

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV062320\
 Data File : VV017038.D
 Acq On : 22 Jun 2020 23:45
 Operator : SY/MD
 Sample : L3067-08
 Misc : 25.0mL/MSVOA V/WATER
 ALS Vial : 20 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	1.116	4	8	20	rVB2	13579	17502	2.14%	0.218%
2	1.316	61	70	78	rBV	82442	89770	10.99%	1.117%
3	1.425	91	104	106	rBV2	31653	55021	6.74%	0.685%
4	1.579	146	152	166	rVB2	63164	109514	13.41%	1.363%
5	2.123	312	321	334	rVB2	133875	200943	24.60%	2.501%
6	2.775	516	524	536	rBV2	18988	33613	4.12%	0.418%
7	3.209	650	659	676	rVB3	20193	43150	5.28%	0.537%
8	3.315	679	692	708	rVB4	31287	75165	9.20%	0.936%
9	3.939	869	886	928	rBV3	116122	419496	51.36%	5.221%
10	4.377	1005	1022	1043	rBV3	110193	270378	33.10%	3.365%
11	4.634	1085	1102	1120	rBV	49555	126430	15.48%	1.574%
12	5.071	1220	1238	1246	rBV2	254373	593504	72.66%	7.387%
13	5.122	1247	1254	1275	rVB	342342	724337	88.68%	9.016%
14	5.640	1403	1415	1436	rBV	206026	424244	51.94%	5.281%
15	6.097	1542	1557	1578	rBV	140313	289060	35.39%	3.598%
16	6.344	1619	1634	1650	rBV	160784	335698	41.10%	4.178%
17	6.778	1755	1769	1777	rBV9	8613	18457	2.26%	0.230%
18	6.955	1812	1824	1831	rBV4	11145	21924	2.68%	0.273%
