

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV062320\
 Data File : VV017041.D
 Acq On : 23 Jun 2020 00:57
 Operator : SY/MD
 Sample : L3067-20
 Misc : 25.0mL/MSVOA V/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BFXH7

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	1.595	145	157	172	rVB2	146227	233296	1.27%	0.899%
2	2.122	312	321	334	rVB2	137314	215542	1.17%	0.830%
3	3.209	641	659	681	rBV	8846880	18417756	100.00%	70.941%
4	3.315	682	692	711	rVB	91601	221404	1.20%	0.853%
5	3.946	874	888	927	rBV3	53572	252432	1.37%	0.972%
6	4.376	1007	1022	1041	rBV	106763	261760	1.42%	1.008%
7	5.071	1221	1238	1259	rBV2	249631	608209	3.30%	2.343%
8	5.640	1401	1415	1433	rBV	229048	460500	2.50%	1.774%
9	6.097	1544	1557	1579	rBV2	137301	282906	1.54%	1.090%
10	6.344	1619	1634	1649	rBV	185504	377081	2.05%	1.452%
11	7.164	1869	1889	1904	rBV2	192576	367326	1.99%	1.415%
12	7.338	1931	1943	1960	rBV	313457	539074	2.93%	2.076%
13	8.113	2169	2184	2215	rBV	283002	534943	2.90%	2.060%
14	8.871	2409	2420	2435	rBV	345154	556130	3.02%	2.142%
15	9.752	2677	2694	2726	rBV	541218	890344	4.83%	3.429%
16	10.502	2914	2927	2943	rBV	405039	678963	3.69%	2.615%
17	11.270	3154	3166	3186	rVB	366607	571496	3.10%	2.201%
18	11.646	3272	3283	3298	rBV	310648	492942	2.68%	1.899%

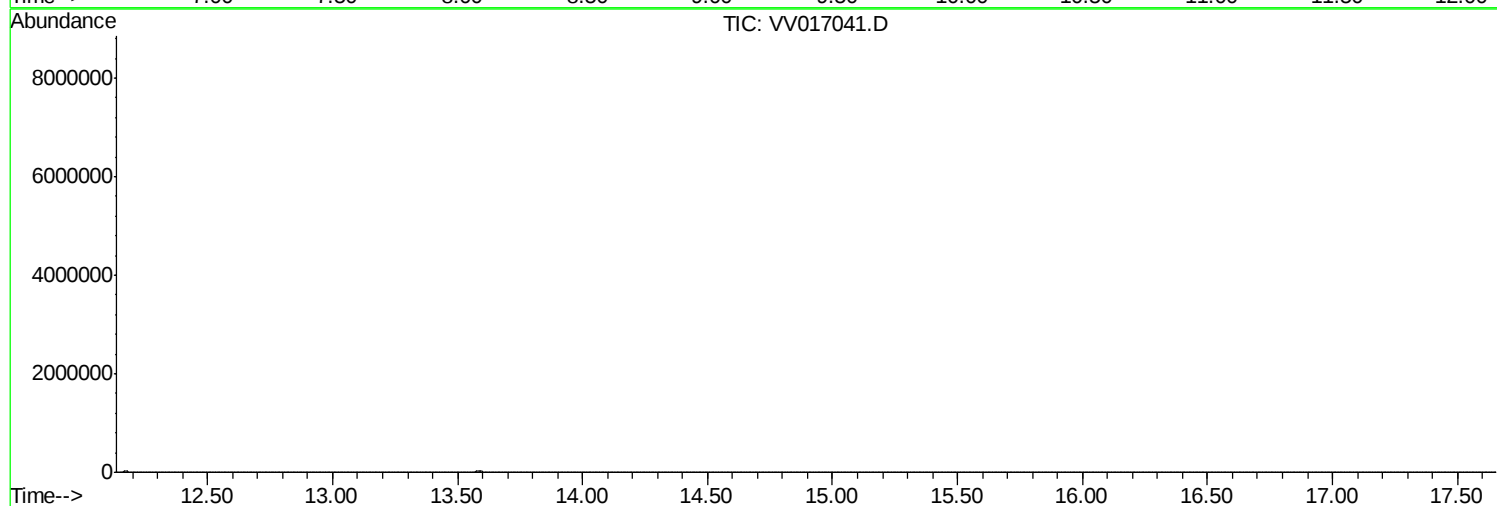
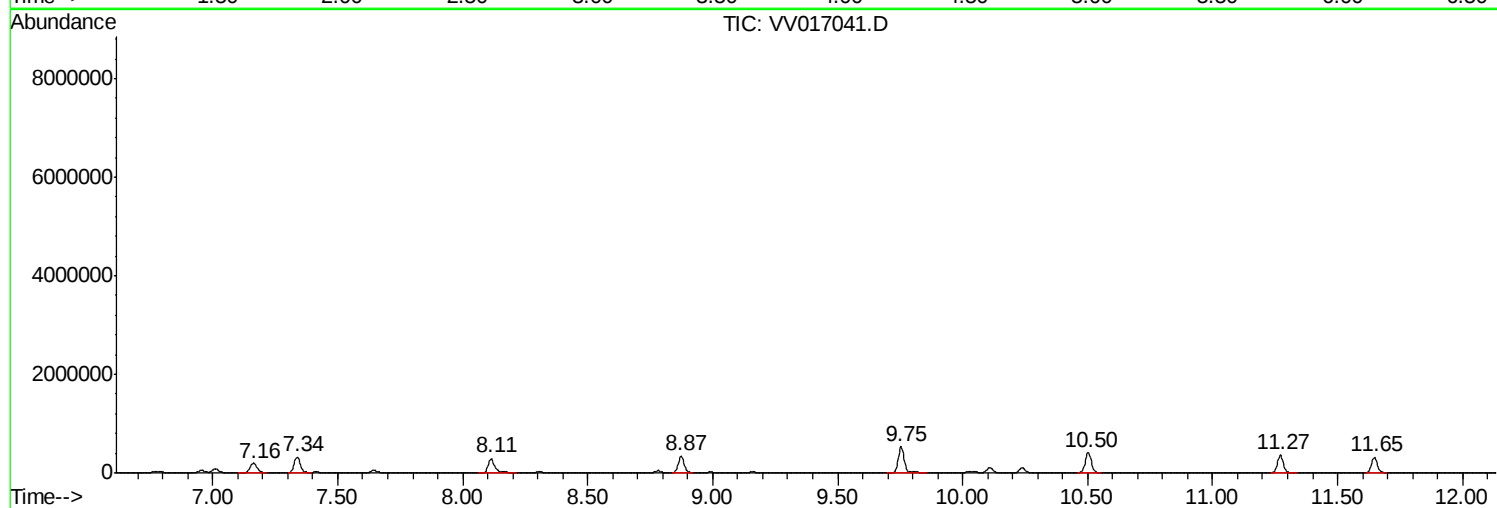
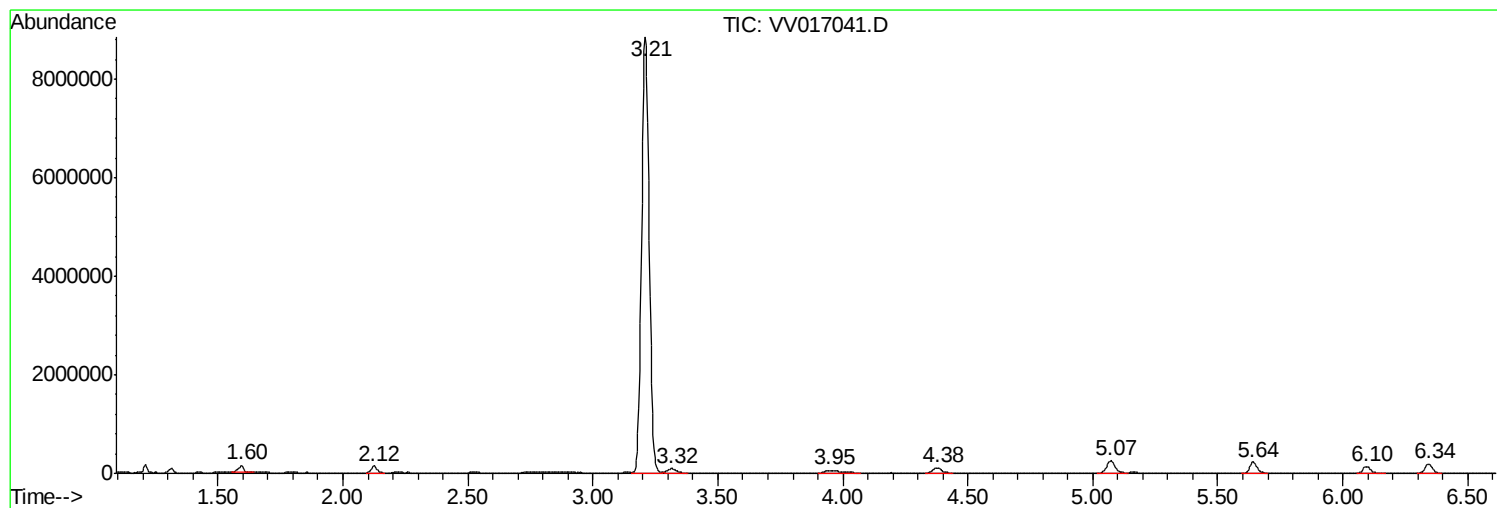
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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



