

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062420\
 Data File : VU039059.D
 Acq On : 24 Jun 2020 13:17
 Operator : SY/MD
 Sample : L3061-03
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFXJ0

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

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062320WMA.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	2.591	376	389	404	rBV2	262261	445840	1.00%	0.748%
2	4.674	1022	1037	1083	rVB3	223094	756104	1.70%	1.268%
3	5.102	1150	1170	1192	rBV	231613	517967	1.16%	0.869%
4	5.761	1352	1375	1385	rBV2	463093	1227798	2.76%	2.060%
5	6.279	1521	1536	1560	rBV	332118	627858	1.41%	1.053%
6	6.722	1659	1674	1690	rBV	287547	568830	1.28%	0.954%
7	6.944	1726	1743	1764	rBV	1625935	3112213	6.98%	5.221%
8	7.738	1975	1990	2009	rBV	440718	817220	1.83%	1.371%
9	7.922	2032	2047	2063	rBV	560201	958098	2.15%	1.607%
10	8.658	2262	2276	2299	rBV	895768	1574497	3.53%	2.641%
11	9.436	2504	2518	2538	rBV2	499657	991250	2.22%	1.663%
12	10.279	2766	2780	2800	rBV	971655	1712680	3.84%	2.873%
13	11.047	2997	3019	3050	rBV	26564081	44561551	100.00%	74.749%
14	11.825	3249	3261	3278	rBV	485555	787325	1.77%	1.321%
15	12.208	3365	3380	3399	rVB2	535897	955681	2.14%	1.603%