19	7.010	1831	1841	1856	rVB	70183	127438	15.60%	1.586%
20	7.164	1876	1889	1906	rVB4	30374	66913	8.19%	0.833%
21	7.338	1930	1943	1958	rBV	315337	546156	66.87%	6.798%
22	7.412	1958	1966	1982	rVB3	10394	23596	2.89%	0.294%
23	7.643	2029	2038	2054	rBV	43093	77873	9.53%	0.969%
24	8.113	2174	2184	2215	rBV	280836	542966	66.48%	6.758%
25	8.875	2409	2421	2438	rBV	316566	524193	64.18%	6.525%
26	8.994	2449	2458	2466	rVB	6835	12360	1.51%	0.154%
27	9.756	2681	2695	2709	rBV	73966	127706	15.64%	1.590%
28	10.238	2830	2845	2856	rBV	102701	163691	20.04%	2.037%
29	10.502	2913	2927	2942	rBV	492837	816792	100.00%	10.167%
30	10.601	2951	2958	2966	rBV9	8661	13159	1.61%	0.164%
31	11.270	3155	3166	3189	rVB	330328	516634	63.25%	6.431%
32	11.556	3244	3255	3262	rBV7	14040	24499	3.00%	0.305%
33	11.646	3270	3283	3298	rBV	320867	506867	62.06%	6.309%
34	13.485	3844	3855	3864	rBV	8356	16445	2.01%	0.205%

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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 >
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Title : TRACE VOA SOM01.0

35	13.624	3888	3898	3909	rbV4	25522	43282	5.30%	0.539%
36	16.334	4732	4741	4751	rbV2	21790	35324	4.32%	0.440%