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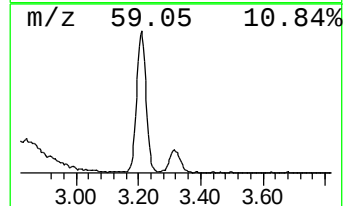
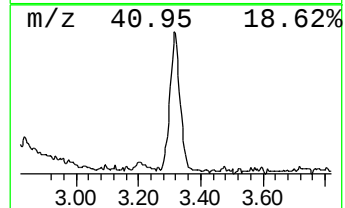
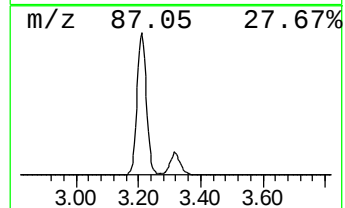
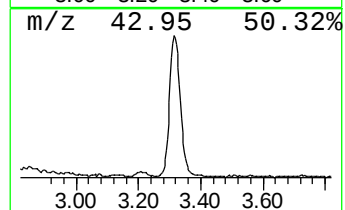
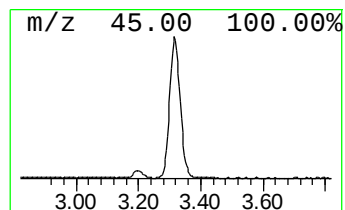
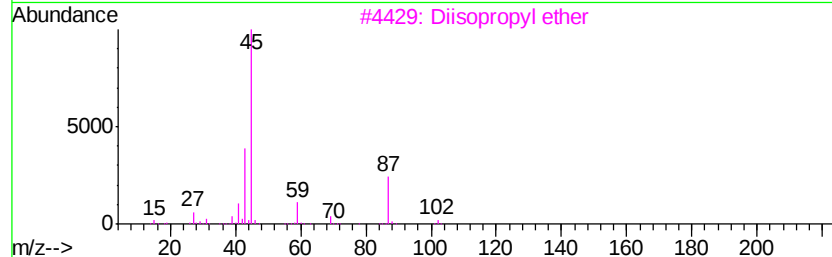
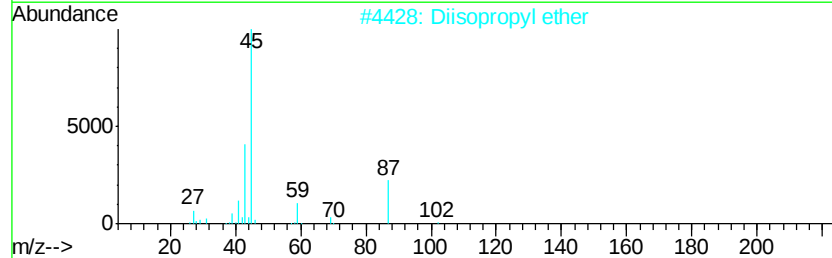
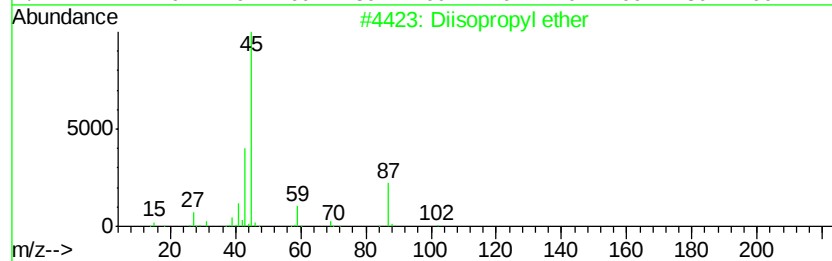
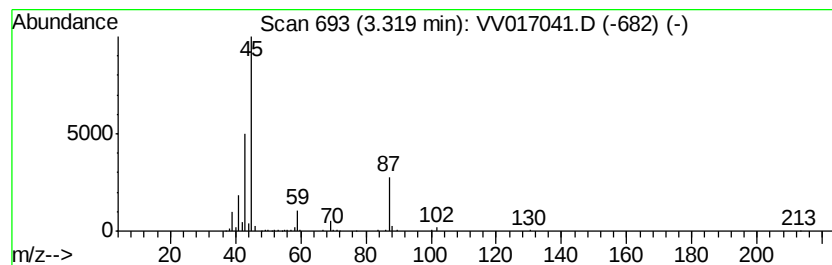
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Diisopropyl ether Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.32	2.40 ug/L	221404	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Diisopropyl ether	102	C6H14O	000108-20-3	83
2		Diisopropyl ether	102	C6H14O	000108-20-3	83
3		Diisopropyl ether	102	C6H14O	000108-20-3	83
4		1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	72
