	rBV6	130390	243927	2.67%	0.560%
36	14.853	4063	4068	4077	rVV3	149287	250961	2.75%	0.576%
37	14.911	4078	4086	4099	rVB2	124484	218517	2.39%	0.502%
38	15.130	4140	4154	4165	rVB	66958	157212	1.72%	0.361%

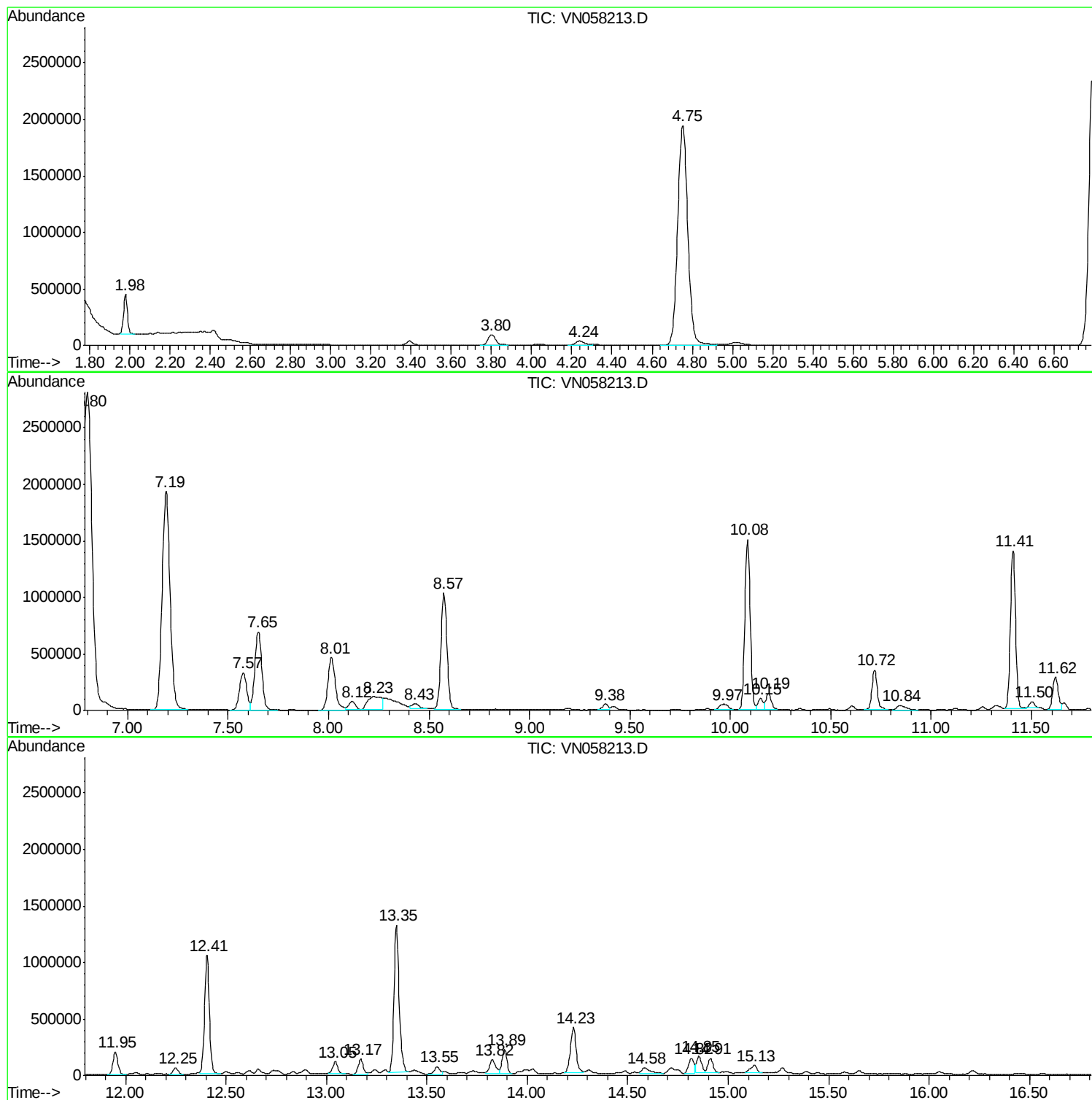
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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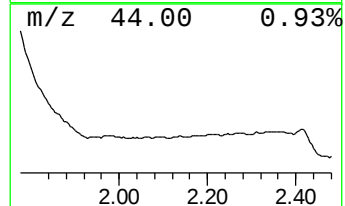
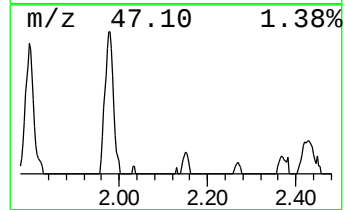
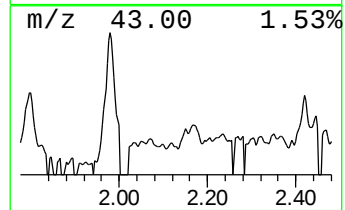
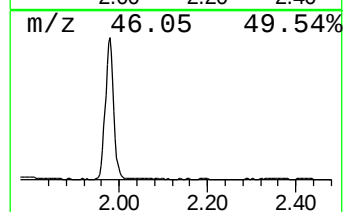
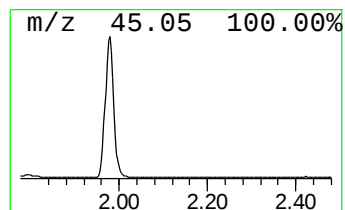
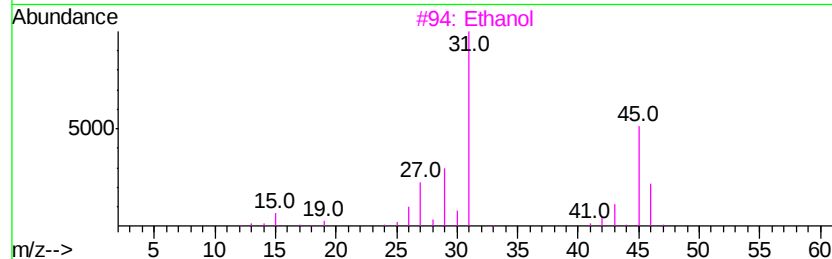
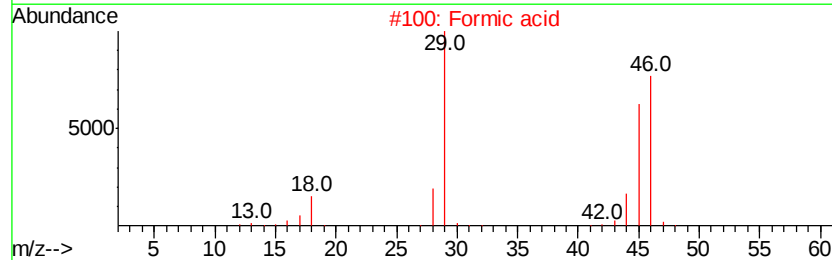
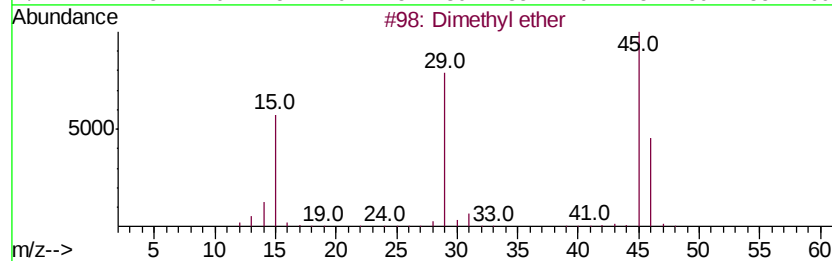
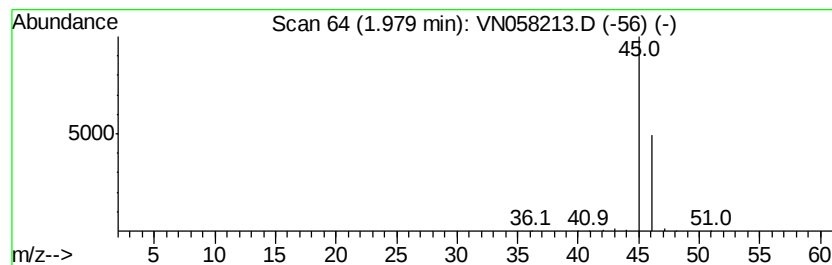
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N091819W.M
Quant Title : SW846 8260

