

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV062320\
 Data File : VV017048.D
 Acq On : 23 Jun 2020 12:11
 Operator : SY/MD
 Sample : L3067-08
 Misc : 25.0mL/MSVOA V/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BFXG5

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

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_V\METHOD\SOMVTR061720WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.113	4	7	16	rVB2	12633	12761	1.70%	0.161%
2	1.315	61	70	79	rVB	91940	94284	12.58%	1.192%
3	1.579	145	152	165	rVB2	70623	107458	14.34%	1.358%
4	2.122	312	321	332	rBV	139515	201604	26.90%	2.549%
5	2.200	336	345	354	rBV3	6012	11807	1.58%	0.149%
6	2.778	519	525	542	rVB2	20982	39116	5.22%	0.494%
7	3.312	679	691	710	rVB2	32864	79217	10.57%	1.001%
8	3.936	869	885	917	rBV2	116819	369164	49.27%	4.667%
9	4.376	1005	1022	1044	rVB2	117451	292849	39.08%	3.702%
10	5.071	1222	1238	1246	rBV2	281598	651368	86.93%	8.234%
11	5.122	1247	1254	1275	rVB	328151	706578	94.29%	8.932%
12	5.643	1400	1416	1438	rBV	226940	465795	62.16%	5.888%
13	6.096	1535	1557	1583	rBV	156676	327610	43.72%	4.141%
14	6.341	1620	1633	1649	rBV	149871	309908	41.36%	3.918%
15	6.778	1756	1769	1778	rBV	7559	16733	2.23%	0.212%
16	6.958	1814	1825	1831	rBV4	12083	22807	3.04%	0.288%
17	7.010	1831	1841	1857	rVB2	79924	143929	19.21%	1.819%
18	7.161	1876	1888	1902	rVB3	28249	55009	7.34%	0.695%
19	7.338	1928	1943	1959	rBV	343123	594546	79.34%	7.516%
20	7.643	2028	2038	2052	rBV	48511	83831	11.19%	1.060%
21	8.112	2174	2184	2221	rBV2	261282	519120	69.28%	6.562%
22	8.875	2408	2421	2443	rBV	345087	566670	75.62%	7.163%
23	8.993	2448	2458	2470	rVB	6314	13293	1.77%	0.168%
24	9.752	2685	2694	2714	rVB2	54292	90833	12.12%	1.148%
25	10.238	2835	2845	2858	rBV	104536	166525	22.22%	2.105%
26	10.501	2912	2927	2949	rBV2	446678	749332	100.00%	9.472%
27	10.601	2952	2958	2966	rVV9	6476	9614	1.28%	0.122%
28	10.678	2976	2982	2988	rVB8	6570	8524	1.14%	0.108%
29	10.720	2989	2995	3003	rVV8	5413	8616	1.15%	0.109%
30	10.820	3019	3026	3034	rVB8	4507	7863	1.05%	0.099%
31	11.199	3136	3144	3152	rVB8	4718	8349	1.11%	0.106%
32	11.270	3154	3166	3179	rBV	368062	571499	76.27%	7.224%
33	11.550	3245	3253	3264	rVB5	8939	14862	1.98%	0.188%
34	11.646	3271	3283	3299	rBV	344044	541861	72.31%	6.850%

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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: 0.1 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 : TRACE VOA SOM01.0

35	13.488	3848	3856	3864	rVB10	6201	10545	1.41%	0.133%
36	13.627	3887	3899	3913	rBV4	21792	36811	4.91%	0.465%

