

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062420\
 Data File : VU039057.D
 Acq On : 24 Jun 2020 11:42
 Operator : SY/MD
 Sample : L3061-02
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFXH9

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_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	2.594	377	390	404	rBV2	276099	471696	1.06%	0.787%
2	4.674	1022	1037	1081	rVB2	235040	790056	1.77%	1.317%
3	5.102	1153	1170	1200	rBV	244090	543258	1.22%	0.906%
4	5.758	1352	1374	1385	rBV2	476512	1282712	2.88%	2.139%
5	6.279	1516	1536	1559	rVB	346346	649147	1.46%	1.083%
6	6.719	1659	1673	1692	rBV	308861	602890	1.35%	1.005%
7	6.944	1722	1743	1764	rBV	1629613	3120427	7.01%	5.204%
8	7.739	1974	1990	2007	rBV	434026	811133	1.82%	1.353%
9	7.922	2033	2047	2062	rBV	591007	996657	2.24%	1.662%
10	8.658	2261	2276	2308	rBV	920784	1648152	3.70%	2.748%
11	9.436	2505	2518	2539	rBV2	509484	1004470	2.26%	1.675%
12	10.279	2765	2780	2800	rBV	971799	1717882	3.86%	2.865%
13	11.047	2995	3019	3061	rBV	26666975	44530022	100.00%	74.258%
14	11.825	3248	3261	3278	rBV	495601	803457	1.80%	1.340%
15	12.208	3364	3380	3401	rVB	564155	994423	2.23%	1.658%

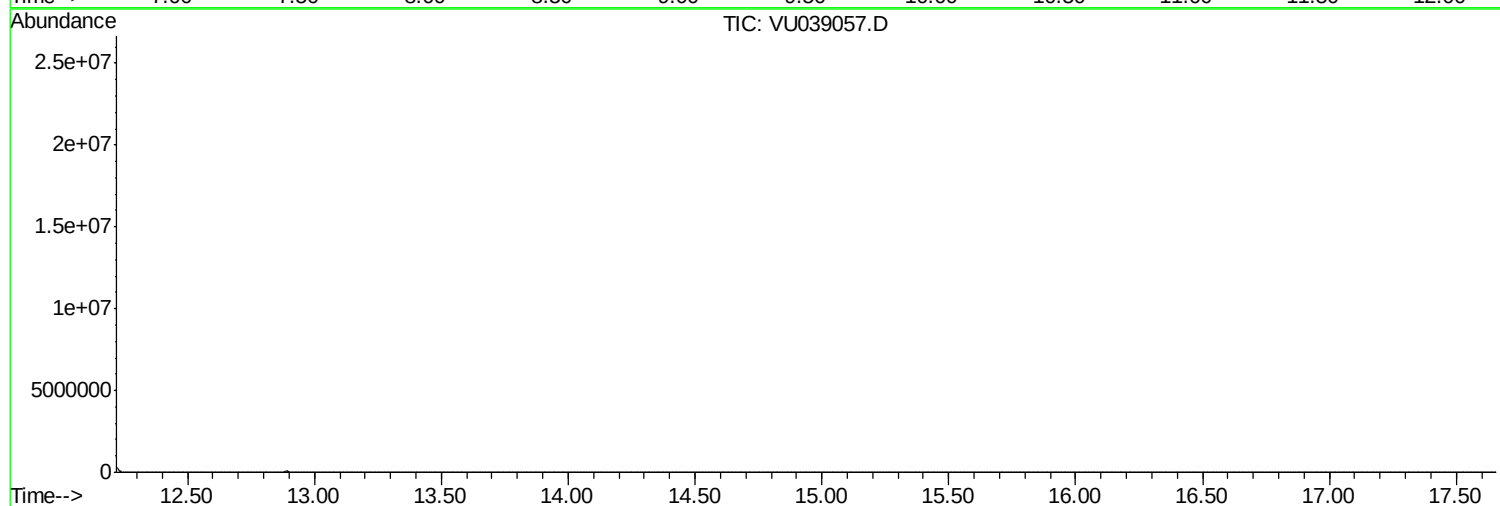
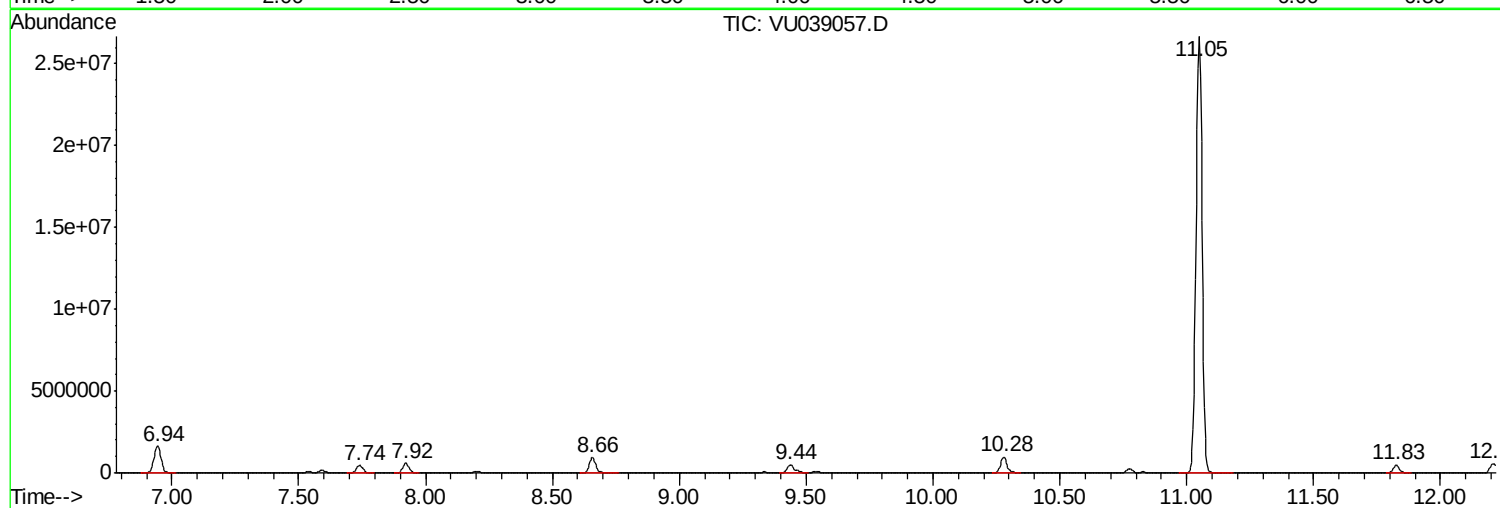
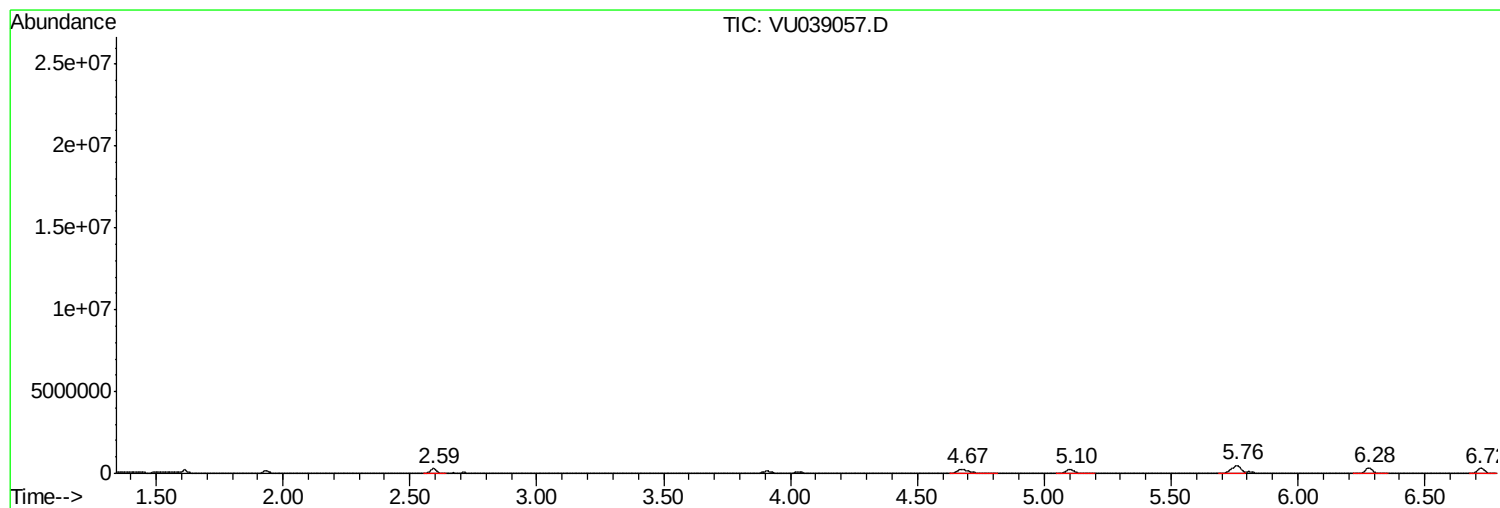
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062320WMA.M
Quant Title : TRACE VOA SOM01.0

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



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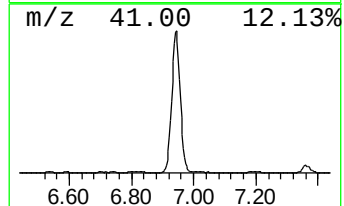