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

Peak Number 1 Dimethyl ether Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.98	14.17 ug/l	469474	Pentafluorobenzene	7.65	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl ether	46	C2H6O	000115-10-6	90
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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ClientSampleId :
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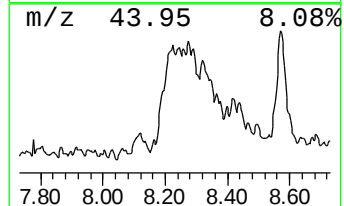
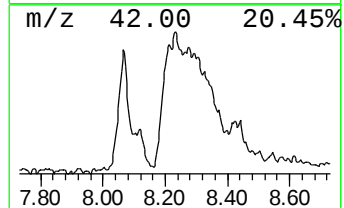
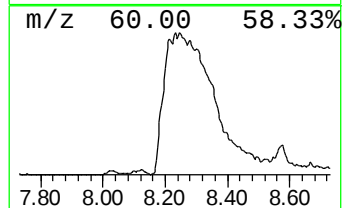
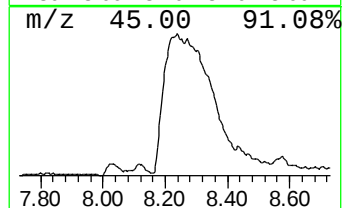
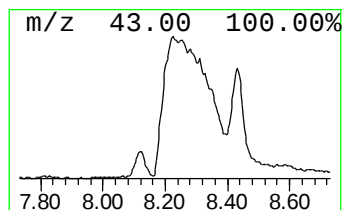
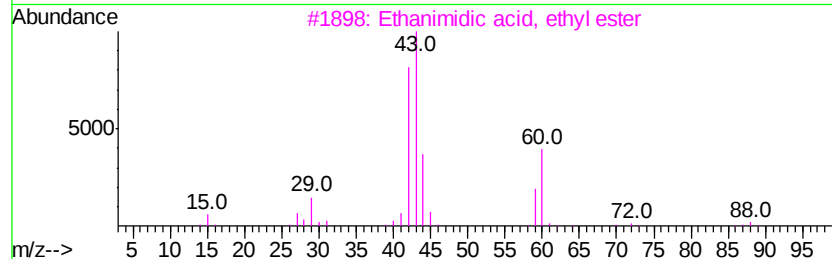
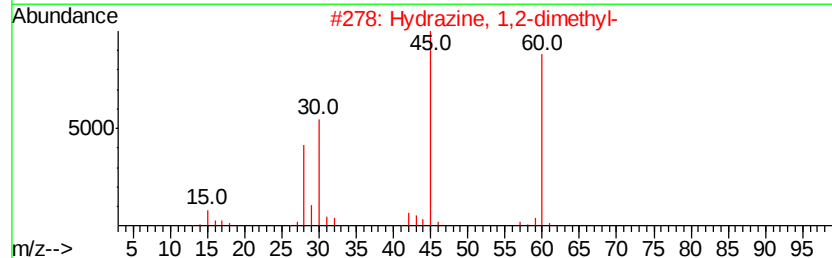
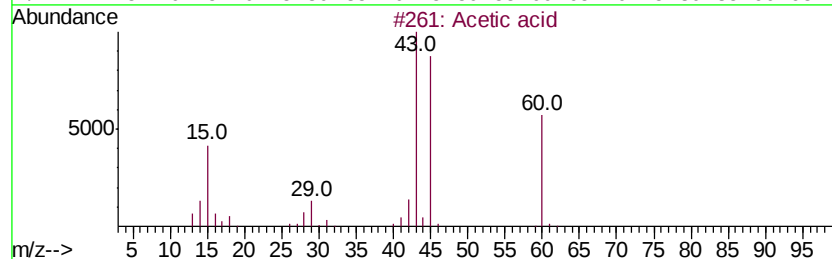
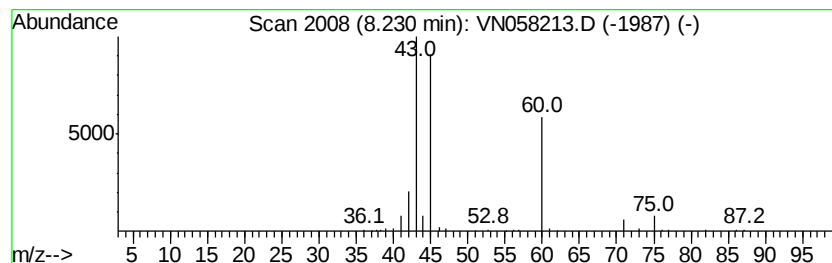
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Acetic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.23	12.35 ug/l	523720	1,4-Difluorobenzene	8.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid	60	C2H4O2	000064-19-7	86
2		Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	42
3		Ethanimidic acid, ethyl ester	87	C4H9NO	001000-84-6	12
4		o-Acetyl-L-serine	147	C5H9NO4	005147-00-2	10
5		Thiirane	60	C2H4S	000420-12-2	9



