

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV062320\
 Data File : VV017034.D
 Acq On : 22 Jun 2020 22:09
 Operator : SY/MD
 Sample : L3067-15
 Misc : 25.0mL/MSVOA V/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BFXH2

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	2.135	312	325	337	rBV2	928724	1444112	3.62%	2.319%
2	3.212	641	660	680	rBV	5534214	11623650	29.14%	18.663%
3	3.936	868	885	913	rBV3	349451	949184	2.38%	1.524%
4	4.640	1078	1104	1142	rBV	15707425	39893777	100.00%	64.054%
5	5.074	1223	1239	1249	rBV2	257533	618963	1.55%	0.994%
6	5.640	1403	1415	1434	rBV	219741	444475	1.11%	0.714%
7	6.341	1616	1633	1656	rBV	191488	403996	1.01%	0.649%
8	7.338	1932	1943	1957	rBV	318587	544380	1.36%	0.874%
9	8.109	2172	2183	2208	rBV	304851	548985	1.38%	0.881%
10	8.875	2407	2421	2446	rBV2	350442	701936	1.76%	1.127%
11	9.752	2682	2694	2706	rBV	410328	644396	1.62%	1.035%
12	10.501	2916	2927	2940	rVB	1712821	2739082	6.87%	4.398%
13	11.270	3154	3166	3184	rBV	376475	604389	1.51%	0.970%
14	11.556	3240	3255	3272	rBV3	288246	489977	1.23%	0.787%
15	11.646	3272	3283	3302	rVB2	342805	630389	1.58%	1.012%

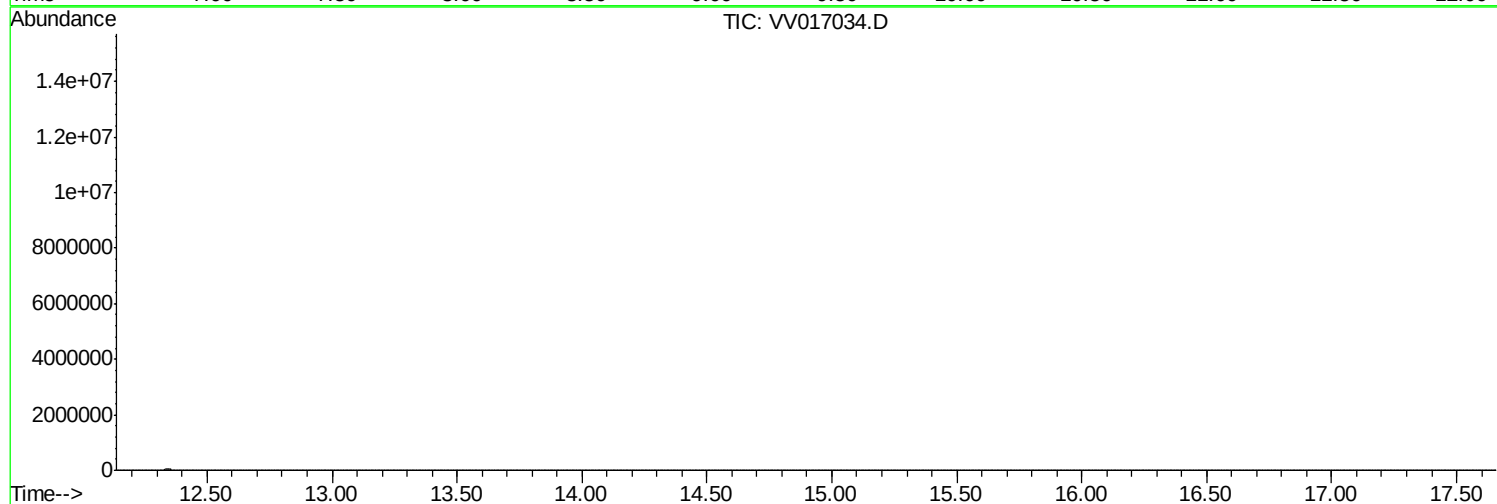
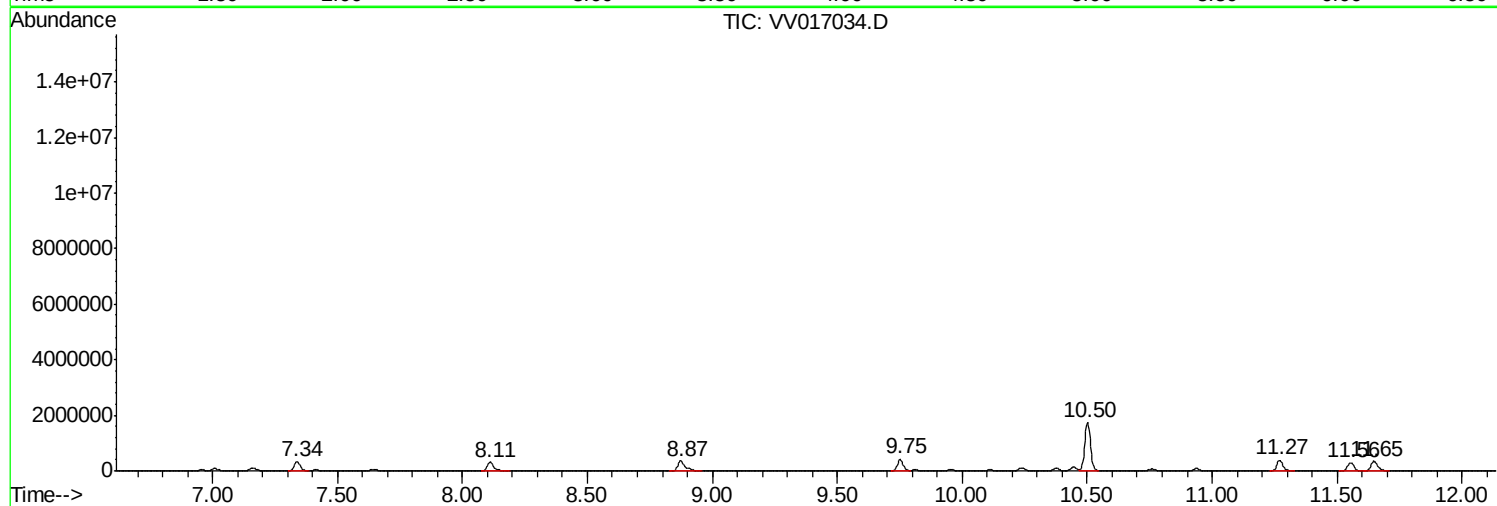
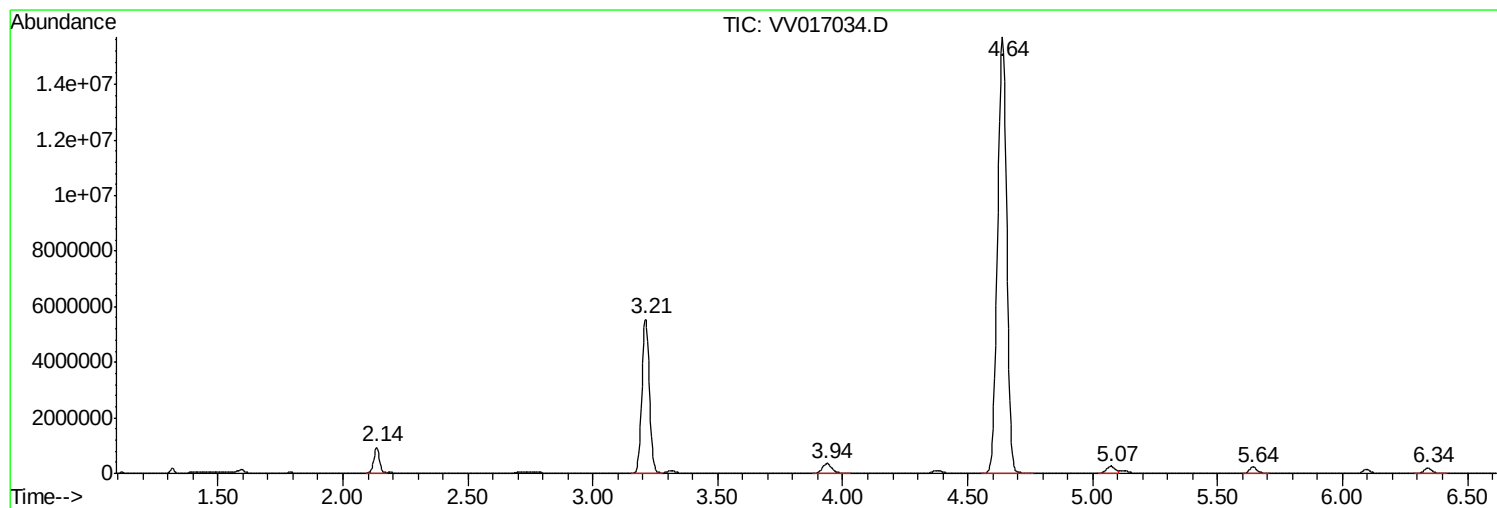
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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