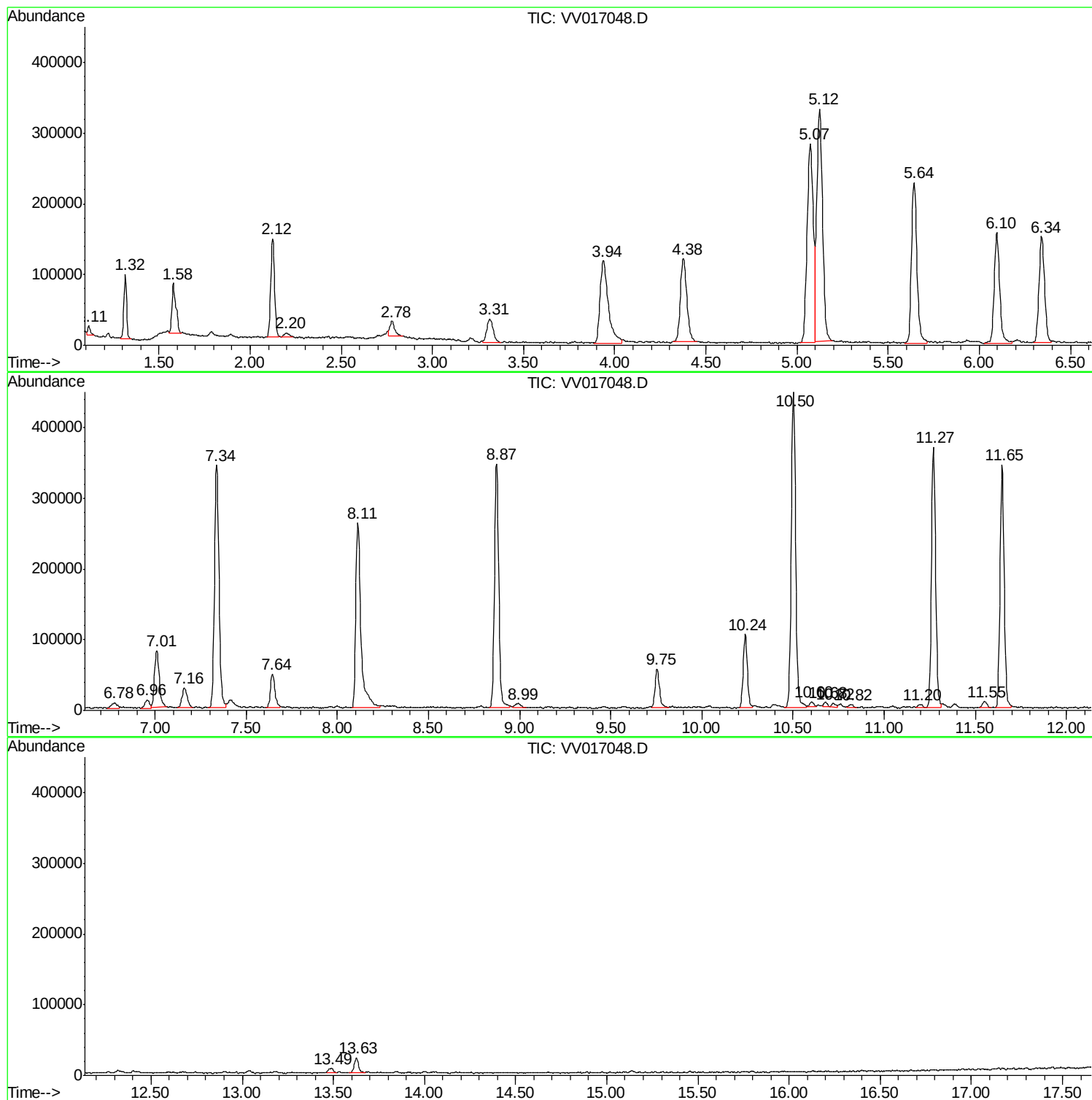
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Quant Title : TRACE VOA SOM01.0