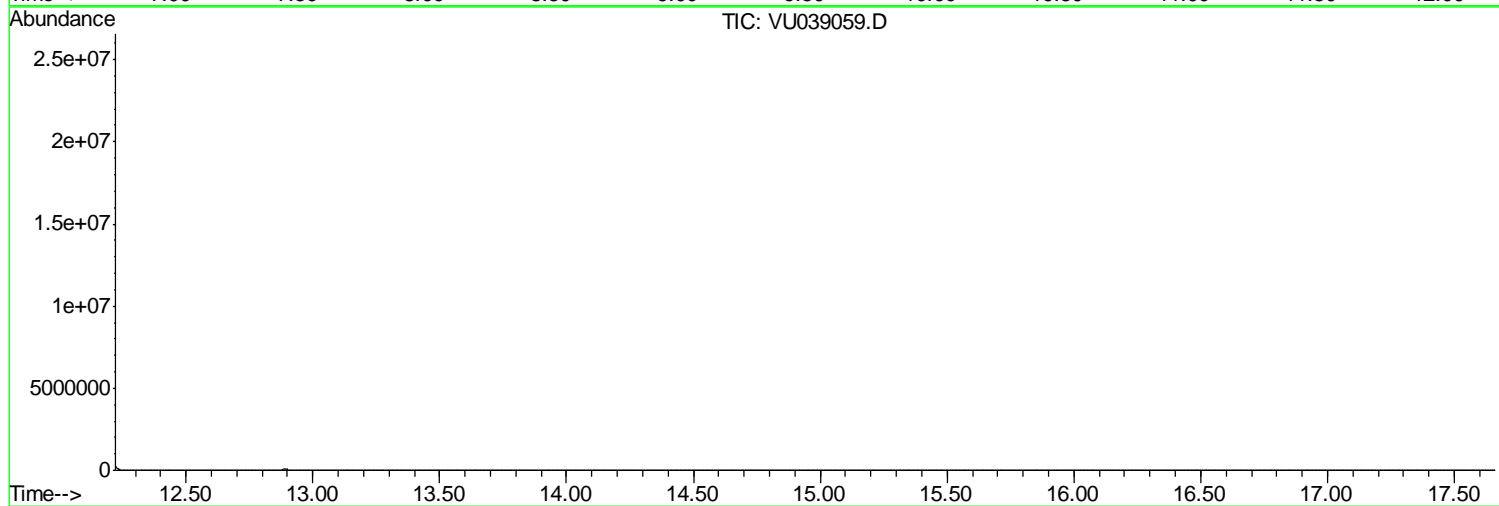
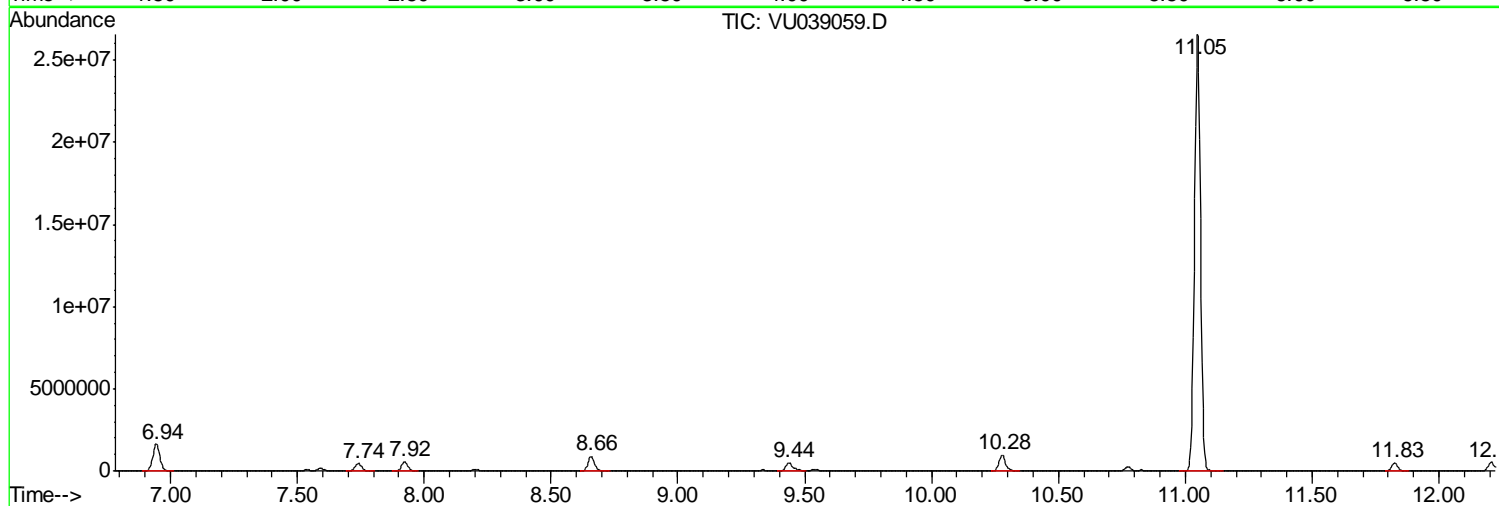