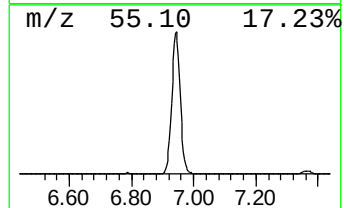
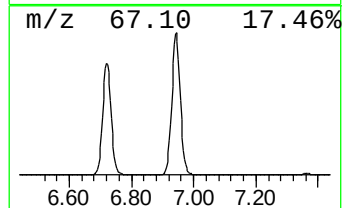
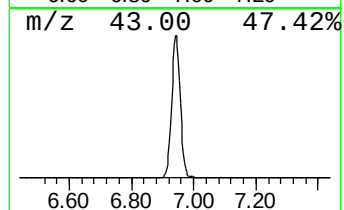
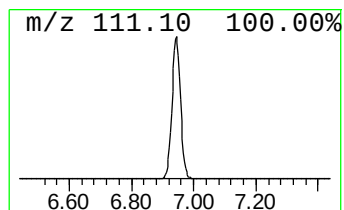
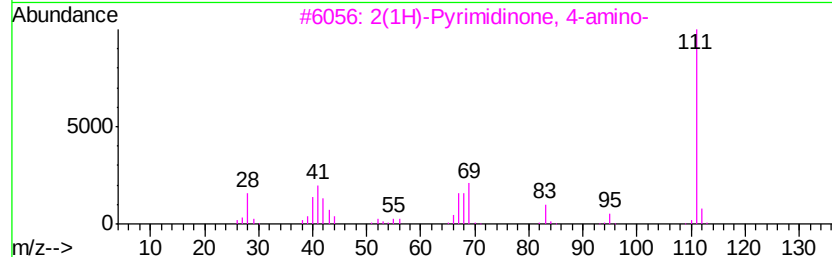
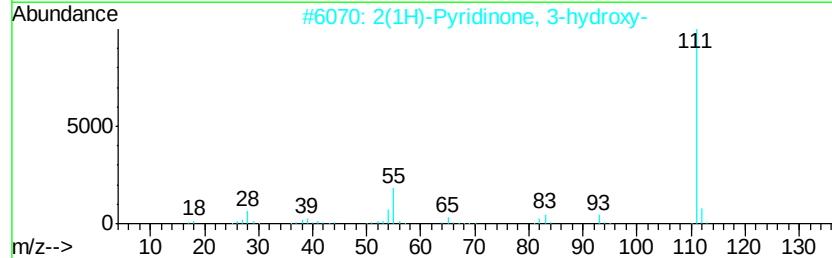
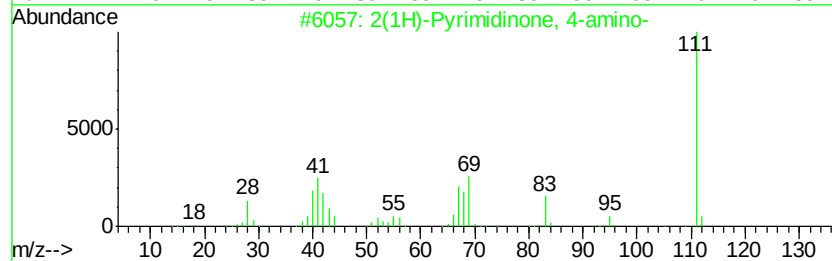
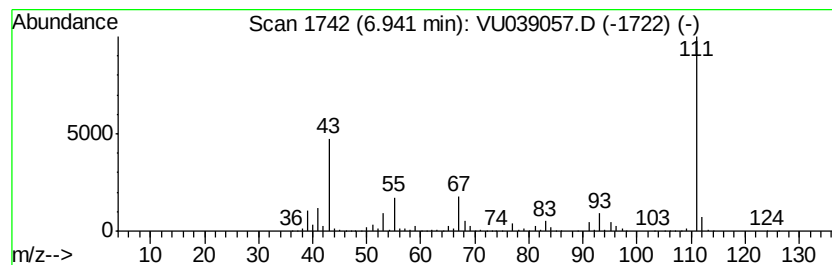
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Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.94	24.03 ug/L	3120430	1,4-Difluorobenzene	6.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	50
2			2(1H)-Pyridinone, 3-hydroxy-	111	C5H5N02	016867-04-2	45
3			2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	45
4			2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	42