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



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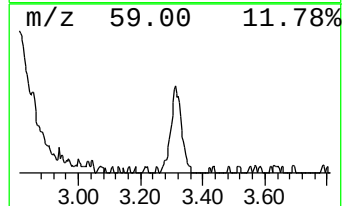
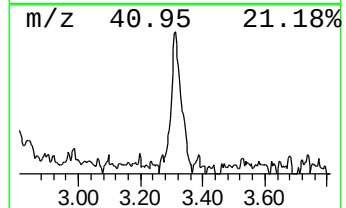
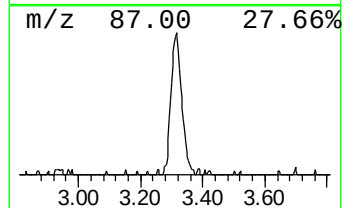
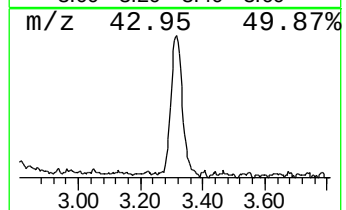
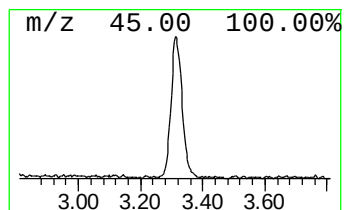
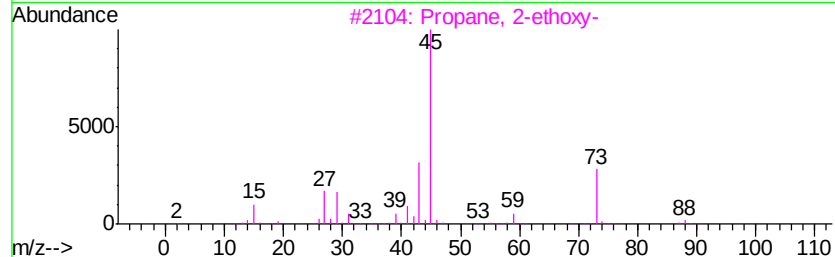
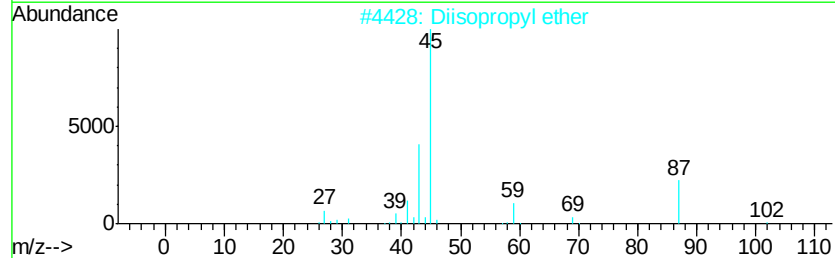
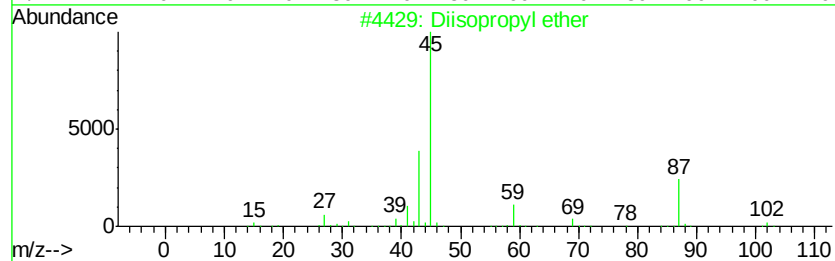
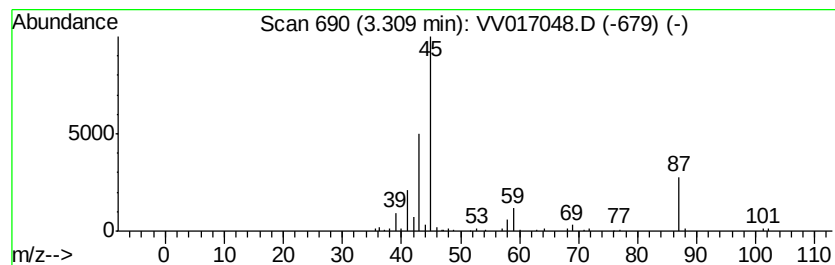
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Diisopropyl ether Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.31	0.85 ug/L	79217	1,4-Difluorobenzene	5.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diisopropyl ether	102	C6H14O	000108-20-3	56
2			Diisopropyl ether	102	C6H14O	000108-20-3	56
3			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	53
4			Ether, sec-butyl isopropyl	116	C7H16O	018641-81-1	43
5			1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	39