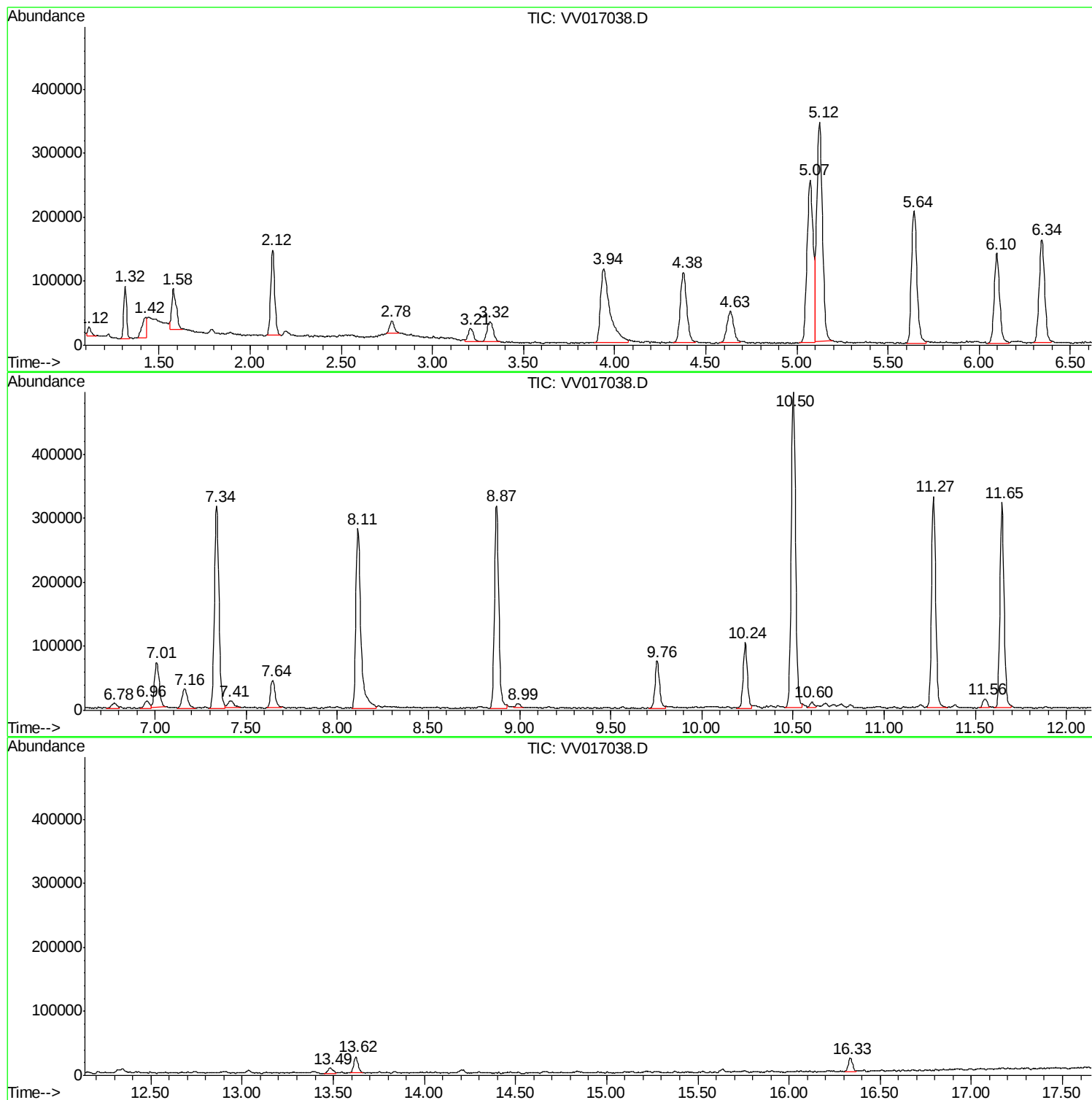
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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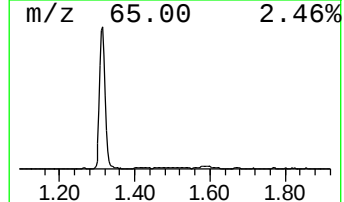
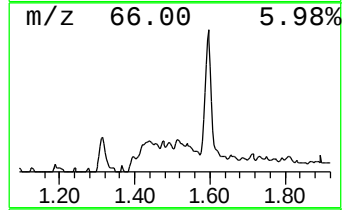
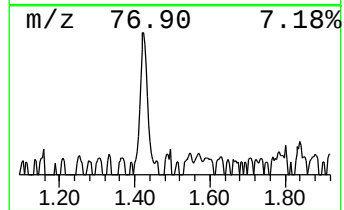
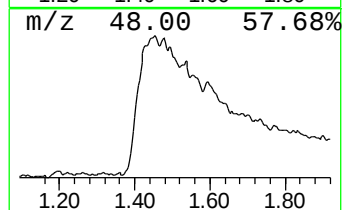
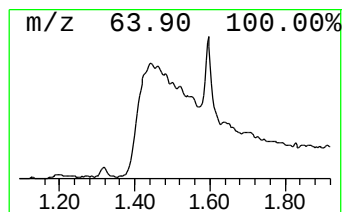
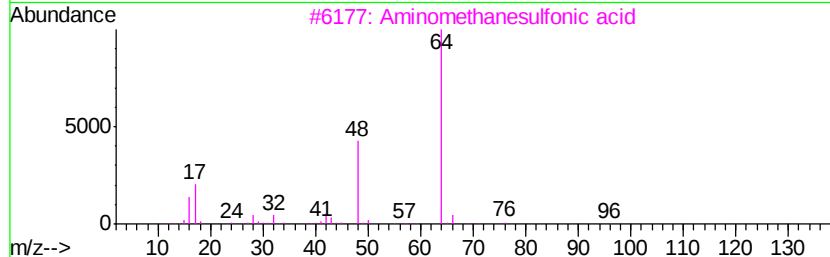
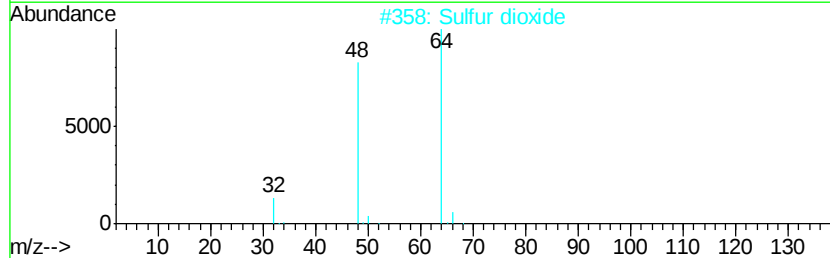
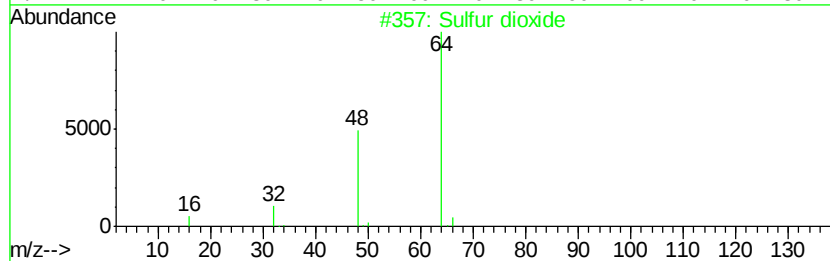
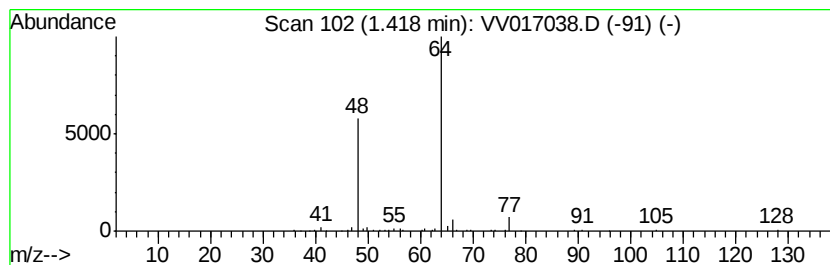
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.42	0.65 ug/L	55021	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfur dioxide	64	O2S	007446-09-5	83
2		Sulfur dioxide	64	O2S	007446-09-5	74
3		Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
4		Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
5		Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64



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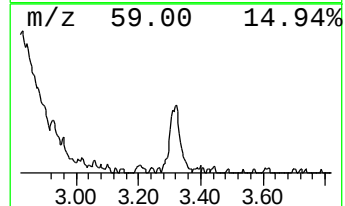
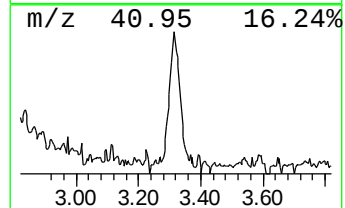
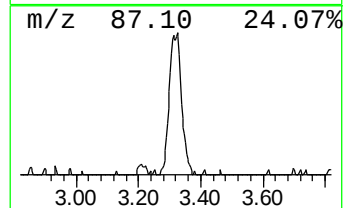
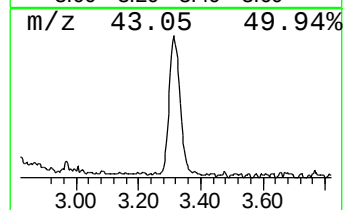
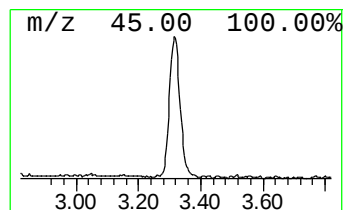