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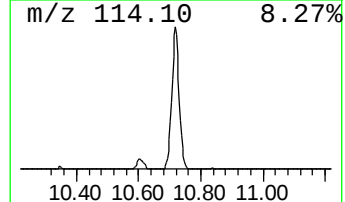
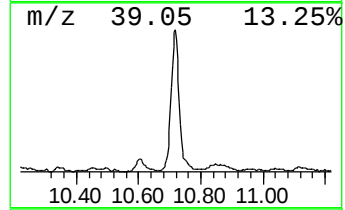
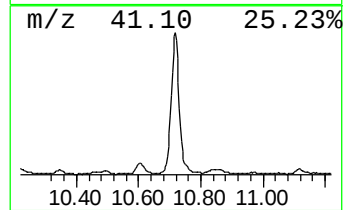
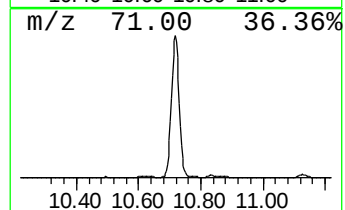
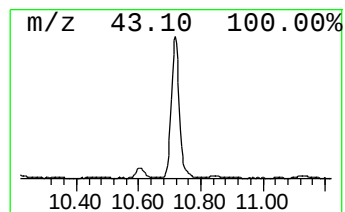
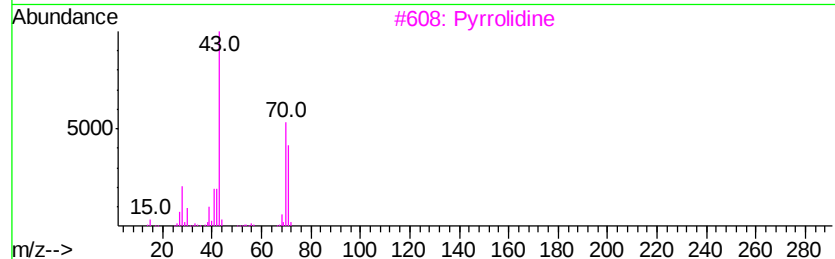
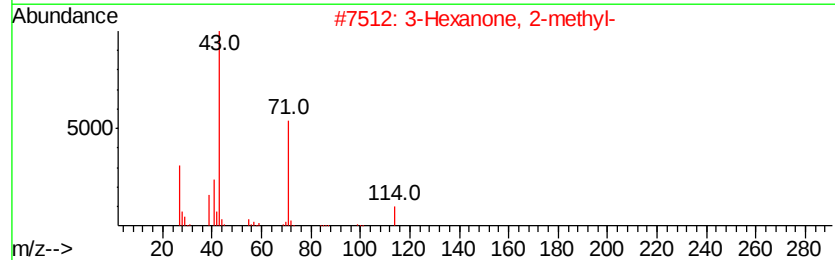
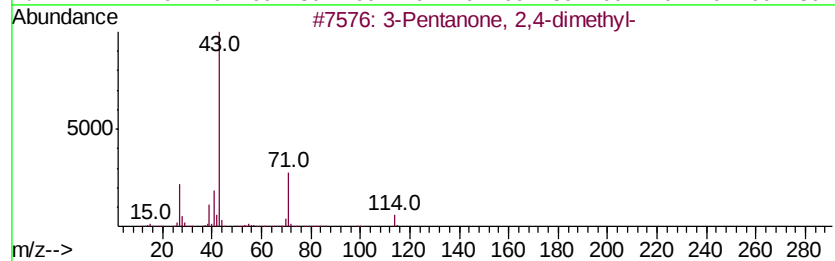
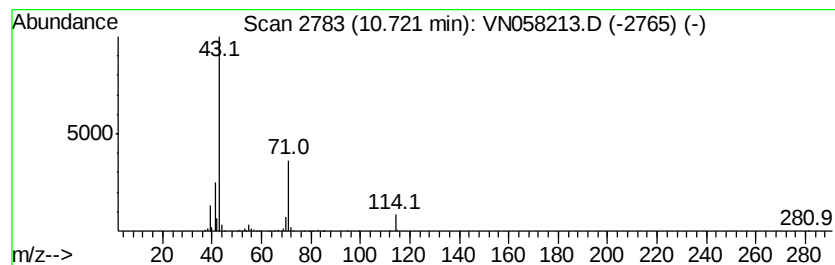
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 3-Pentanone, 2,4-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.72	13.05 ug/l	644877	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	86	
2	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	78	
3	Pyrrolidine	71	C4H9N	000123-75-1	59	
4	2,3-Hexanedione	114	C6H10O2	003848-24-6	53	
5	3,4-Dimethyl-2-pentanone	114	C7H14O	1000202-23-1	45	