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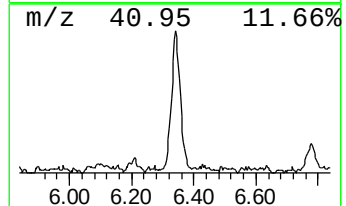
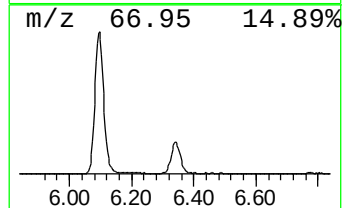
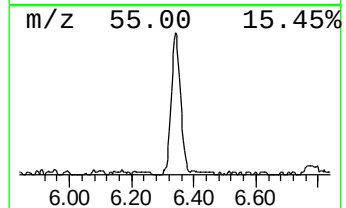
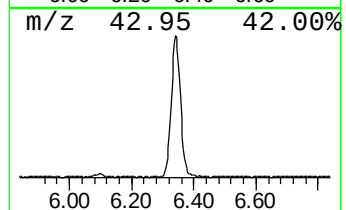
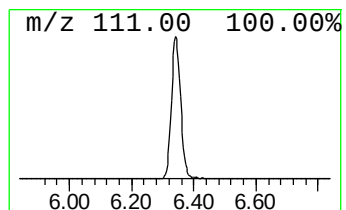
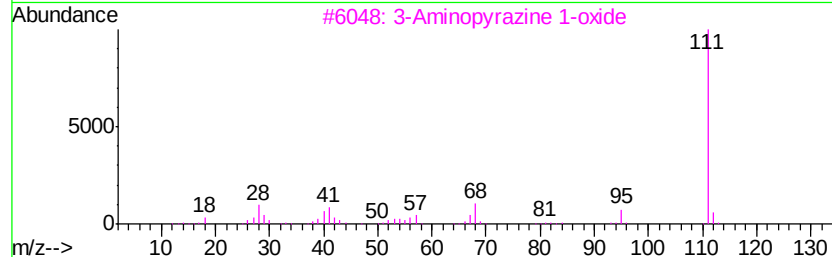
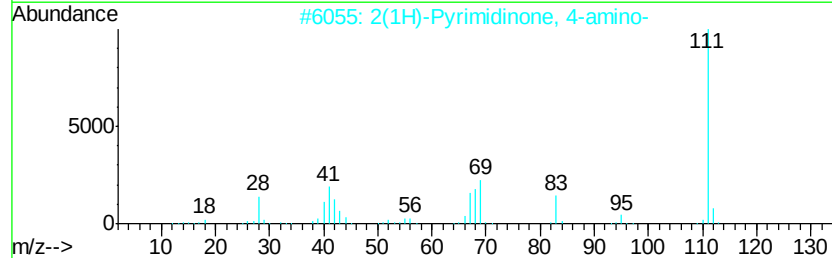
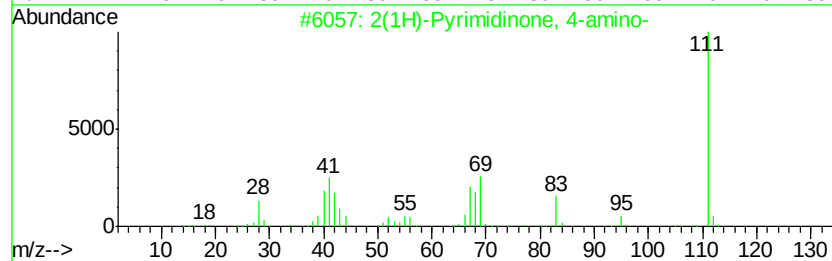
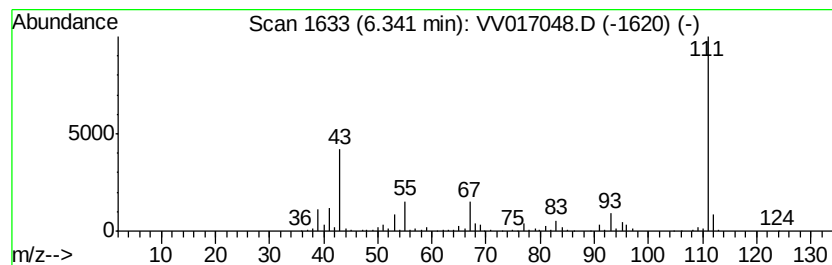
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 2(1H)-Pyrimidinone, 4-amino- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	3.33 ug/L	309908	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	64
2		2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	50
3		3-Aminopyrazine 1-oxide	111	C4H5N3O	006863-77-0	45
4		2(1H)-Pyridinone, 3-hydroxy-	111	C5H5N02	016867-04-2	42
5		2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	39