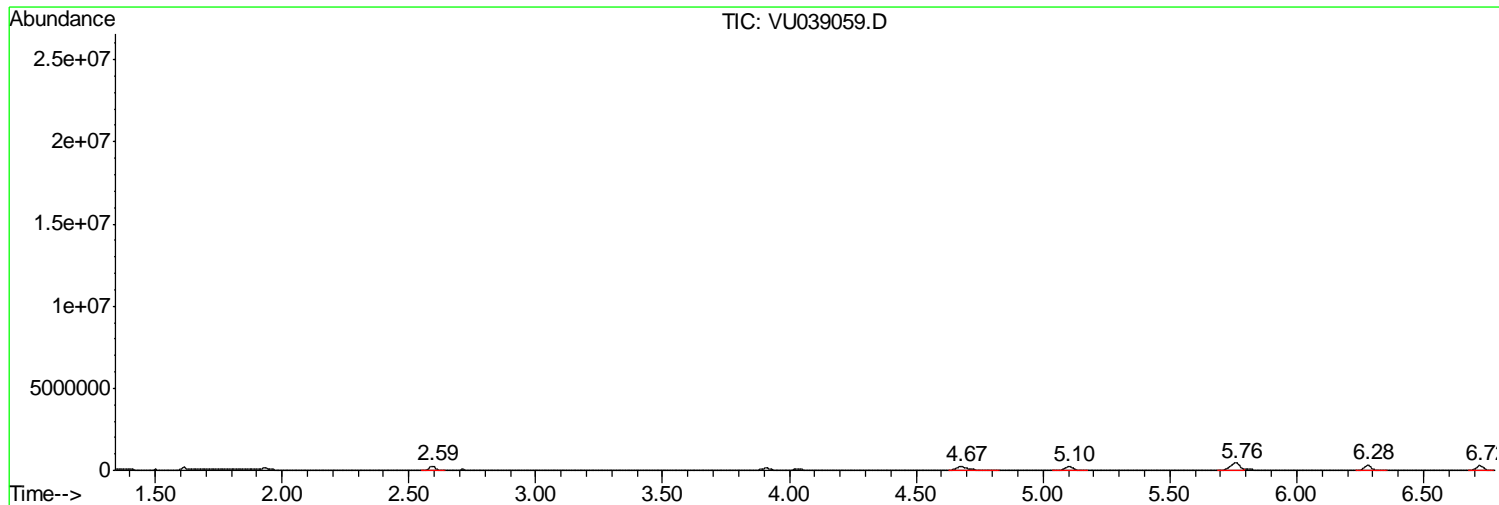
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ClientSampled :
BFXJO