5			2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	39



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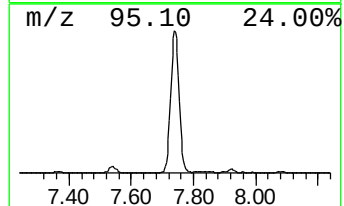
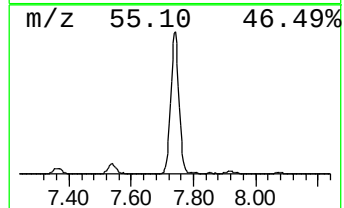
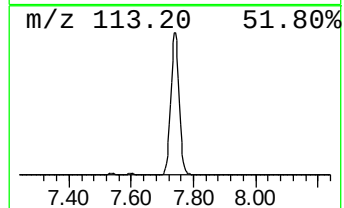
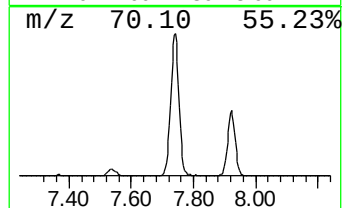
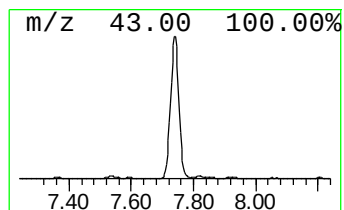
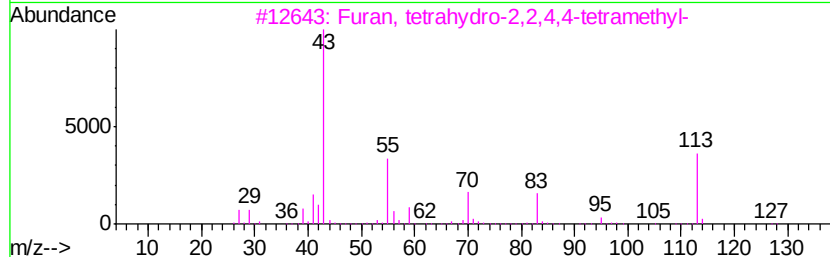
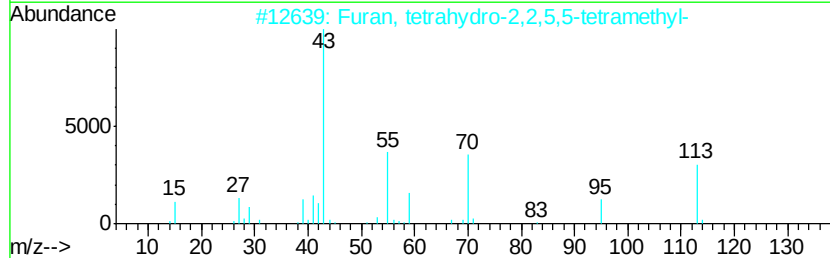
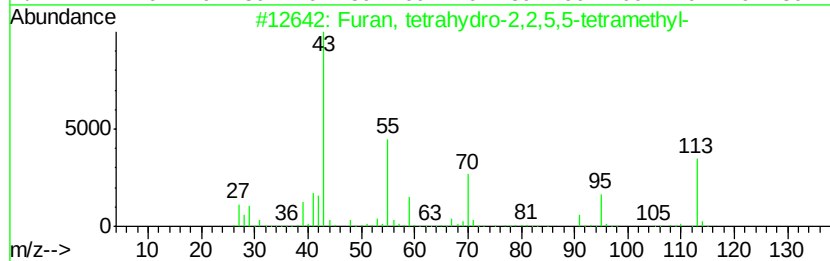
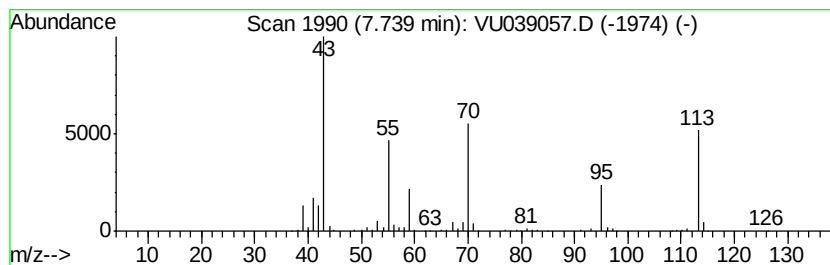
Instrument :
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ClientSampleId :
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Quant Title : TRACE VOA SOM01.0

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	6.25 ug/L	811133	1,4-Difluorobenzene	6.28	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	64