5		1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	64



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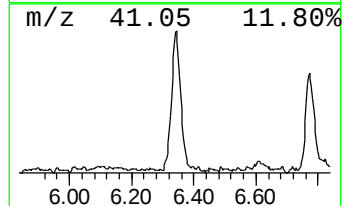
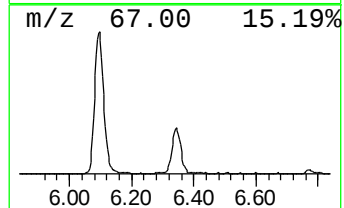
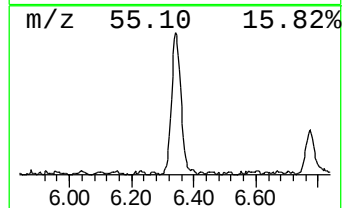
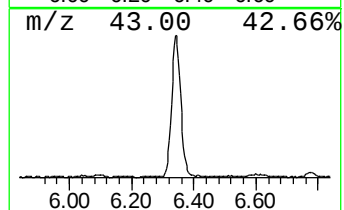
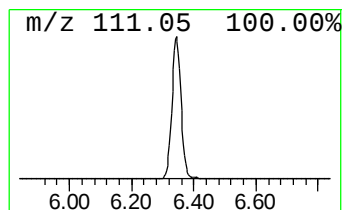
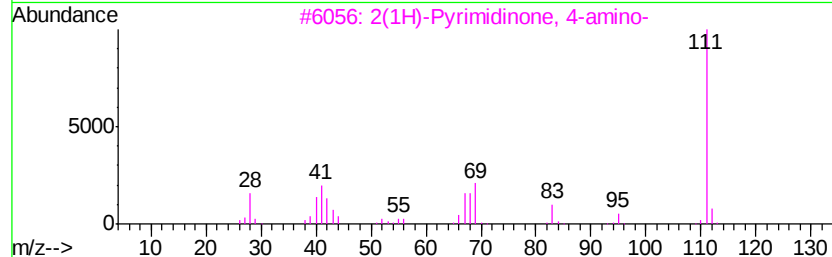
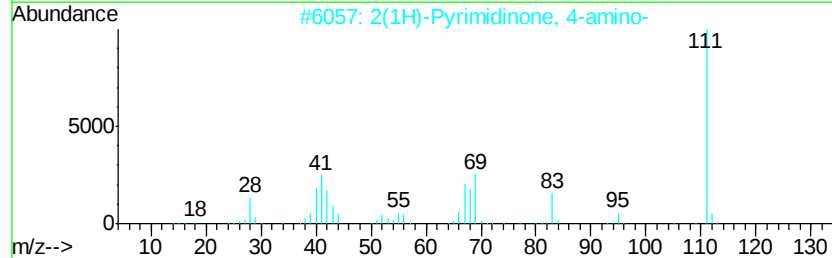
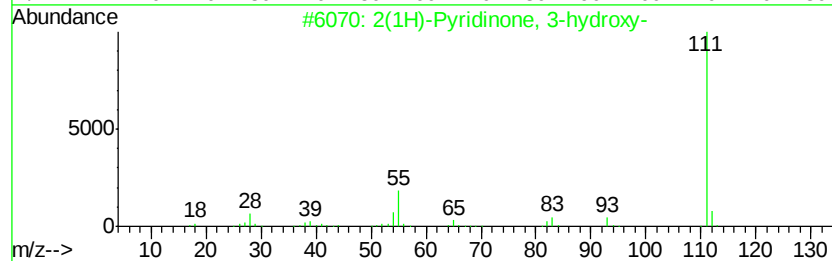
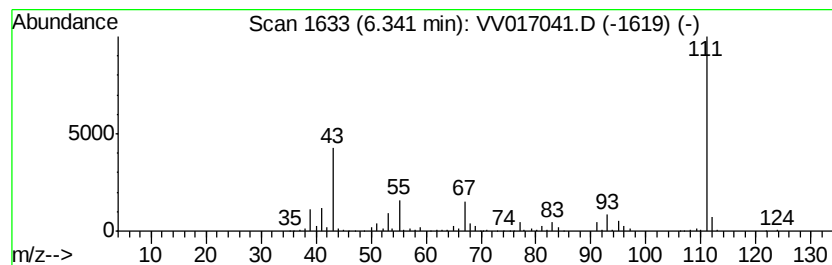
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 2(1H)-Pyridinone, 3-hydroxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	4.09 ug/L	377081	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2(1H)-Pyridinone, 3-hydroxy-	111	C5H5NO2	016867-04-2	59