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062320WMA.M
Quant Title : TRACE VOA SOM01.0

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



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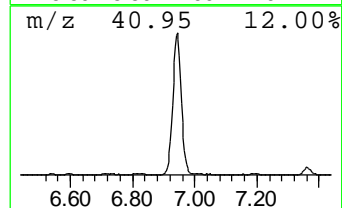
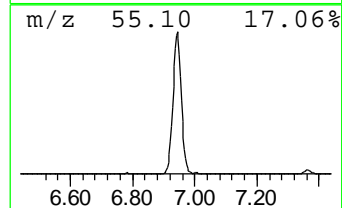
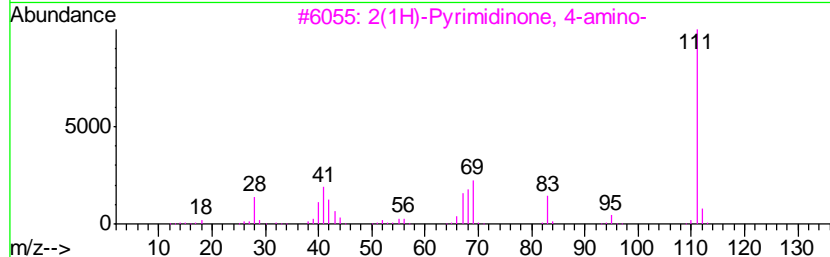
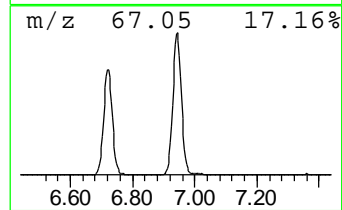
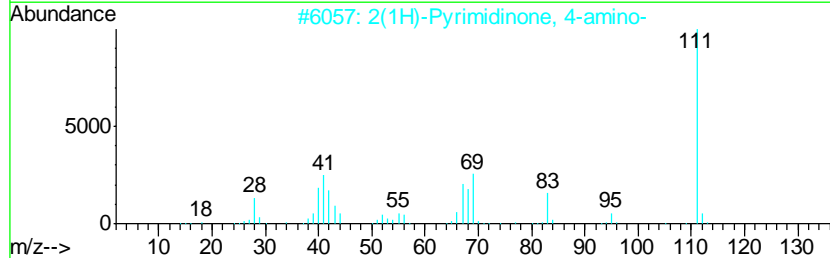
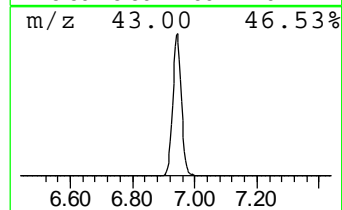
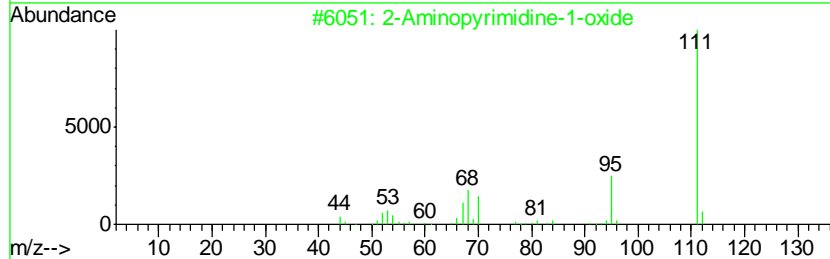
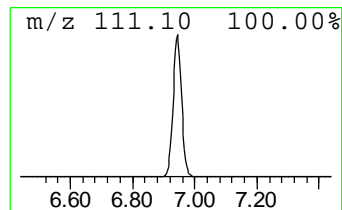
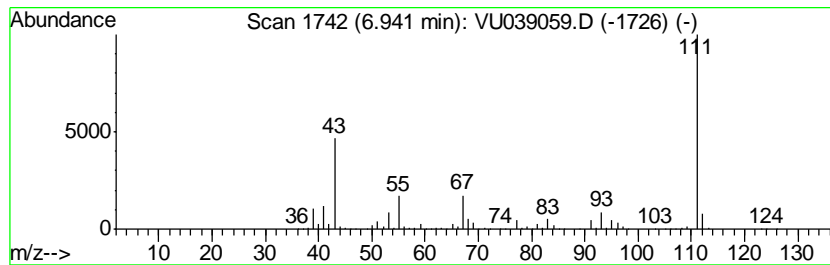
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062320WMA.M
 Quant Title : TRACE VOA SOM01.0