3	Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	53
4	4-Piperidinone, 1-methyl-	113	C6H11NO	001445-73-4	50
5	Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	45



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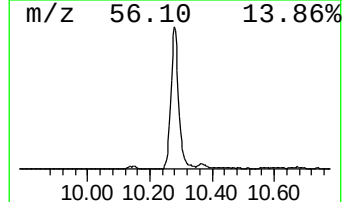
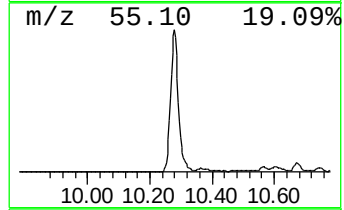
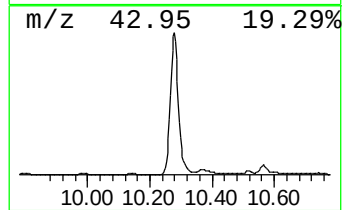
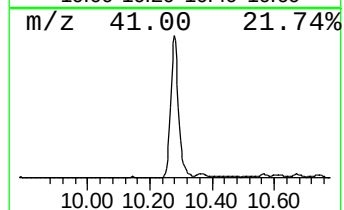
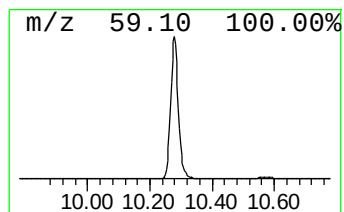
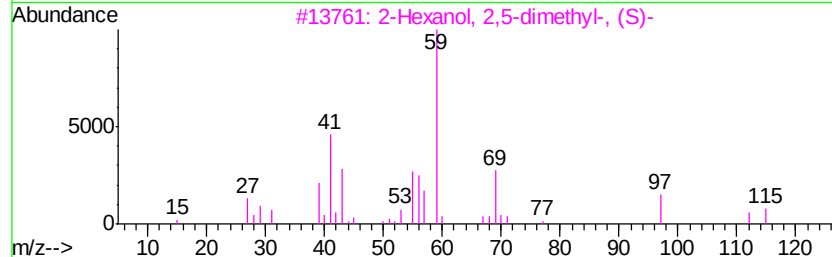
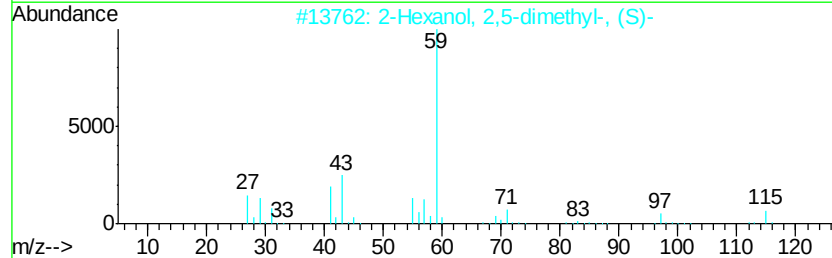
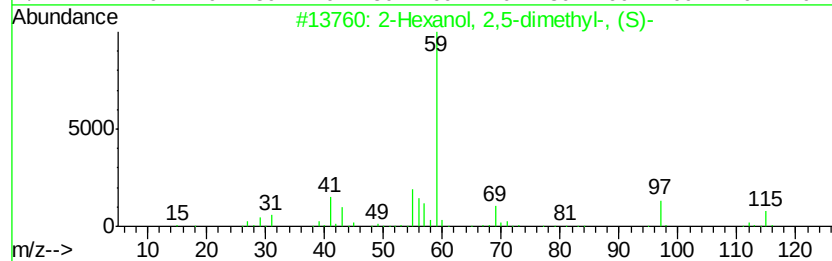
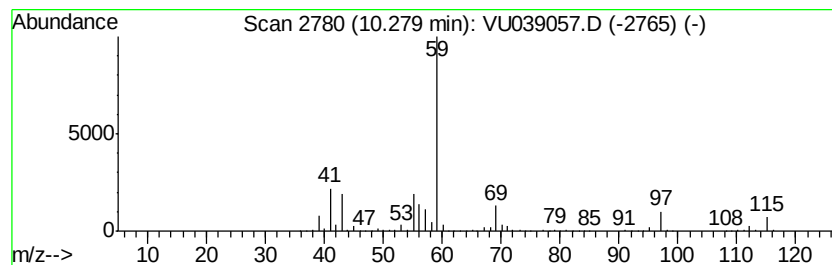