2		2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	56
3		2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	40
4		Bruceantin	548	C28H36O11	041451-75-6	39
5		2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	39



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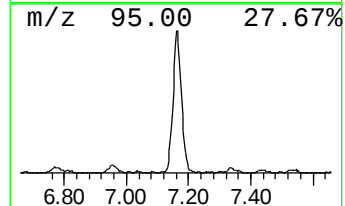
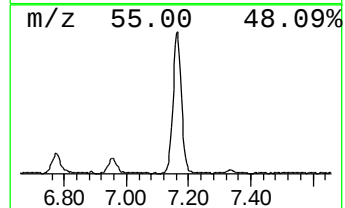
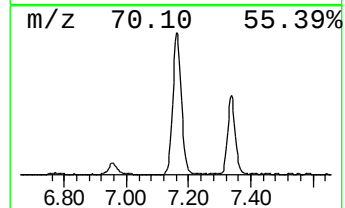
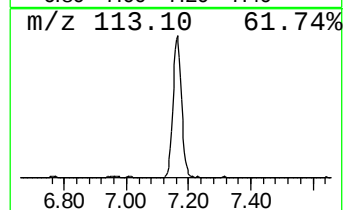
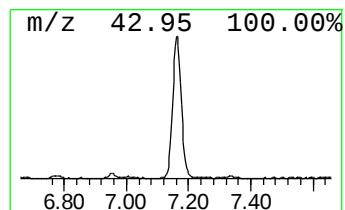
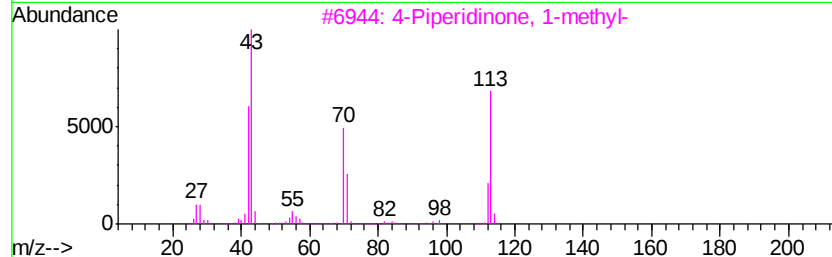
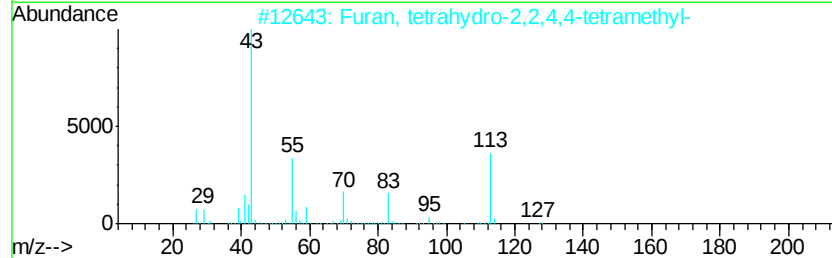
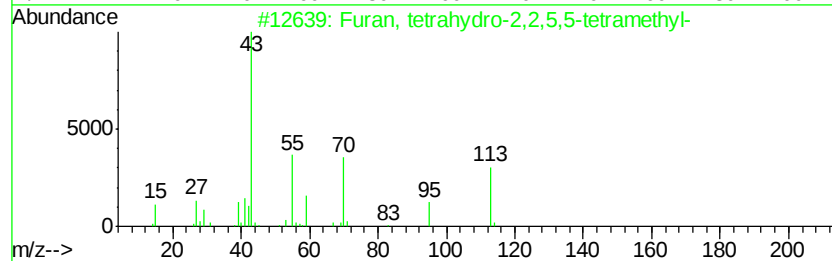
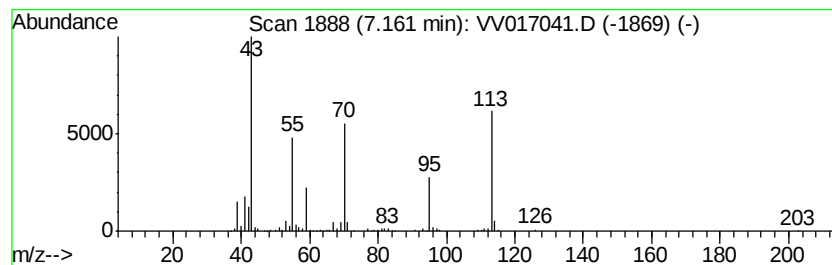
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 Furan, tetrahydro-2,2,5,5-t... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.16	3.99 ug/L	367326	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	83