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Instrument :
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ClientSampled :
BFXG5

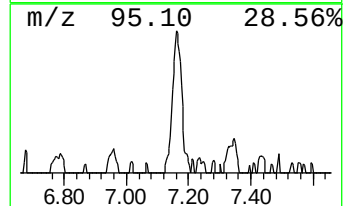
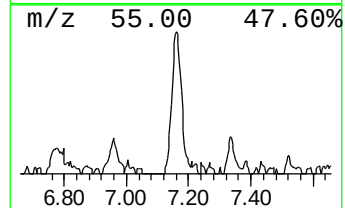
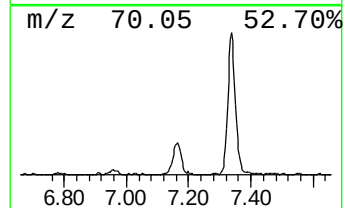
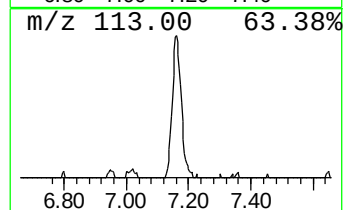
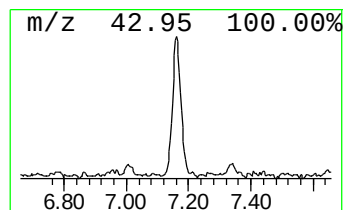
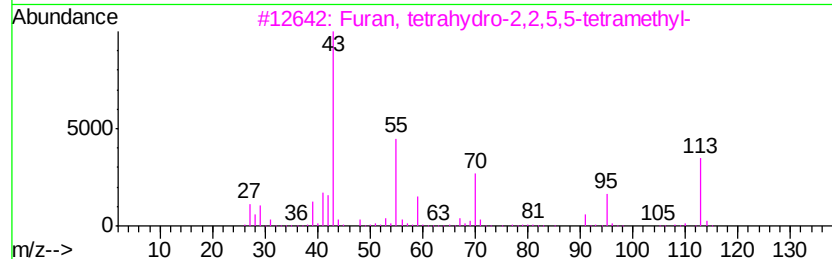
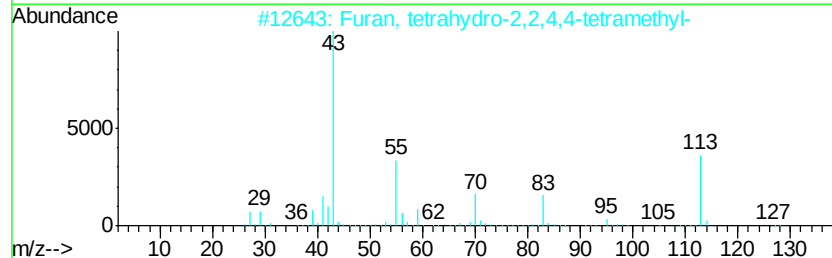
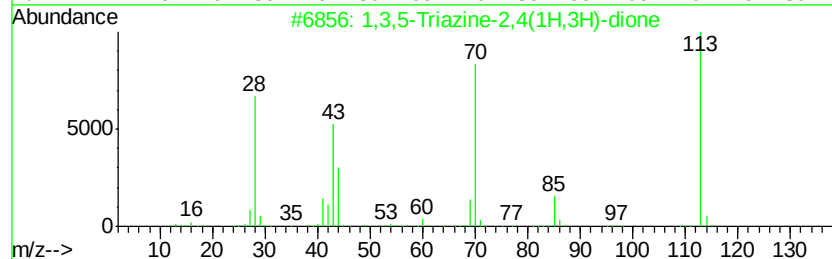
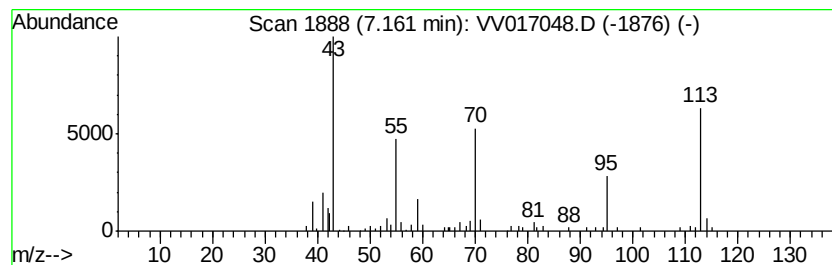
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 1,3,5-Triazine-2,4(1H,3H)-d... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.16	0.59 ug/L	55009	1,4-Difluorobenzene	5.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4(1H,3H)-dione	113	C3H3N3O2	000071-33-0	53	
2	Furan, tetrahydro-2,2,4,4-tetramethyl-	128	C8H16O	003358-28-9	53	
3	Furan, tetrahydro-2,2,5,5-tetramethyl-	128	C8H16O	015045-43-9	50	
4	Furan, tetrahydro-2,2,5,5-tetramethyl-	128	C8H16O	015045-43-9	50	
5	4-Piperidinone, 1-methyl-	113	C6H11NO	001445-73-4	50	