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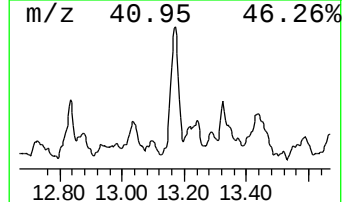
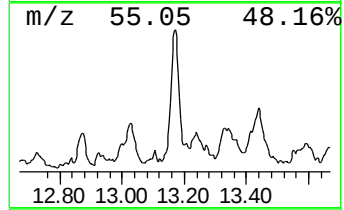
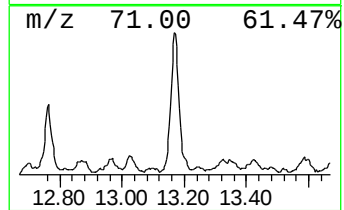
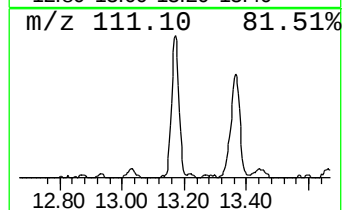
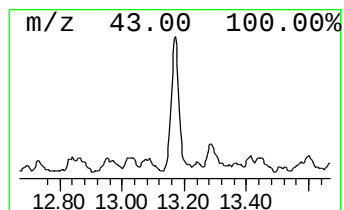
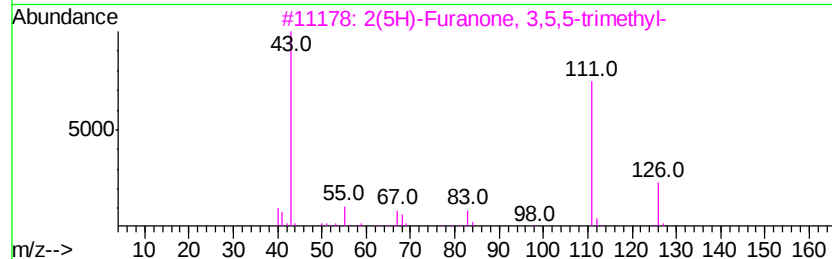
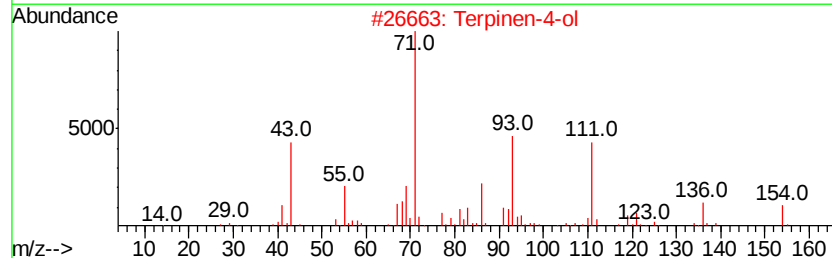
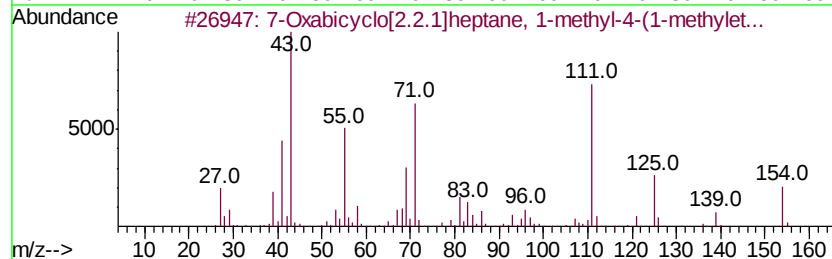
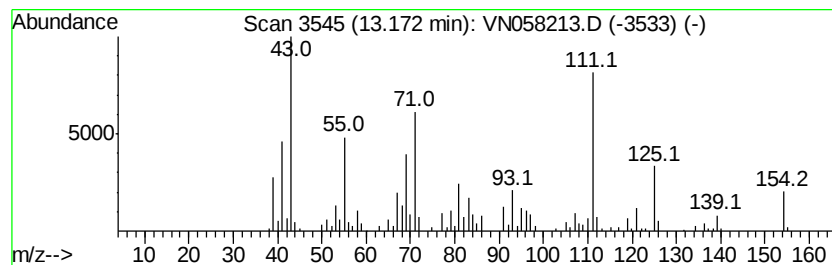
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Peak Number 4 7-Oxabicyclo[2.2.1]heptane,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.17	5.09 ug/l	237709	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		7-Oxabicyclo[2.2.1]heptane, 1-me...	154 C10H18O	000470-67-7 93
2		Terpinen-4-ol	154 C10H18O	000562-74-3 43
3		2(5H)-Furanone, 3,5,5-trimethyl-	126 C7H10O2	050598-50-0 42
4		Tetrahydrocarvone	154 C10H18O	000499-70-7 38
5		2(3H)-Furanone, 5-ethenyldihydro...	126 C7H10O2	001073-11-6 38