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

 Peak Number 1 2-Aminopyrimidine-1-oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.94	24.78 ug/L	3112210	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	64
2		2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	64
3		2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	50
4		2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	50
5		2(1H)-Pyridinone, 3-hydroxy-	111	C5H5NO2	016867-04-2	45



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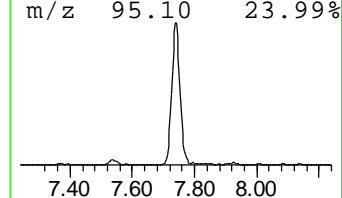
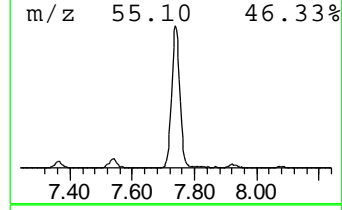
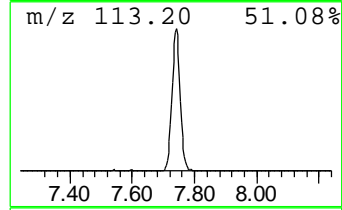
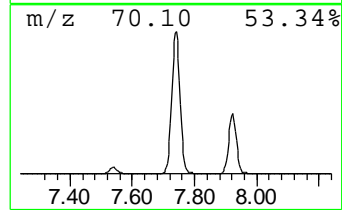
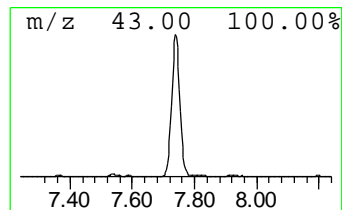
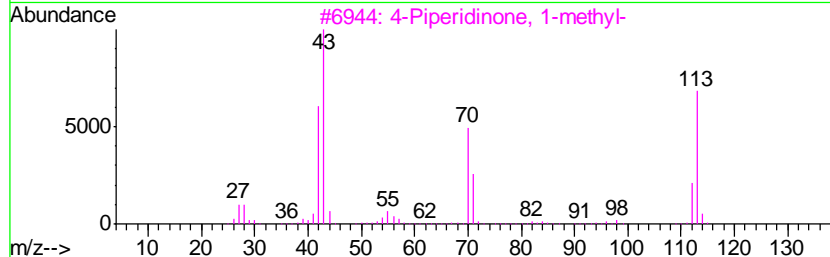
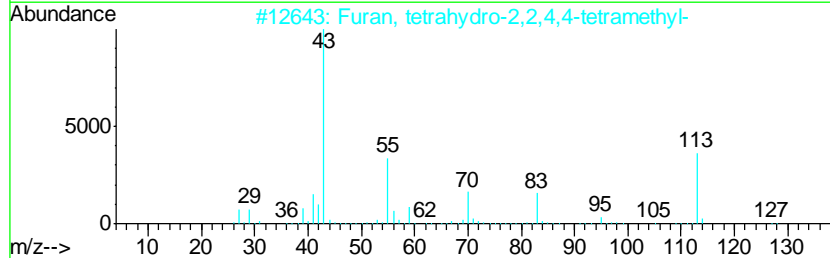
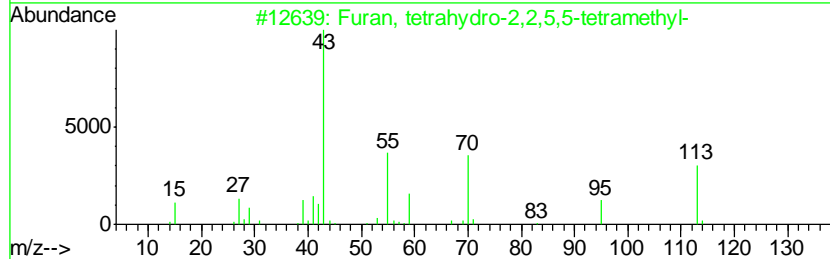
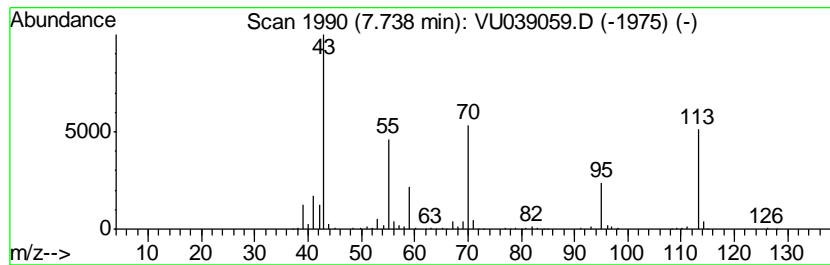
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 Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.74	6.51 ug/L	817220	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	64
2		Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	53
3		4-Piperidinone, 1-methyl-	113	C6H11NO	001445-73-4	50
4		2,5-Hexanediol, 2,5-dimethyl-	146	C8H18O2	000110-03-2	50
5		Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	47