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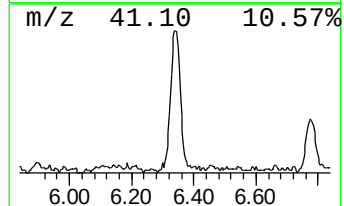
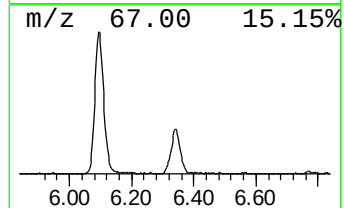
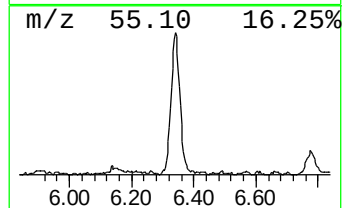
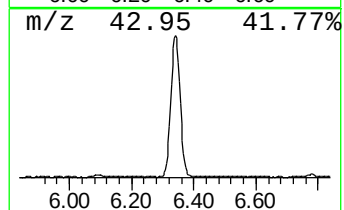
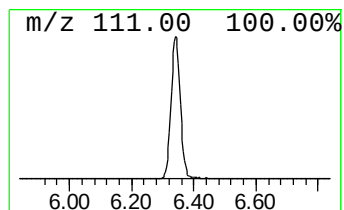
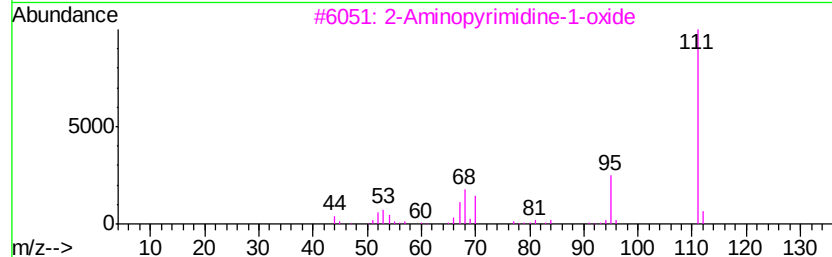
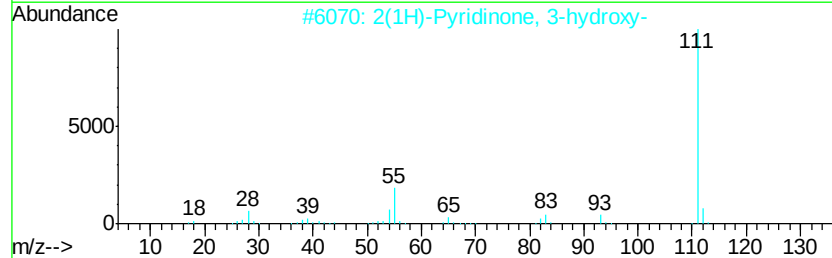
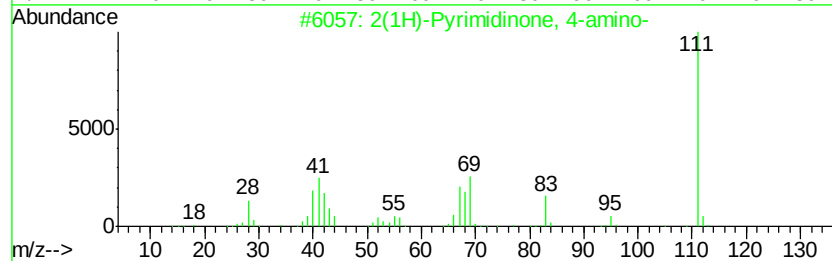
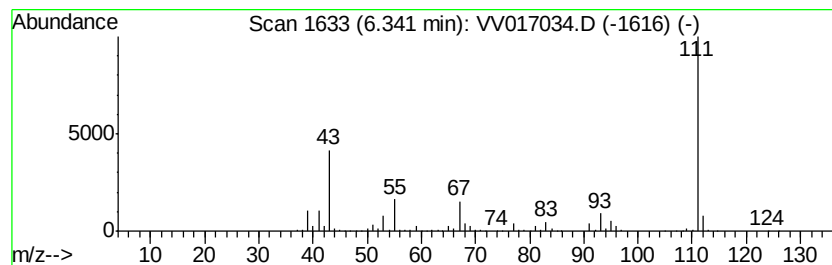
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	4.54 ug/L	403996	1,4-Difluorobenzene	5.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	64