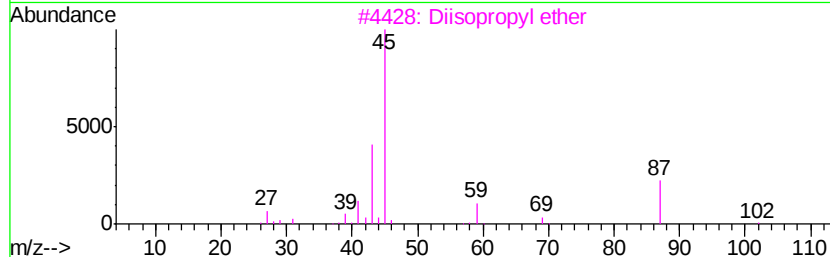
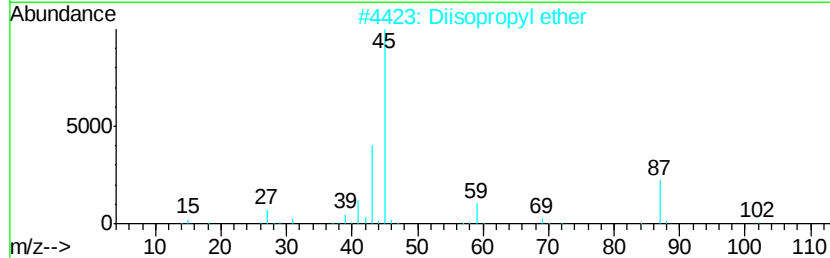
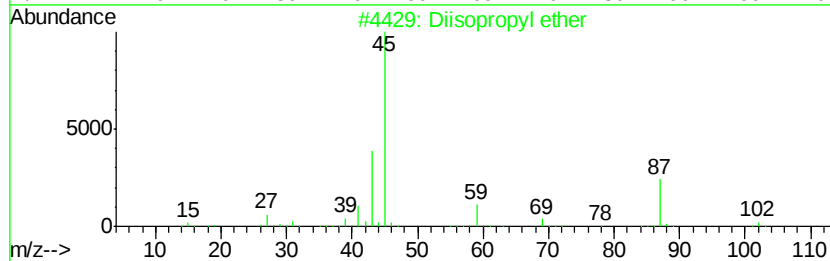
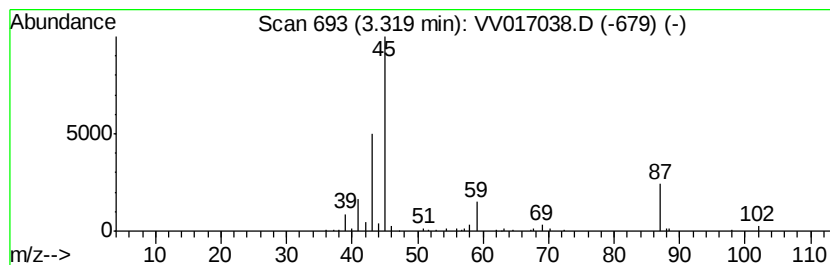
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 Diisopropyl ether Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.32	0.89 ug/L	75165	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Diisopropyl ether	102	C6H14O	000108-20-3	86
2		Diisopropyl ether	102	C6H14O	000108-20-3	78
3		Diisopropyl ether	102	C6H14O	000108-20-3	78
4		Ether, 2-chloro-1-methylethyl is...	136	C6H13ClO	098277-76-0	56
5		Propane, 2-ethoxy-	88	C5H12O	000625-54-7	42



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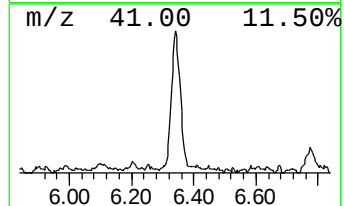
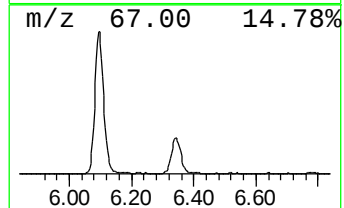
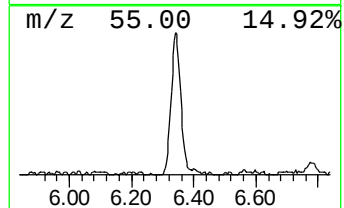
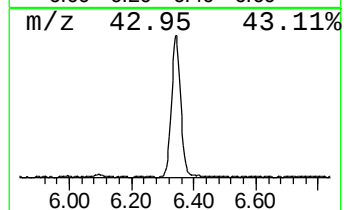
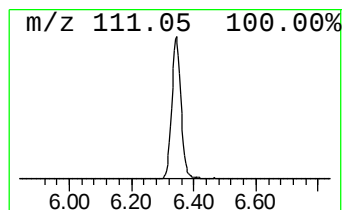
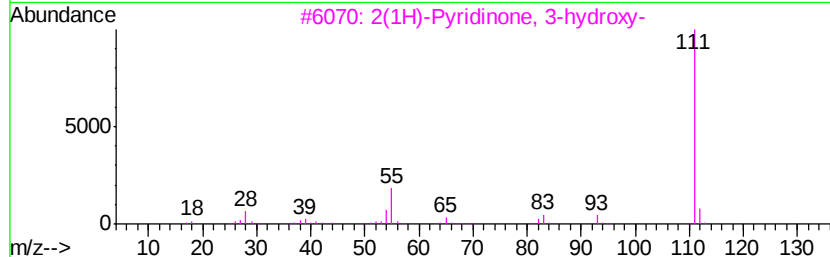
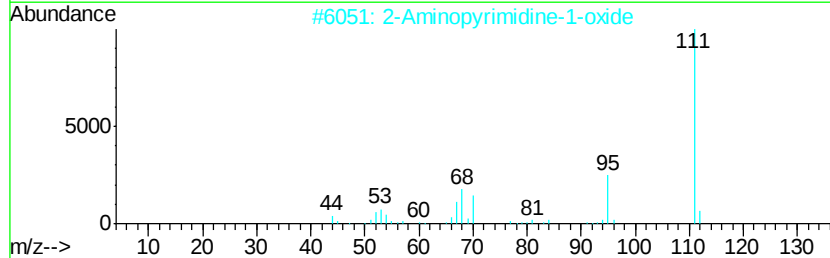
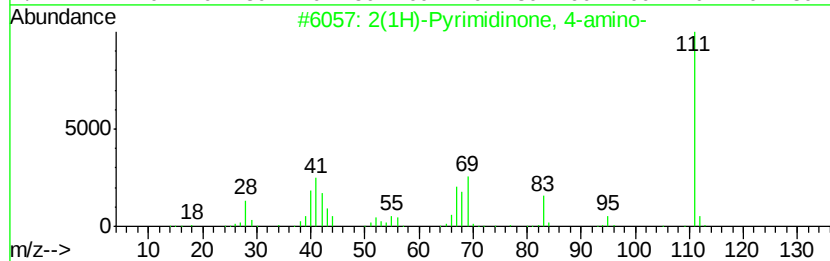
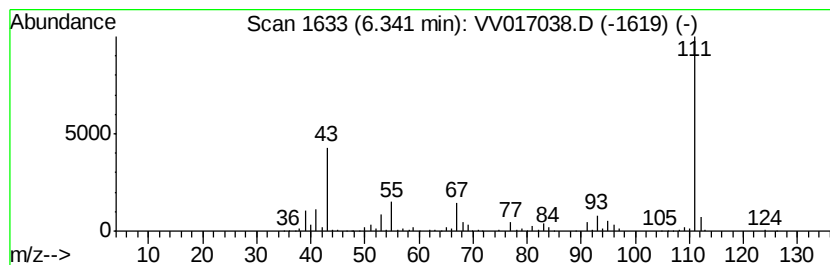
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2(1H)-Pyrimidinone, 4-amino- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	3.96 ug/L	335698	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-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	64