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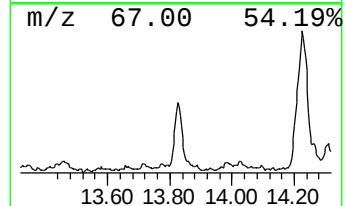
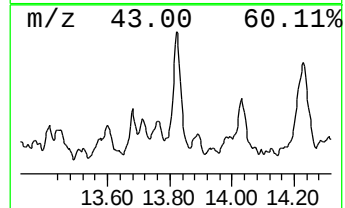
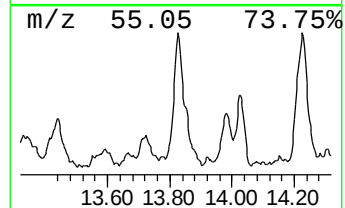
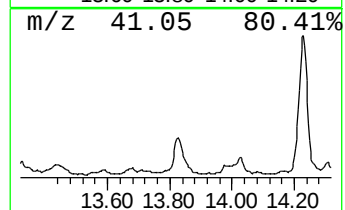
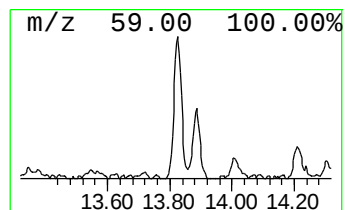
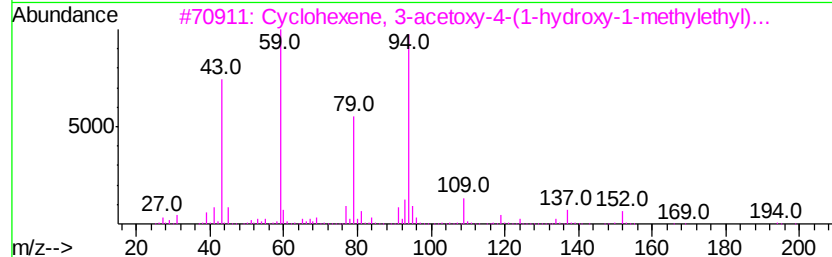
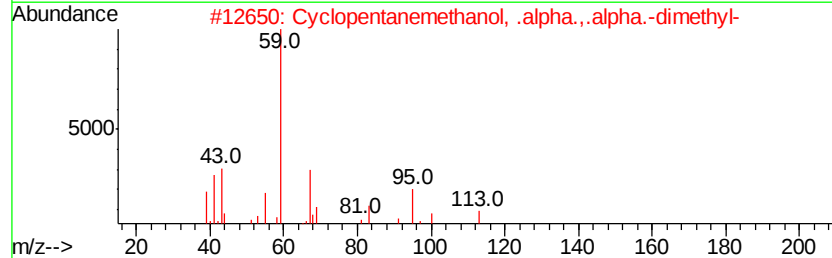
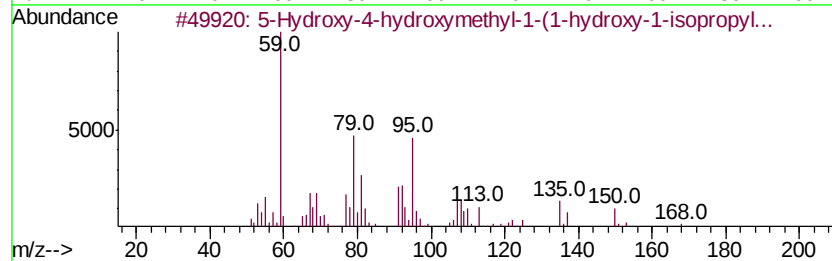
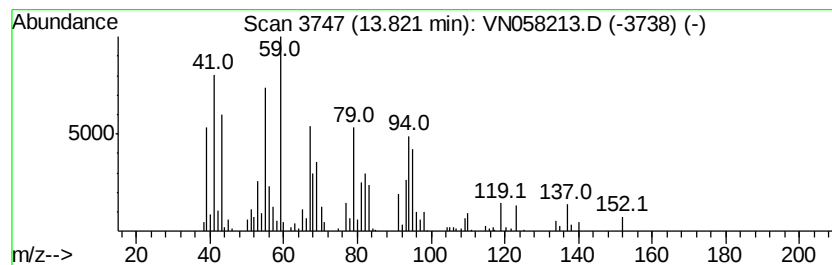
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Peak Number 5 unknown13.82 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	5.66 ug/l	264424	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Hydroxy-4-hydroxymethyl-1-(1-h...	186	C10H18O3	087096-72-8	47
2		Cyclopentanemethanol, .alpha.,.a...	128	C8H16O	001462-06-2	43
3		Cyclohexene, 3-acetoxy-4-(1-hydr...	212	C12H20O3	1000196-01-7	43
4		3-Cyclohexene-1-acetaldehyde, .a...	152	C10H16O	029548-14-9	42
5		Artemiseole	152	C10H16O	060485-46-3	35



Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN091919\
Data File : VN058213.D
Acq On : 19 Sep 2019 18:54
Operator : JC/SP
Sample : K4949-03
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 27 Sample Multiplier: 1

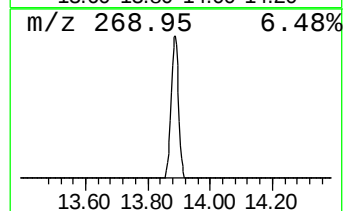
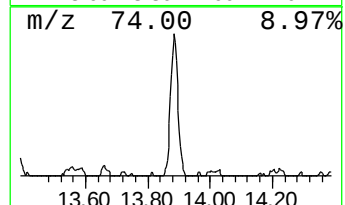
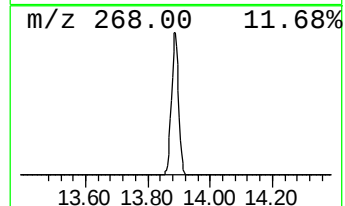
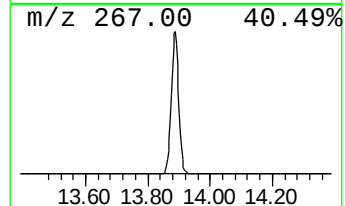
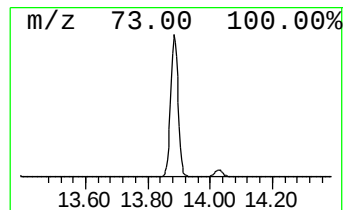
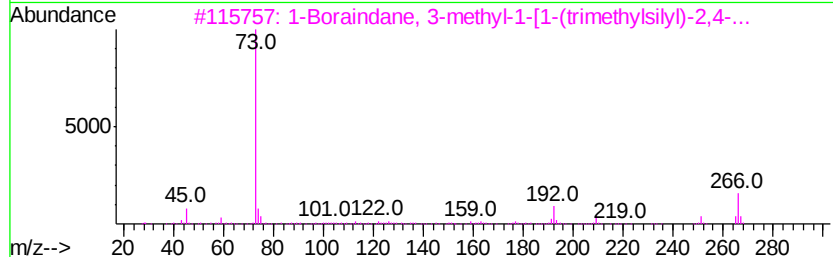
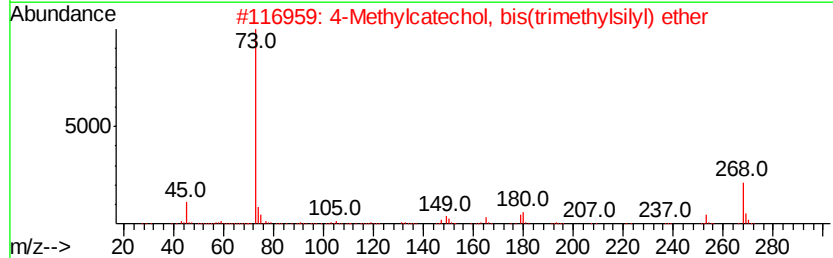
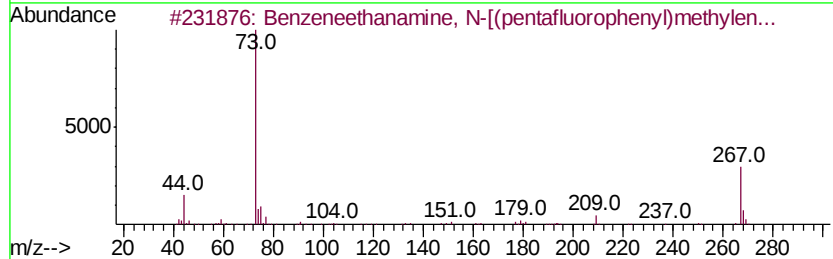
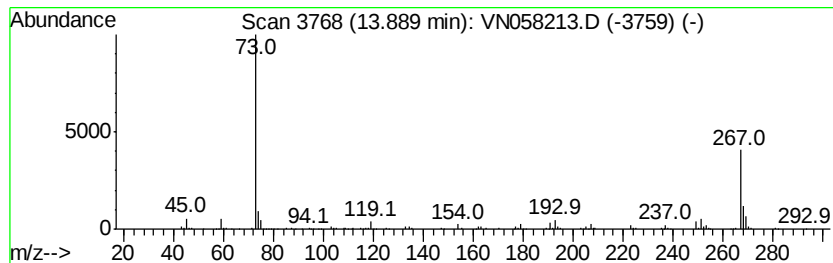
Instrument :
MSVOA_N
ClientSampleId :
390918737.1-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N091819W.M
Quant Title : SW846 8260