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Peak Number 3 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.28	8.55 ug/L	1717880	Chlorobenzene-d5	9.44	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	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-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	50
4	2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	50
5	6-Methyl-2-heptanol, methyl ether	144	C9H20O	1000365-52-0	45



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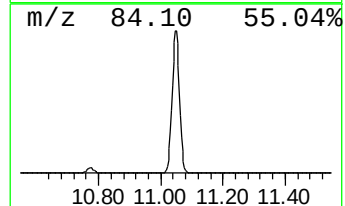
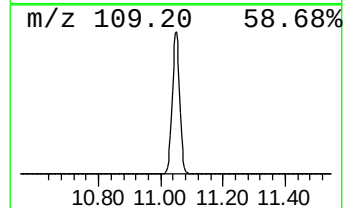
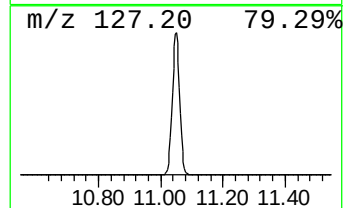
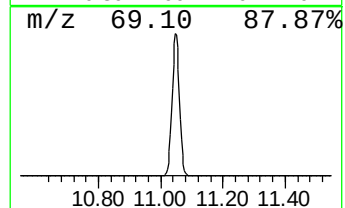
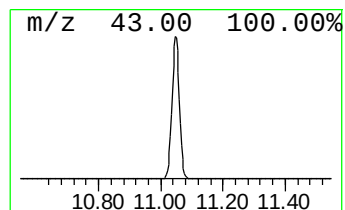
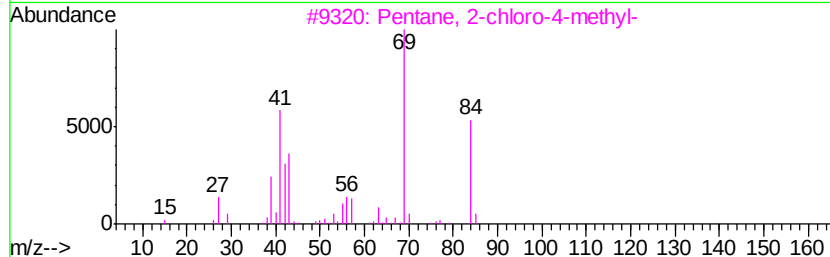
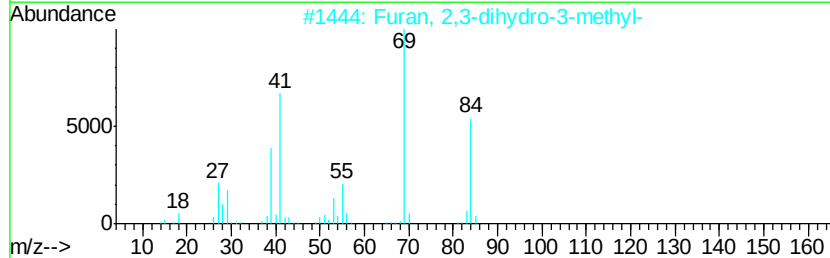
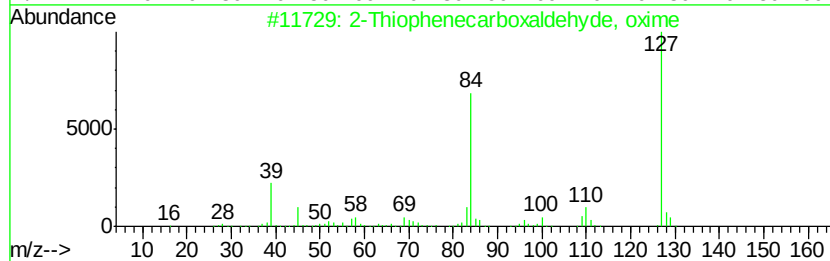
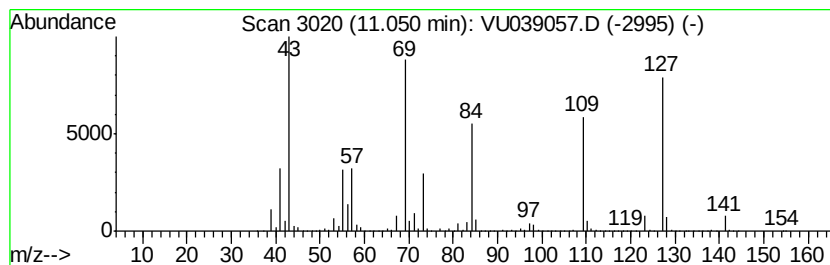
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Peak Number 4 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.05	277.12 ug/L	44530000	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		Furan, 2,3-dihydro-3-methyl-	84	C5H8O	001708-27-6	27
3		Pentane, 2-chloro-4-methyl-	120	C6H13Cl	025346-32-1	27
4		Cyclopropane, (1,2-dimethylpropyl)-	112	C8H16	006976-27-8	27
5		1-Piperidinamine, N-[1-(ethylazo...	184	C9H20N4	059856-64-3	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2(1H)-Pyrimidinon...	6.94	24.0	ug/L	3120430	1	6.28	649147	5.0
Furan, tetrahydro...	7.74	6.3	ug/L	811133	1	6.28	649147	5.0
2-Hexanol, 2,5-di...	10.28	8.6	ug/L	1717880	2	9.44	1004470	5.0
unknown-01	11.05	277.1	ug/L	44530000	3	11.83	803457	5.0