3		2(1H)-Pyrimidinone, 3-hydroxy-	111	C5H5N2O2	016867-04-2	53
4		2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	39
5		2(1H)-Pyridinone, 5-hydroxy-	111	C5H5N2O2	005154-01-8	38



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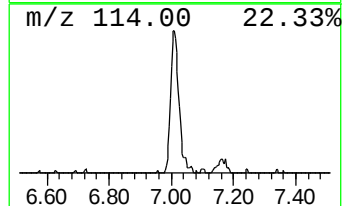
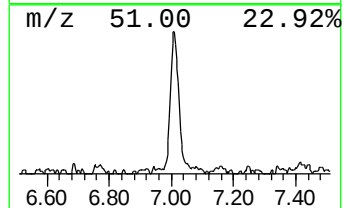
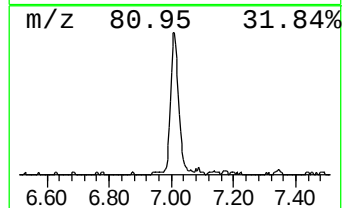
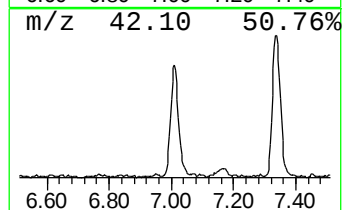
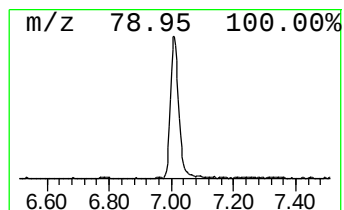
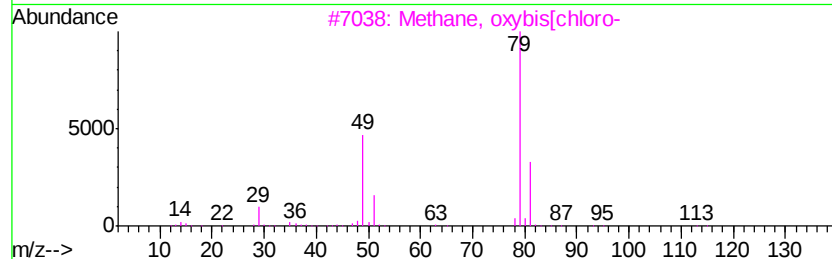
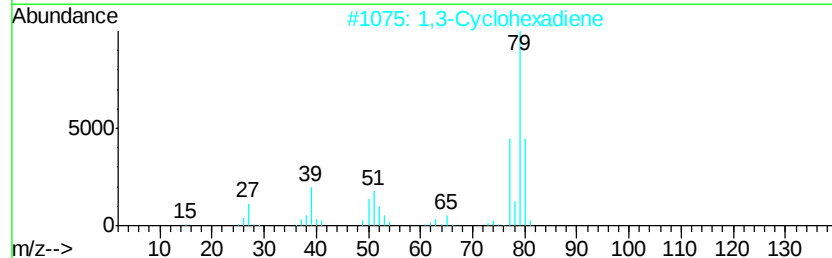
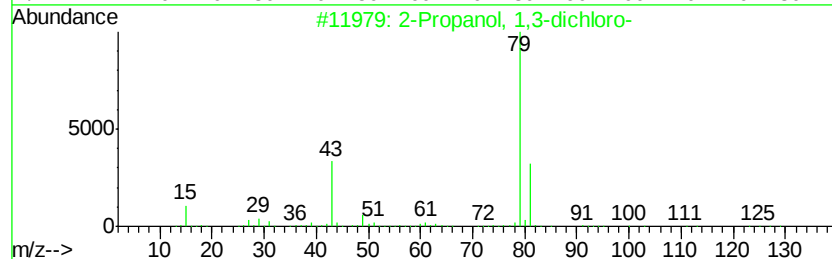
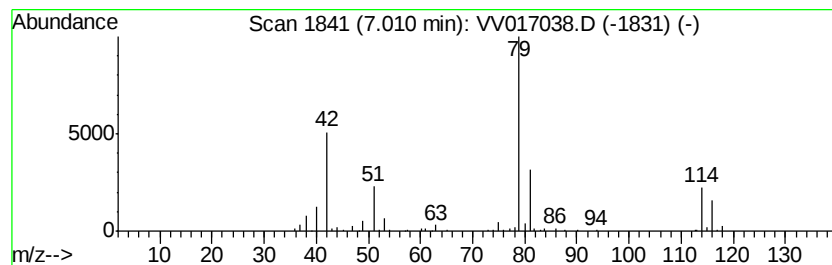
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.01	1.50 ug/L	127438	1,4-Difluorobenzene	5.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1,3-dichloro-			128	C3H6Cl2O	000096-23-1	32
2	1,3-Cyclohexadiene			80	C6H8	000592-57-4	25
3	Methane, oxybis[chloro-			114	C2H4Cl2O	000542-88-1	23
4	2,3-Butanedione, dioxime			116	C4H8N2O2	000095-45-4	9
5	2,4-Imidazolidinedione, 3-methyl-			114	C4H6N2O2	006843-45-4	9