2			2(1H)-Pyridinone, 3-hydroxy-	111	C5H5N2O	016867-04-2	53
3			2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	50
4			3-Aminopyrazine 1-oxide	111	C4H5N3O	006863-77-0	38
5			2(1H)-Pyridinone, 5-hydroxy-	111	C5H5N2O	005154-01-8	38



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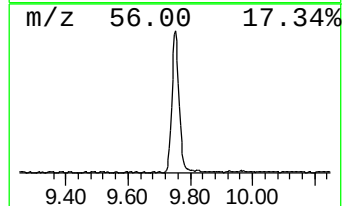
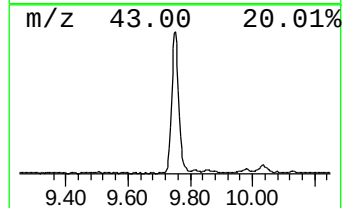
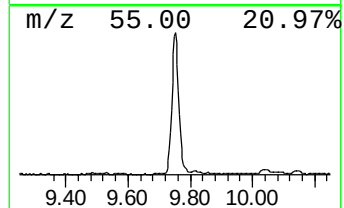
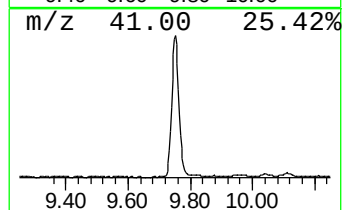
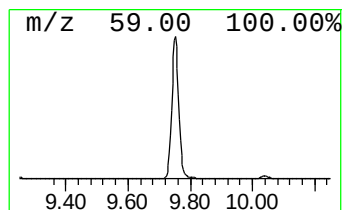
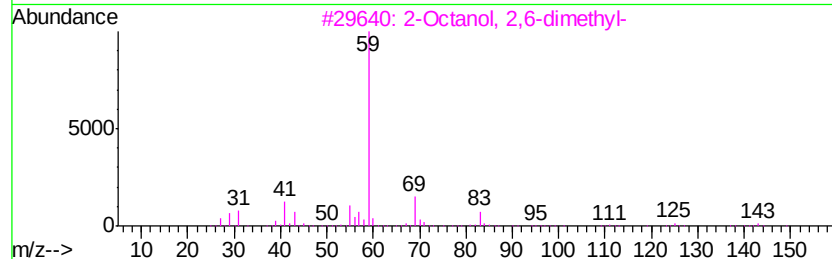
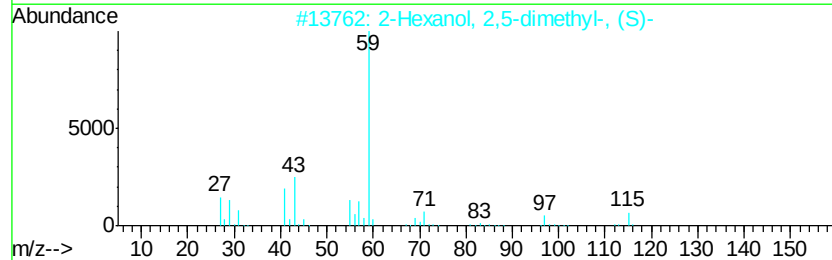
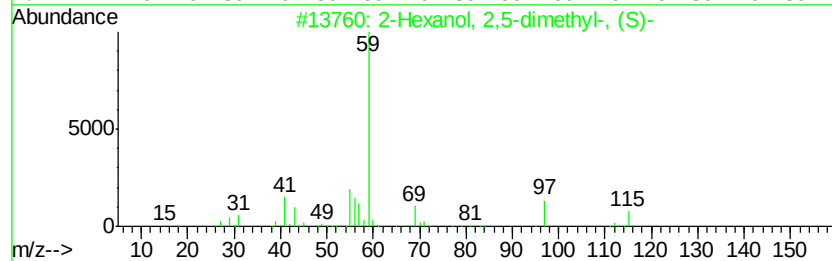
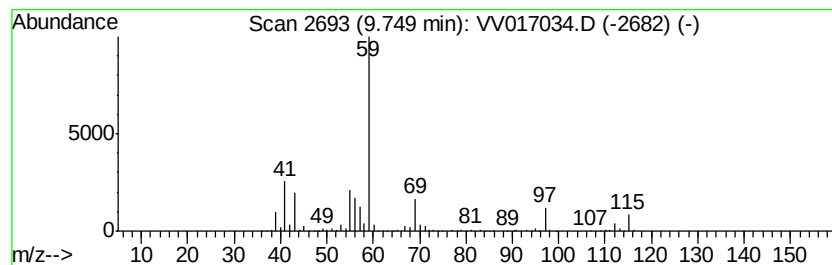