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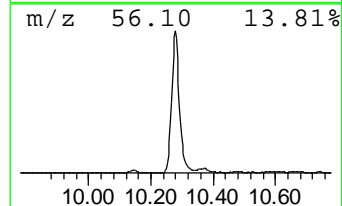
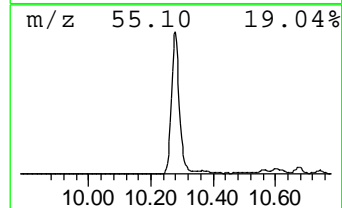
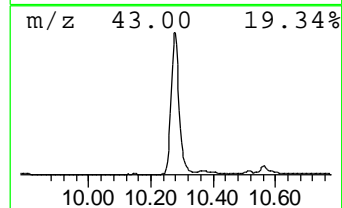
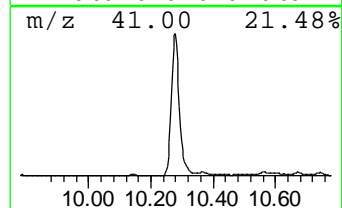
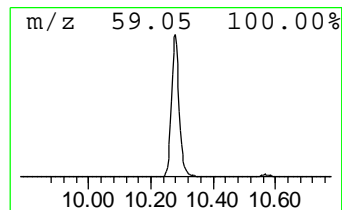
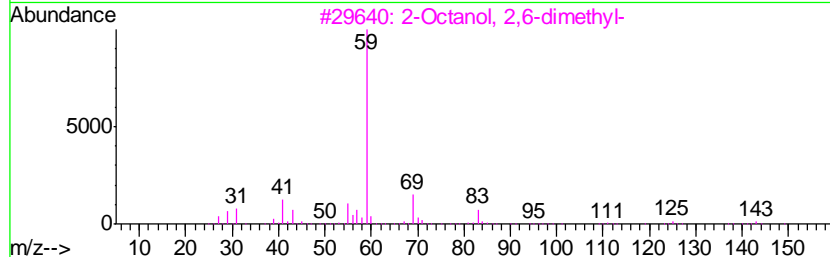
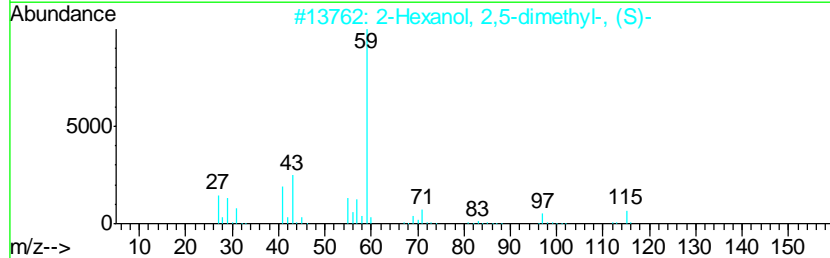
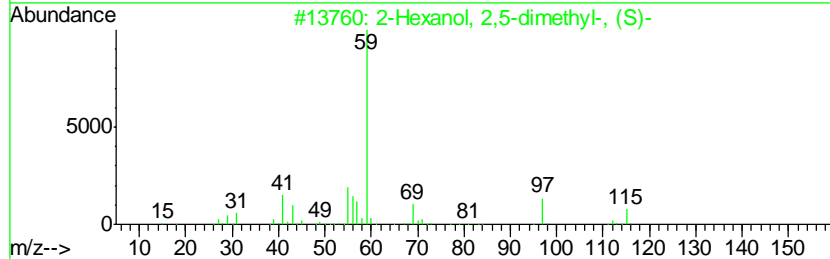
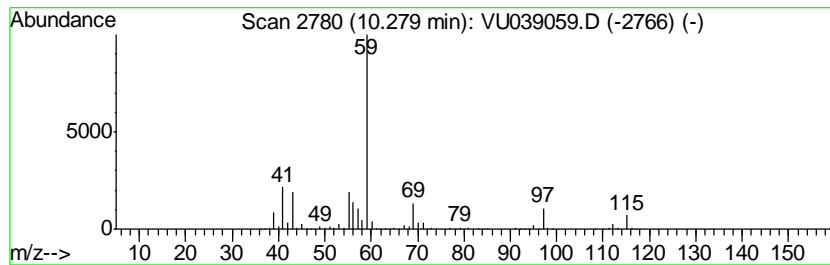
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 Quant Title : TRACE VOA SOM01.0