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

Peak Number 6 unknown13.89 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	7.70 ug/l	359994	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzeneethanamine, N-[(pentafluoro...	475 C21H26F5N02Si2	055429-85-1 42
2		4-Methylcatechol, bis(trimethyls...	268 C13H24O2Si2	1000332-79-9 38
3		1-Boraindane, 3-methyl-1-[1-(tri...	266 C17H23BSi	190316-36-0 35
4		Benzoic acid, 2-[(trimethylsilyl...	282 C13H22O3Si2	003789-85-3 33
5		trans-3-(2,2-Dichlorovinyl)-2,2-...	322 C14H24Cl2O2Si	1000314-29-8 25



Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN091919\
Data File : VN058213.D
Acq On : 19 Sep 2019 18:54
Operator : JC/SP
Sample : K4949-03
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 27 Sample Multiplier: 1

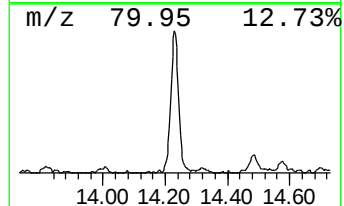
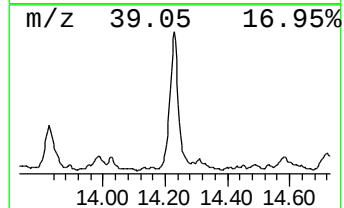
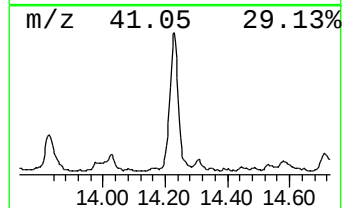
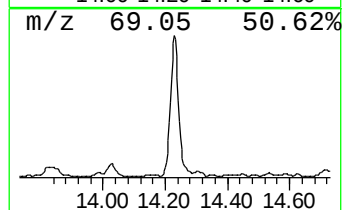
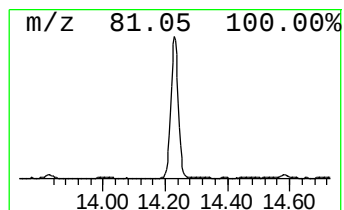
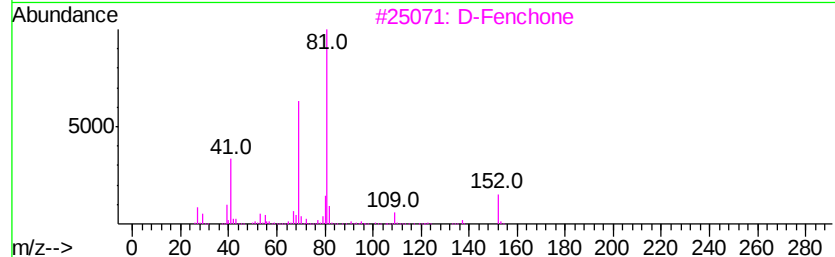
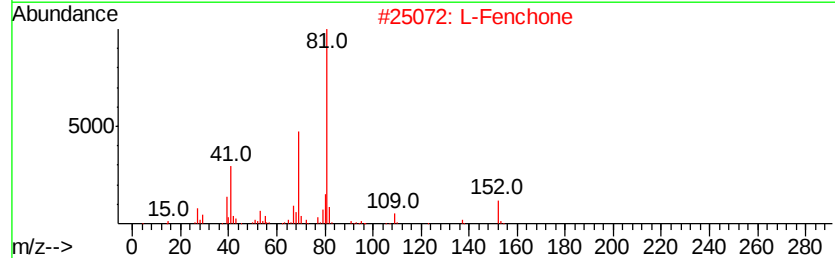
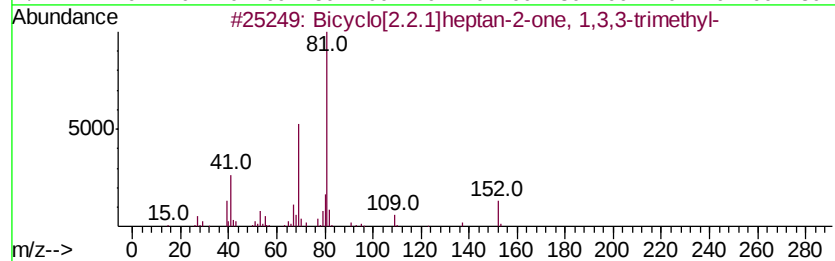
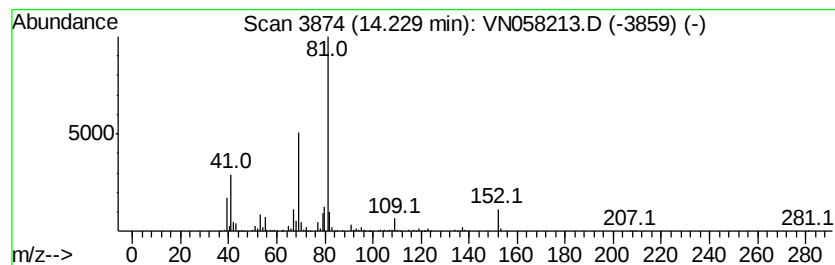
Instrument :
MSVOA_N
ClientSampleId :
390918737.1-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N091819W.M
Quant Title : SW846 8260