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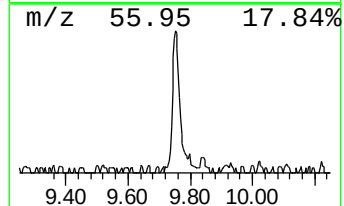
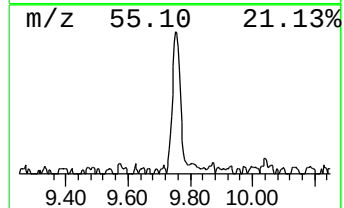
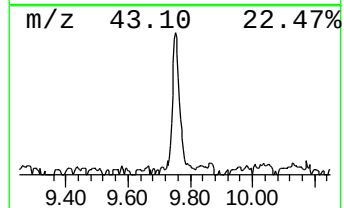
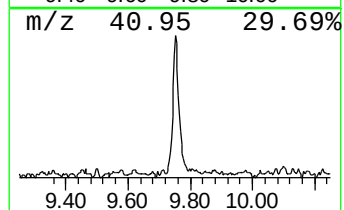
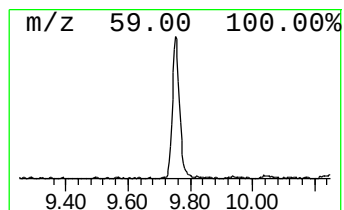
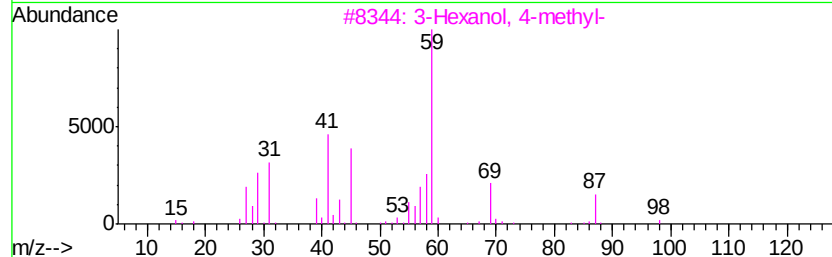
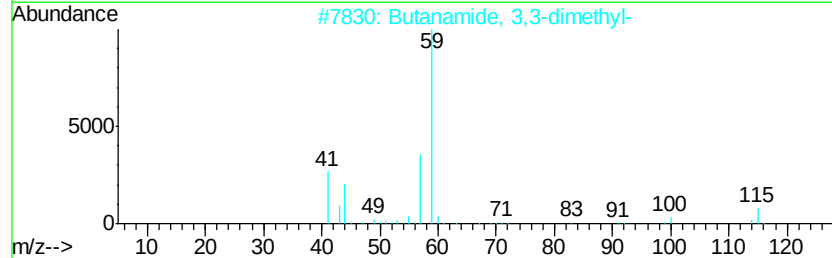
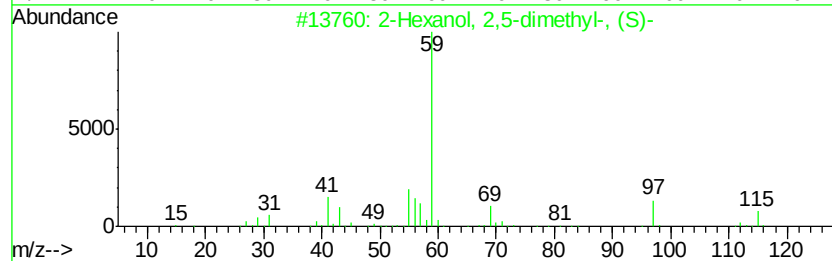
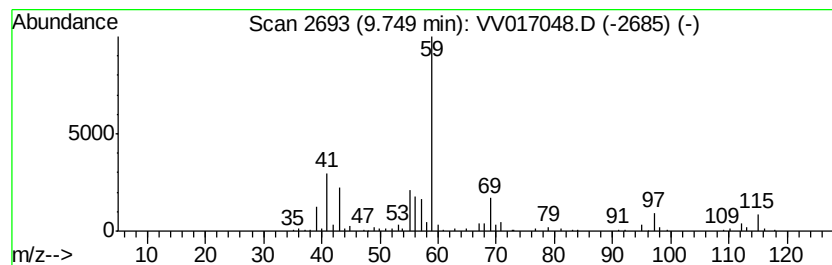
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.75	0.80 ug/L	90833	Chlorobenzene-d5	8.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	83
2		Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	50
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	50
4		2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	50
5		2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	47