2		Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	53
3		4-Piperidinone, 1-methyl-	113	C6H11NO	001445-73-4	52
4		Ethosuximide	141	C7H11NO2	000077-67-8	47
5		1,3,5-Triazine-2,4(1H,3H)-dione	113	C3H3N3O2	000071-33-0	47



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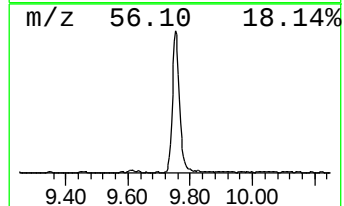
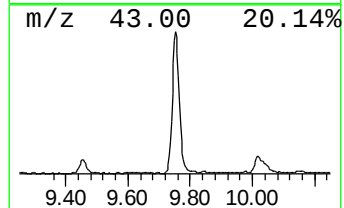
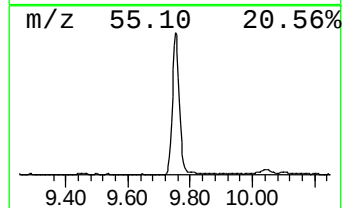
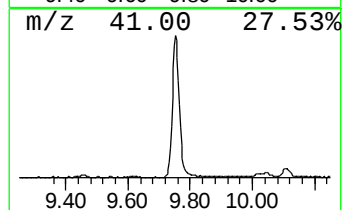
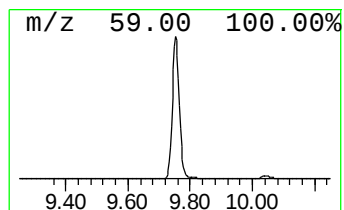
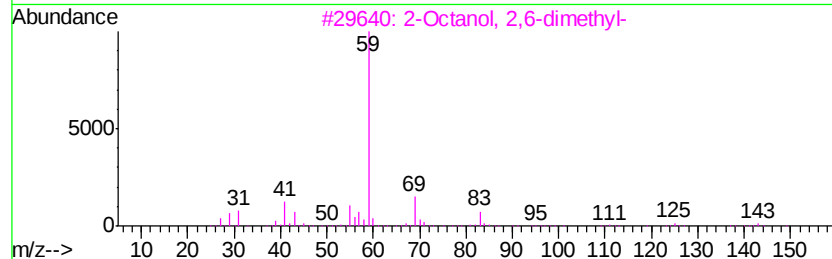
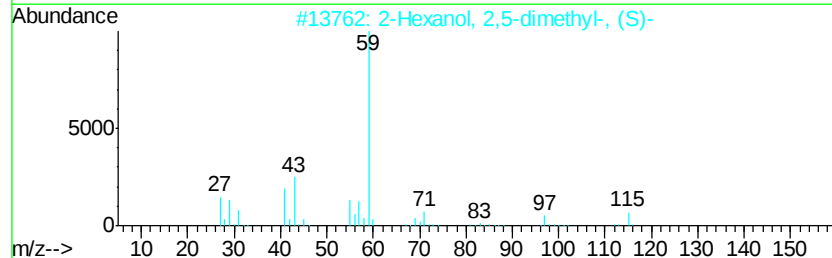
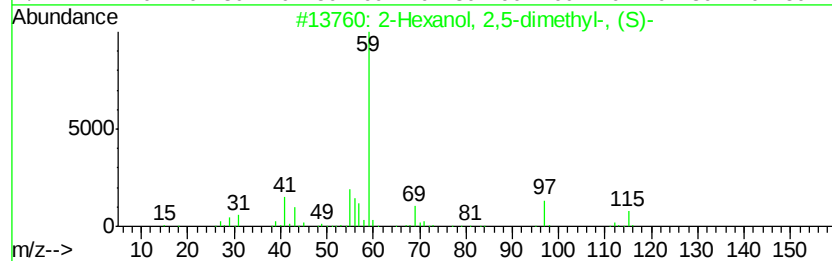
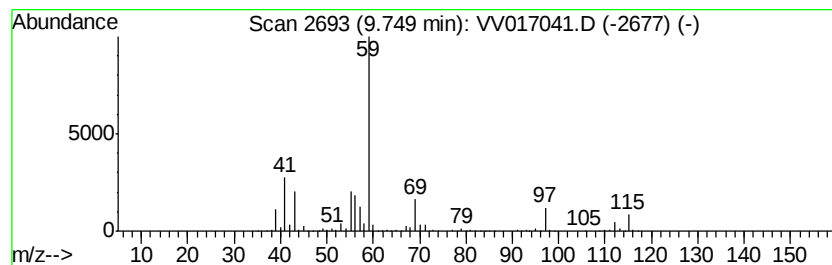