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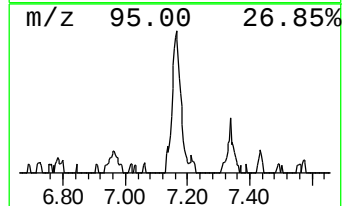
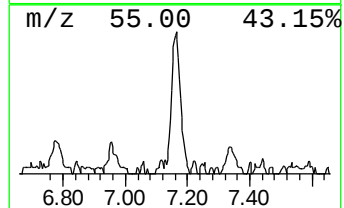
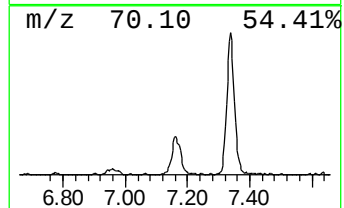
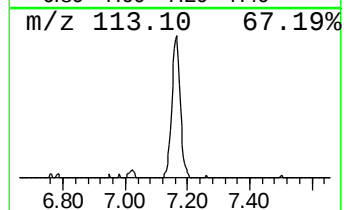
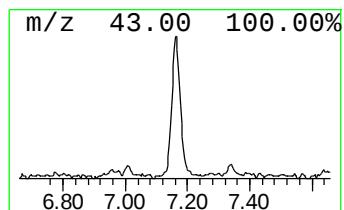
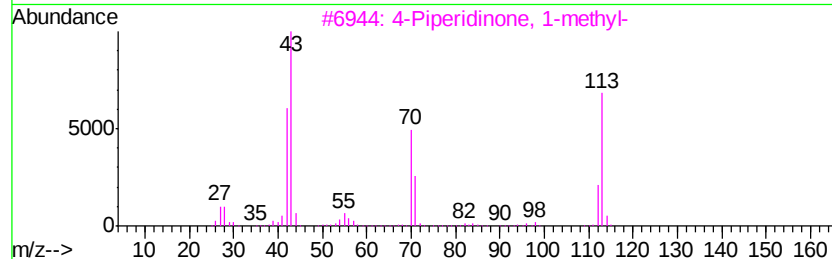
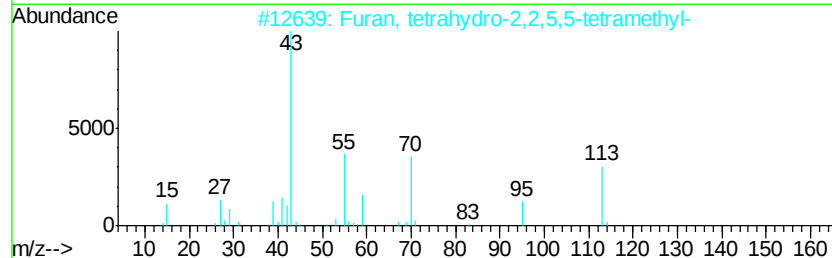
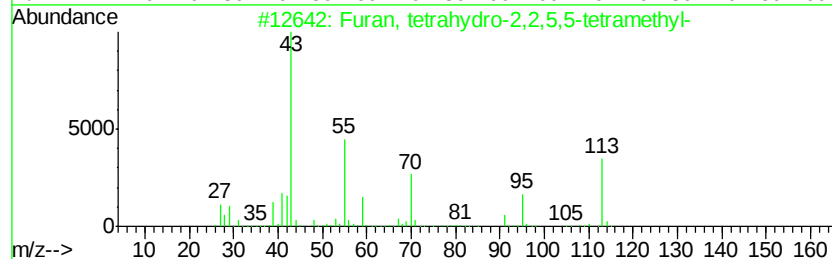
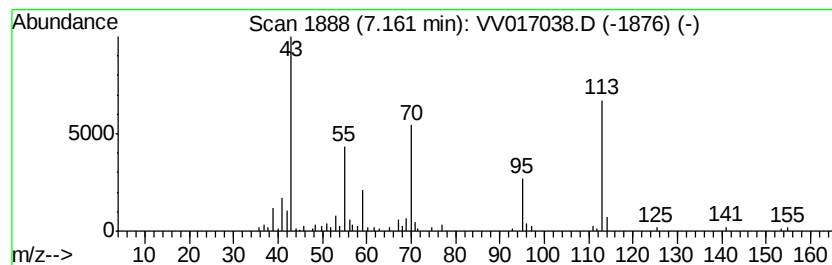
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR061720WMA.M
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Furan, tetrahydro-2,2,5,5-t... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.16	0.79 ug/L	66913	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	72
2		Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	59
3		4-Piperidinone, 1-methyl-	113	C6H11NO	001445-73-4	50
4		Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	50
5		4-Piperidinone, 1-methyl-	113	C6H11NO	001445-73-4	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV062320\
Data File : VV017038.D
Acq On : 22 Jun 2020 23:45
Operator : SY/MD
Sample : L3067-08
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BFXG5

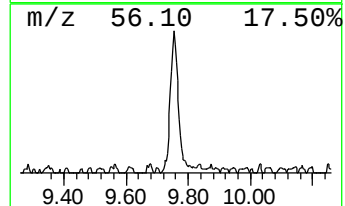
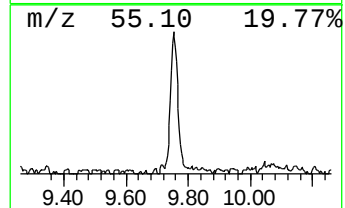