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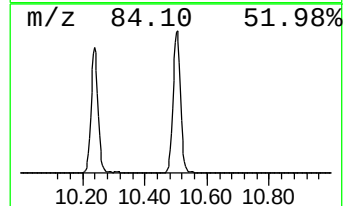
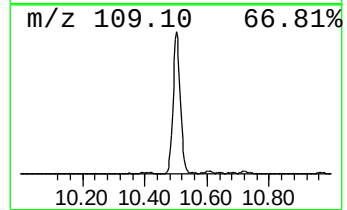
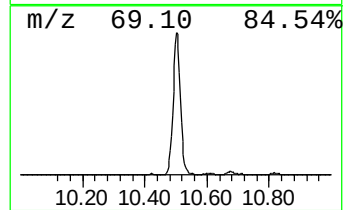
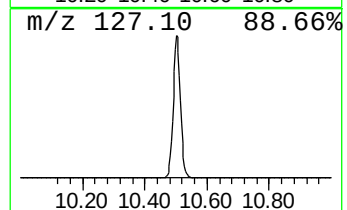
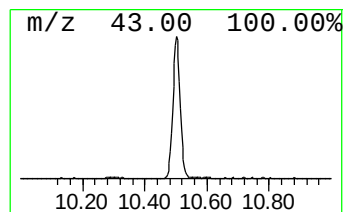
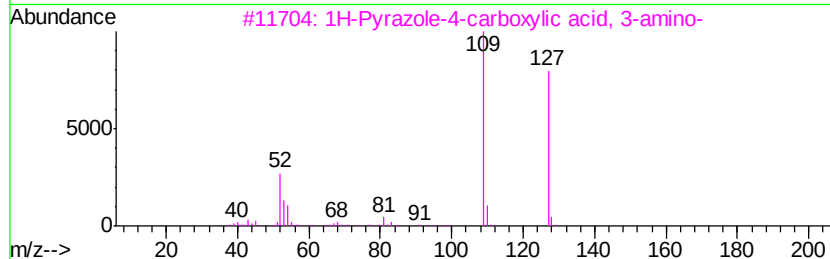
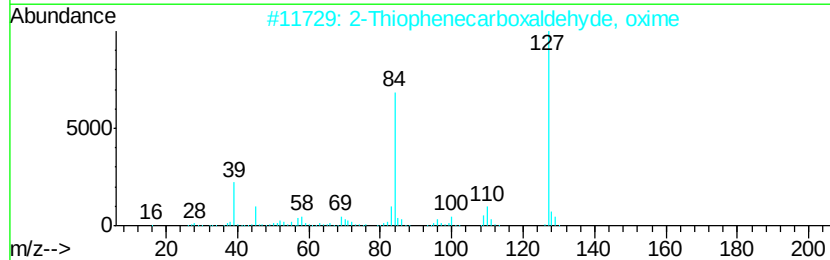
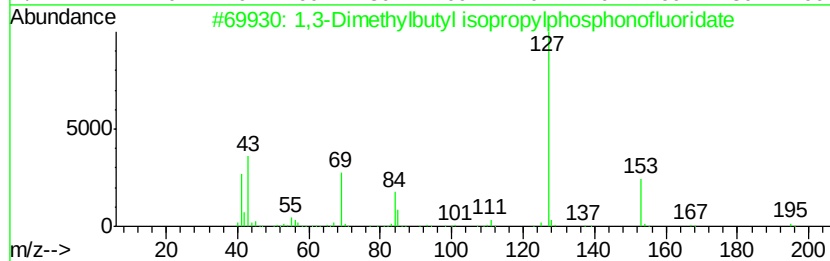
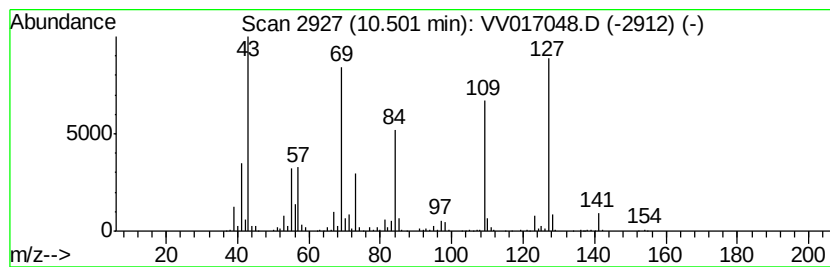
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TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.50	6.56 ug/L	749332	1,4-Dichlorobenzene-d4		11.27
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dimethylbutyl isopropylphosp...	210	C9H20F02P	1000298-25-6	42
2	2-Thiophenecarboxaldehyde, oxime	127	C5H5NOS	029683-84-9	35
3	1H-Pyrazole-4-carboxylic acid, 3...	127	C4H5N3O2	041680-34-6	35
4	3-Hexyne-2,5-diol, 2,5-dimethyl-	142	C8H14O2	000142-30-3	35
5	1H-Pyrazole, 4,5-dihydro-5-methyl-	84	C4H8N2	001568-20-3	27



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV062320\
Data File : VV017048.D
Acq On : 23 Jun 2020 12:11
Operator : SY/MD
Sample : L3067-08
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BFXG5

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Diisopropyl ether	3.31	0.8	ug/L	79217	1	5.64	465795	5.0
2(1H)-Pyrimidinon...	6.34	3.3	ug/L	309908	1	5.64	465795	5.0
1,3,5-Triazine-2,...	7.16	0.6	ug/L	55009	1	5.64	465795	5.0
2-Hexanol, 2,5-di...	9.75	0.8	ug/L	90833	2	8.87	566670	5.0
unknown-01	10.50	6.6	ug/L	749332	3	11.27	571499	5.0