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.75	8.00 ug/L	890344	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	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	72	
3	2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	45	
4	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	40	
5	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	38	



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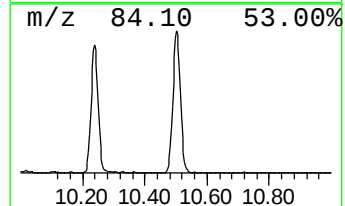
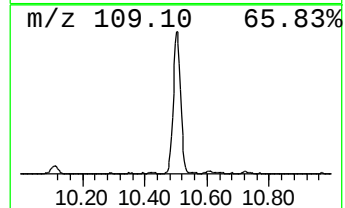
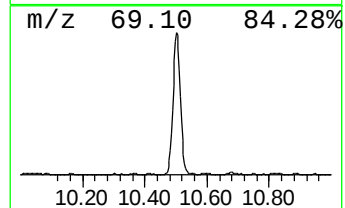
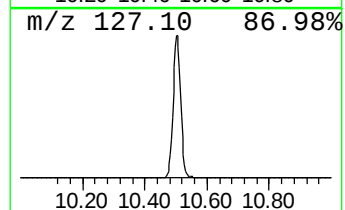
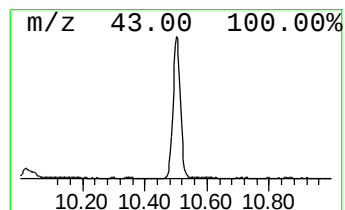
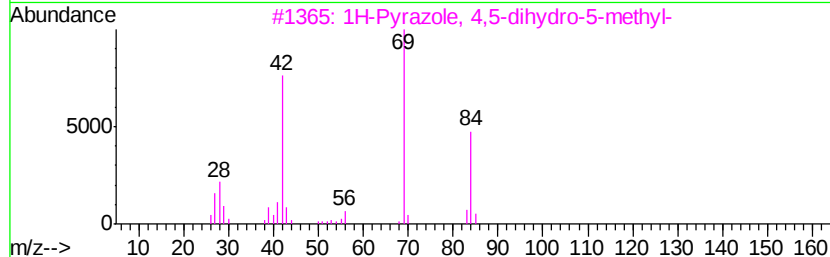
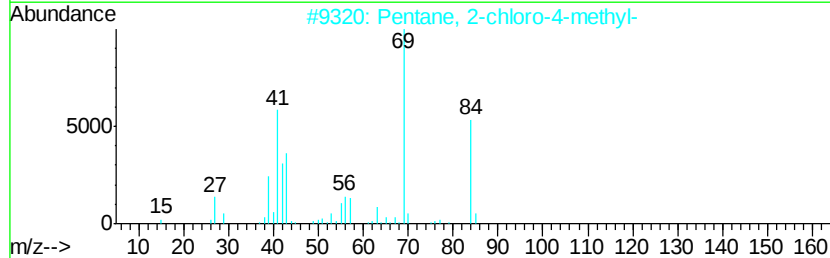
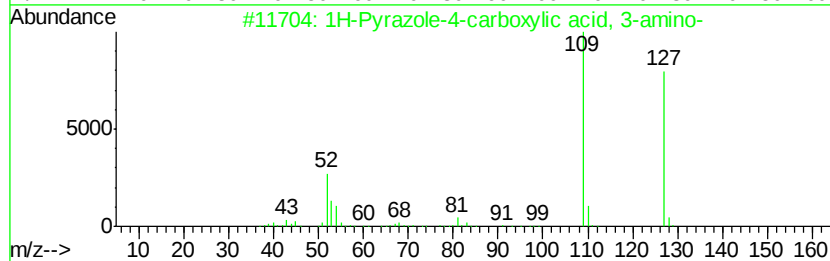
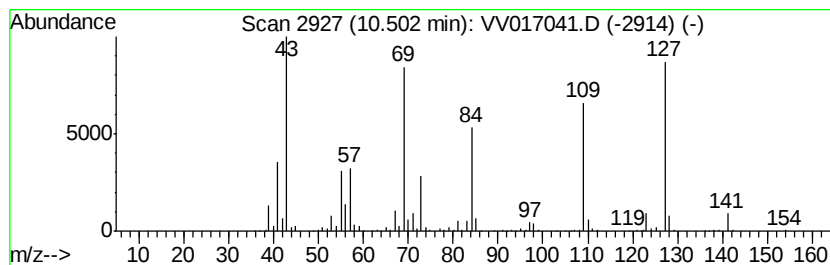
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.50	5.94 ug/L	678963	1,4-Dichlorobenzene-d4	11.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Pyrazole-4-carboxylic acid, 3...	127	C4H5N3O2	041680-34-6	35
2		Pentane, 2-chloro-4-methyl-	120	C6H13Cl	025346-32-1	27
3		1H-Pyrazole, 4,5-dihydro-5-methyl-	84	C4H8N2	001568-20-3	27
4		Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	27
5		1H-Imidazole, 1-methyl-5-nitro-	127	C4H5N3O2	003034-42-2	14



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Diisopropyl ether	3.32	2.4	ug/L	221404	1	5.64	460500	5.0
2(1H)-Pyridinone,...	6.34	4.1	ug/L	377081	1	5.64	460500	5.0
Furan, tetrahydro...	7.16	4.0	ug/L	367326	1	5.64	460500	5.0
2-Hexanol, 2,5-di...	9.75	8.0	ug/L	890344	2	8.87	556130	5.0
unknown-01	10.50	5.9	ug/L	678963	3	11.27	571496	5.0