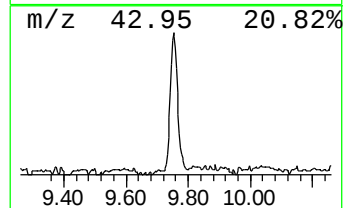
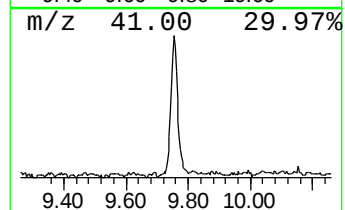
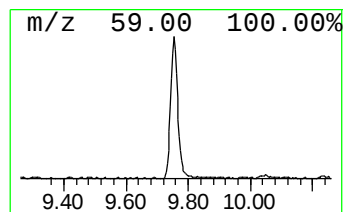
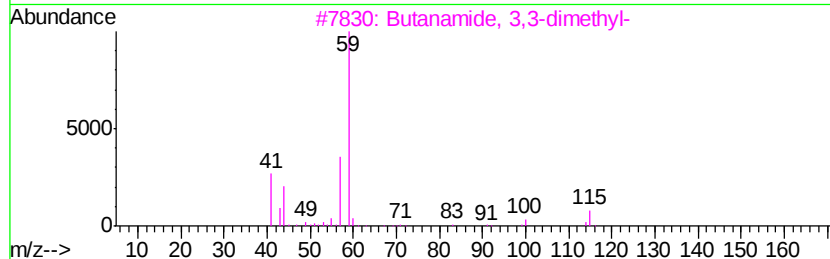
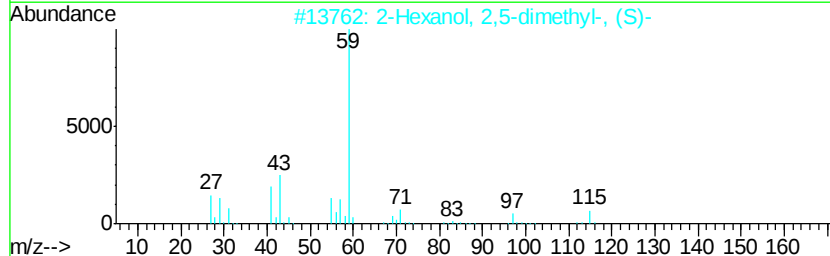
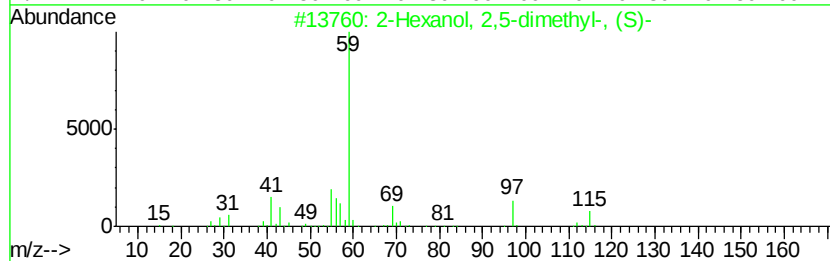
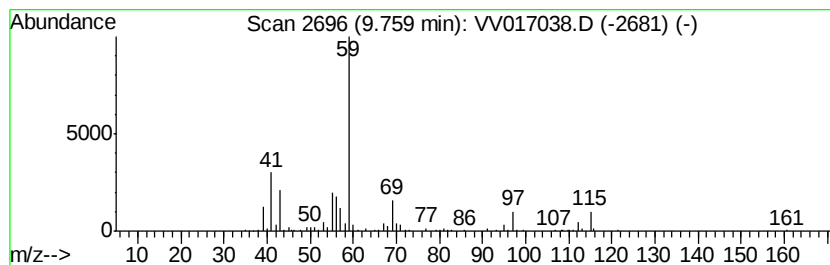
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.76	1.22 ug/L	127706	Chlorobenzene-d5	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	83
2		2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	72
3		Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	50
4		2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	47
5		2-Hexanol, 2,3-dimethyl-	130	C8H18O	019550-03-9	45



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV062320\
Data File : VV017038.D
Acq On : 22 Jun 2020 23:45
Operator : SY/MD
Sample : L3067-08
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BFXG5

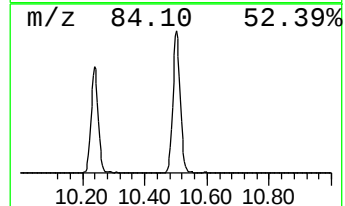
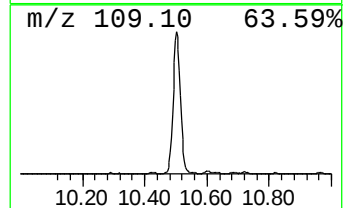
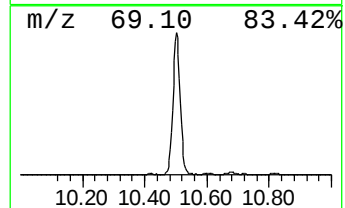
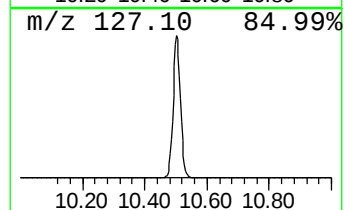
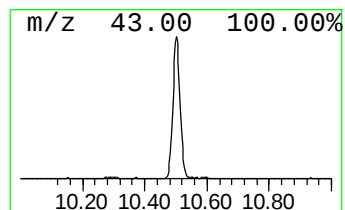
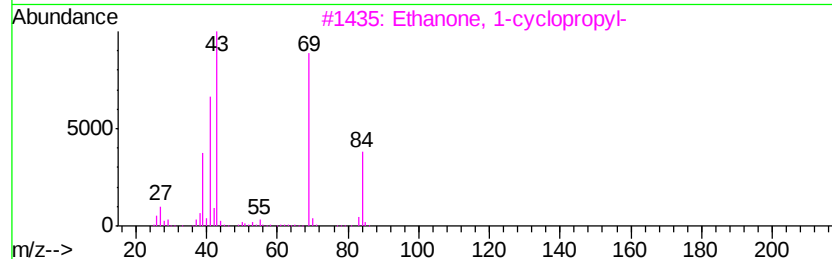
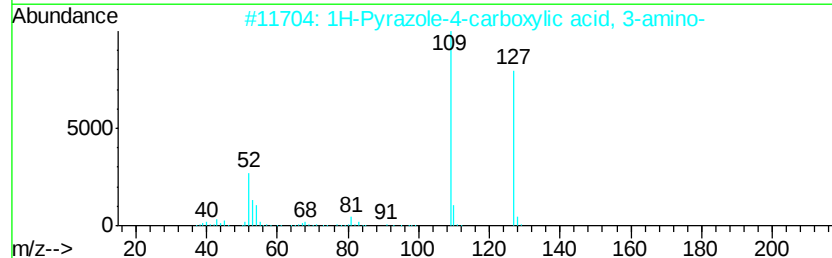