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

 Peak Number 3 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.28	8.64 ug/L	1712680	Chlorobenzene-d5	9.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	90
2		2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	72
3		2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	50
4		6-Methyl-2-heptanol, methyl ether	144	C9H20O	1000365-52-0	45
5		2-Hexanol, 2,3-dimethyl-	130	C8H18O	019550-03-9	45



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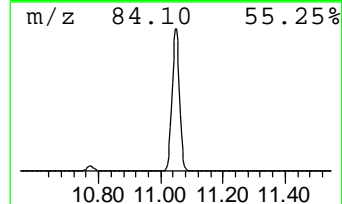
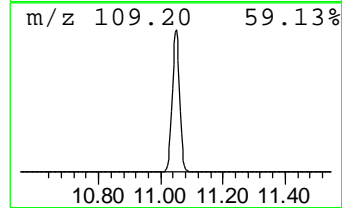
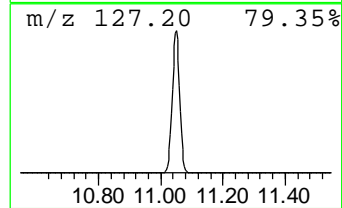
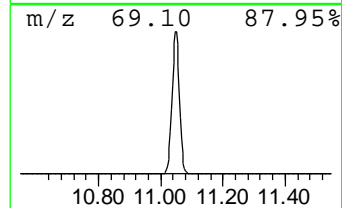
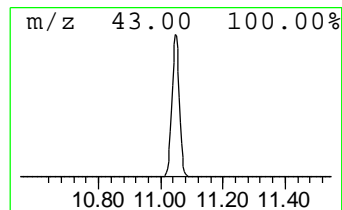
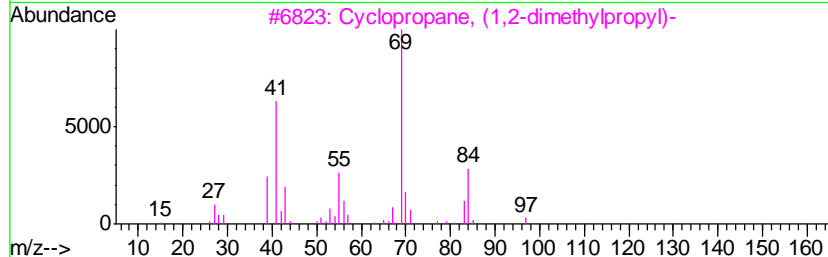
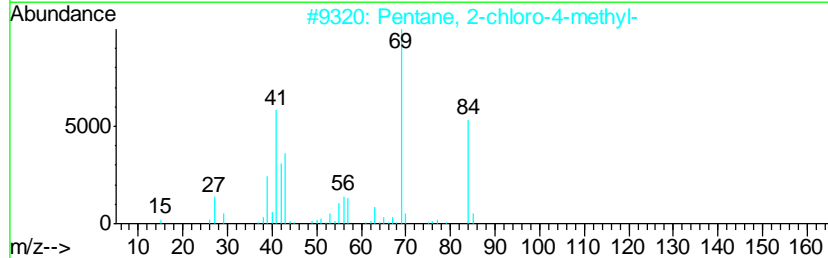
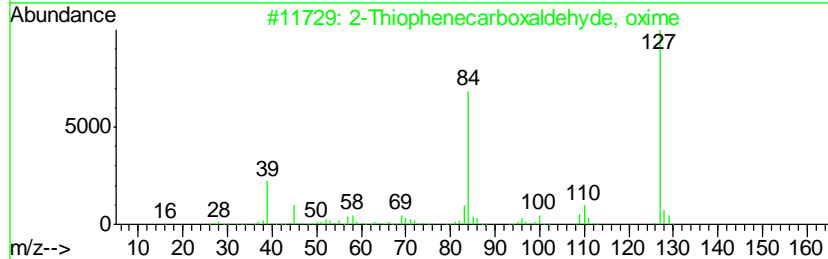
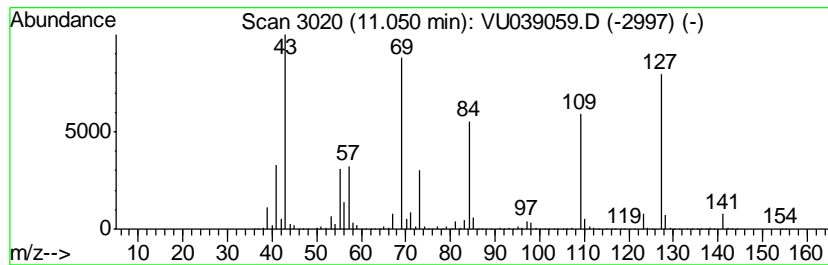
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 4 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.05	282.99 ug/L	44561600	1,4-Dichlorobenzene-d4	11.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Thiophenecarboxaldehyde, oxime	127	C5H5NOS	029683-84-9	35
2		Pentane, 2-chloro-4-methyl-	120	C6H13Cl	025346-32-1	27
3		Cyclopropane, (1,2-dimethylpropyl)-	112	C8H16	006976-27-8	27
4		Furan, 2,3-dihydro-3-methyl-	84	C5H8O	001708-27-6	27
5		4-Amino-2,6-dihydropyrimidine	127	C4H5N3O2	000873-83-6	22



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TIC Library : C:\DATABASE\NIST11.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Aminopyrimidine...	6.94	24.8	ug/L	3112210	1	6.28	627858	5.0
Furan, tetrahydro...	7.74	6.5	ug/L	817220	1	6.28	627858	5.0
2-Hexanol, 2,5-di...	10.28	8.6	ug/L	1712680	2	9.44	991250	5.0
unknown-01	11.05	283.0	ug/L	44561600	3	11.83	787325	5.0