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

Peak Number 7 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.23	17.07 ug/l	797447	1,4-Dichlorobenzene-d4	13.35	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-one, 1,3,...	152	C10H16O	001195-79-5	94
2	L-Fenchone	152	C10H16O	007787-20-4	94
3	D-Fenchone	152	C10H16O	004695-62-9	90
4	2,4-Nonadienal, (E,E)-	138	C9H14O	005910-87-2	45
5	1-[4-(4-tert-Butyl-spirocyclohex...	371	C20H28F3N02	1000301-43-3	40



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN091919\
Data File : VN058213.D
Acq On : 19 Sep 2019 18:54
Operator : JC/SP
Sample : K4949-03
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 27 Sample Multiplier: 1

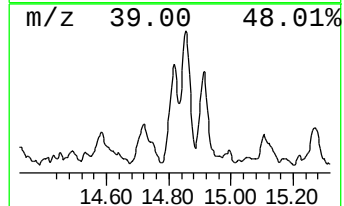
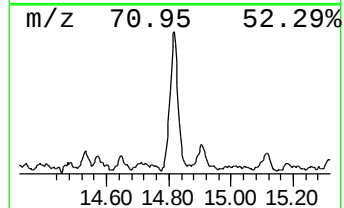
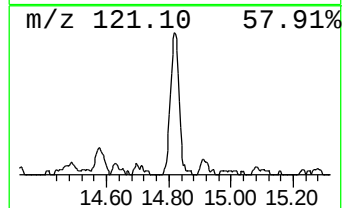
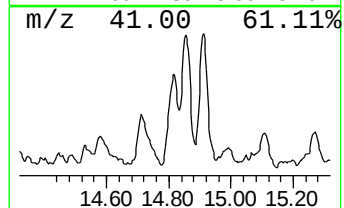
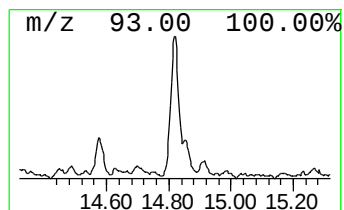
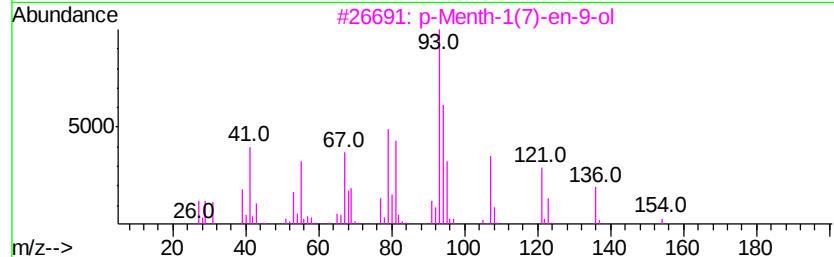
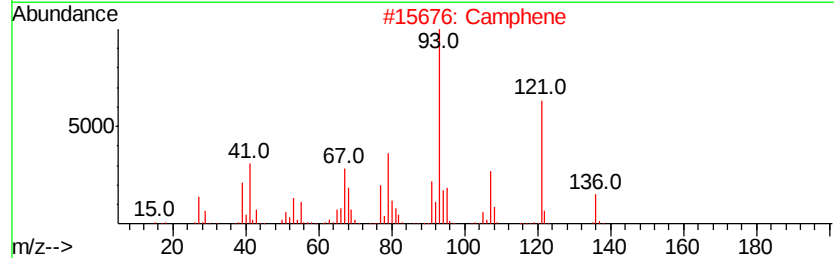
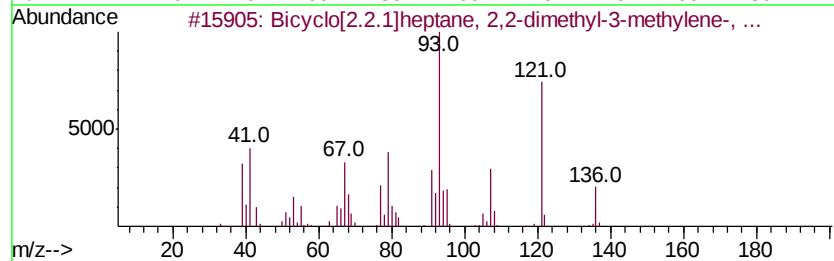
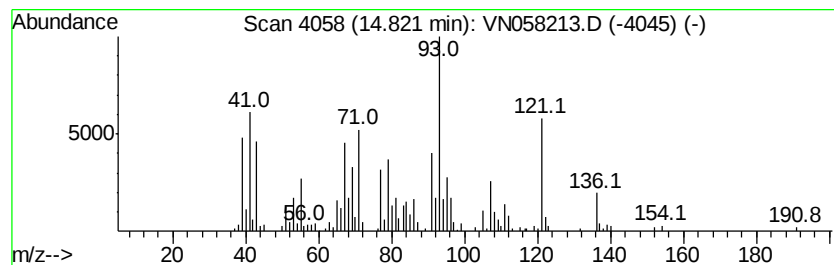
Instrument :
MSVOA_N
ClientSampleId :
390918737.1-VOA

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N091819W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	5.22 ug/l	243927	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Bicyclo[2.2.1]heptane, 2,2-dimet...	136 C10H16	005794-04-7 94
2		Camphene	136 C10H16	000079-92-5 92
3		p-Menth-1(7)-en-9-ol	154 C10H18O	029548-16-1 76
4		2-Carene	136 C10H16	000554-61-0 60
5		Cyclopentene, 4-ethenyl-1,5,5-tr...	136 C10H16	001727-69-1 55



Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN091919\
Data File : VN058213.D
Acq On : 19 Sep 2019 18:54
Operator : JC/SP
Sample : K4949-03
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 27 Sample Multiplier: 1