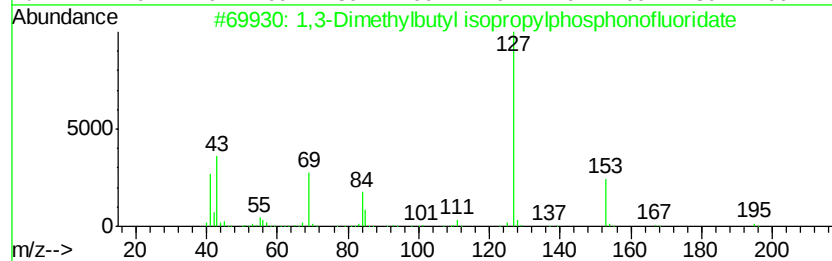
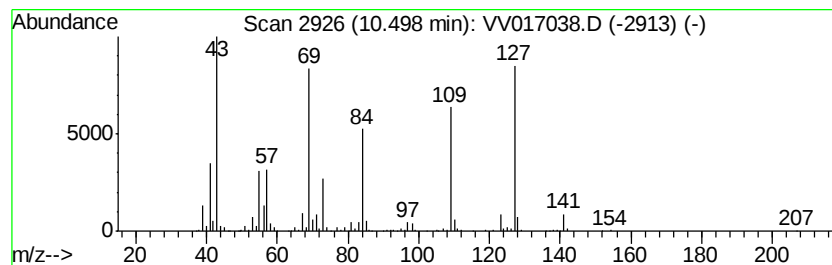
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 unknown-02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.50	7.90 ug/L	816792	1,4-Dichlorobenzene-d4	11.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dimethylbutyl isopropylphosp...	210	C9H20F02P	1000298-25-6	42
2		1H-Pyrazole-4-carboxylic acid, 3...	127	C4H5N3O2	041680-34-6	35
3		Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	27
4		Furan, 2,3-dihydro-3-methyl-	84	C5H8O	001708-27-6	27
5		2-Nonen-4-one	140	C9H16O	032064-72-5	27



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ALS Vial : 20 Sample Multiplier: 1

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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
Sulfur dioxide	1.42	0.7	ug/L	55021	1	5.64	424244	5.0
Diisopropyl ether	3.32	0.9	ug/L	75165	1	5.64	424244	5.0
2(1H)-Pyrimidinon...	6.34	4.0	ug/L	335698	1	5.64	424244	5.0
unknown-01	7.01	1.5	ug/L	127438	1	5.64	424244	5.0
Furan, tetrahydro...	7.16	0.8	ug/L	66913	1	5.64	424244	5.0
2-Hexanol, 2,5-di...	9.76	1.2	ug/L	127706	2	8.87	524193	5.0
unknown-02	10.50	7.9	ug/L	816792	3	11.27	516634	5.0