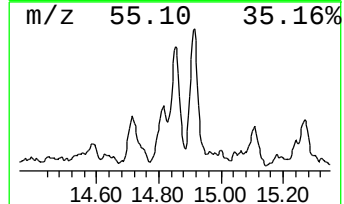
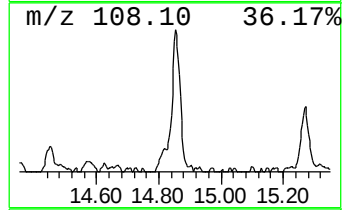
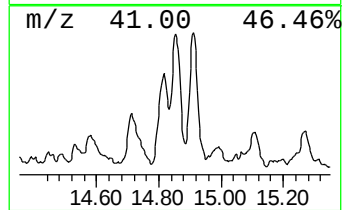
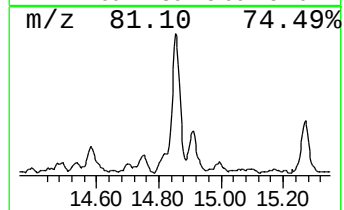
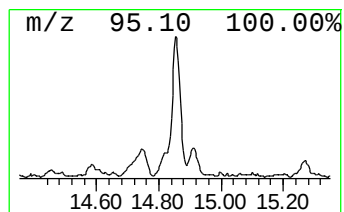
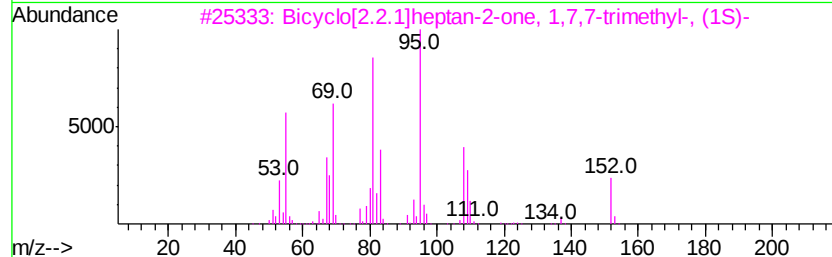
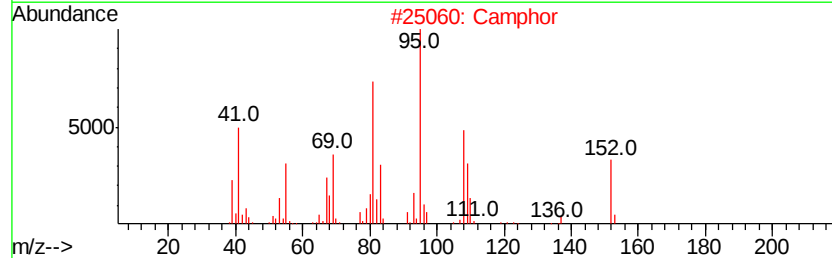
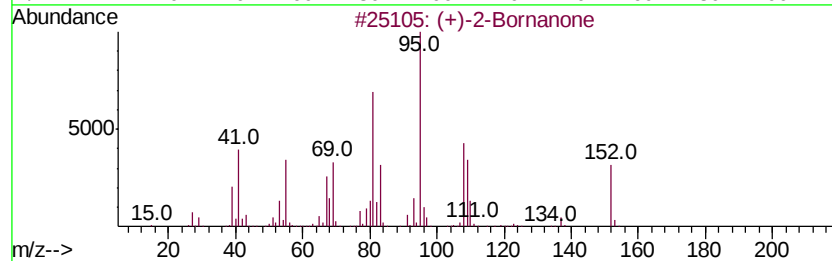
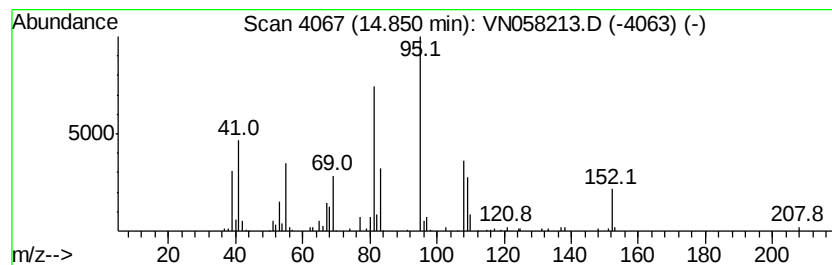
Instrument :
MSVOA_N
ClientSampleId :
390918737.1-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N091819W.M
Quant Title : SW846 8260

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

Peak Number 9 (+)-2-Bornanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.85	5.37 ug/l	250961	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		(+)-2-Bornanone	152 C10H16O	000464-49-3 91
2		Camphor	152 C10H16O	000076-22-2 86
3		Bicyclo[2.2.1]heptan-2-one, 1,7,...	152 C10H16O	000464-48-2 86
4		Cyclohexanone, 5-methyl-2-(1-met...	152 C10H16O	015932-80-6 43
5		Tricyclo[2.2.1.0(2,6)]heptan-3-o...	152 C10H16O	062560-53-6 38



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN091919\
Data File : VN058213.D
Acq On : 19 Sep 2019 18:54
Operator : JC/SP
Sample : K4949-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
390918737.1-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N091819W.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	1.98	14.2	ug/l	469474	1	7.65	1656890	50.0
Acetic acid	8.23	12.4	ug/l	523720	2	8.57	2119670	50.0
3-Pentanone, 2,4-...	10.72	13.1	ug/l	644877	3	11.41	2471290	50.0
7-Oxabicyclo[2.2.1]hept-2-en-5-one	13.17	5.1	ug/l	237709	4	13.35	2336390	50.0
unknown13.82	13.82	5.7	ug/l	264424	4	13.35	2336390	50.0
unknown13.89	13.89	7.7	ug/l	359994	4	13.35	2336390	50.0
Bicyclo[2.2.1]hept-2-en-5-one	14.23	17.1	ug/l	797447	4	13.35	2336390	50.0
Bicyclo[2.2.1]hept-2-en-5-one	14.82	5.2	ug/l	243927	4	13.35	2336390	50.0
(+)-2-Bornanone	14.85	5.4	ug/l	250961	4	13.35	2336390	50.0