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Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.75	4.59 ug/L	644396	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-Propanol, 2-methyl-	74	C4H10O	000075-65-0	42
5			2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	40



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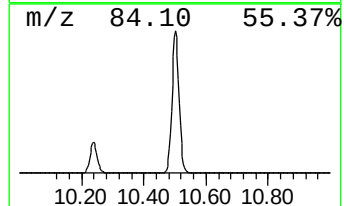
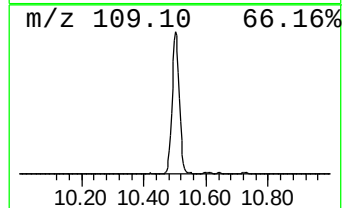
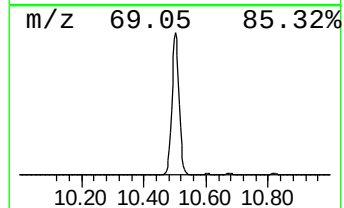
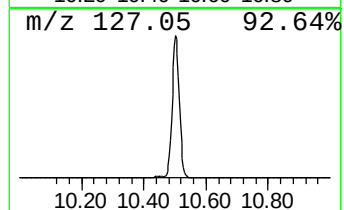
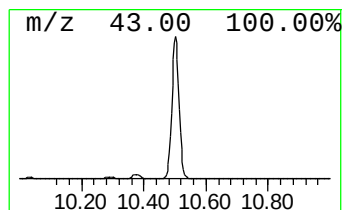
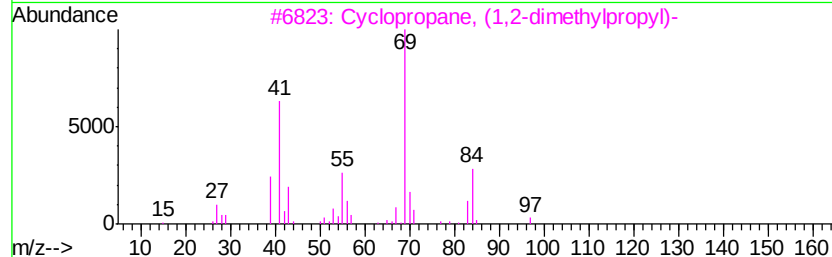
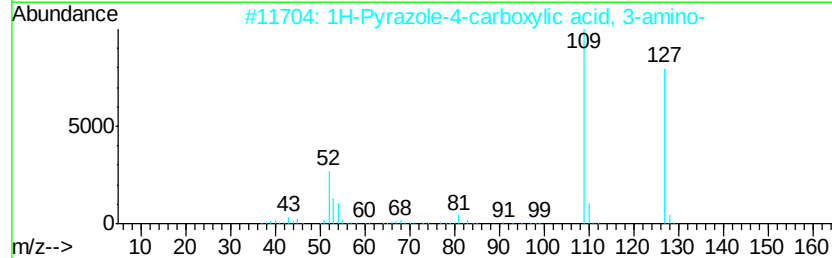
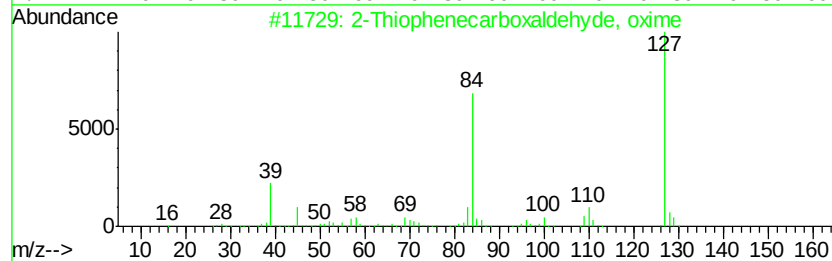
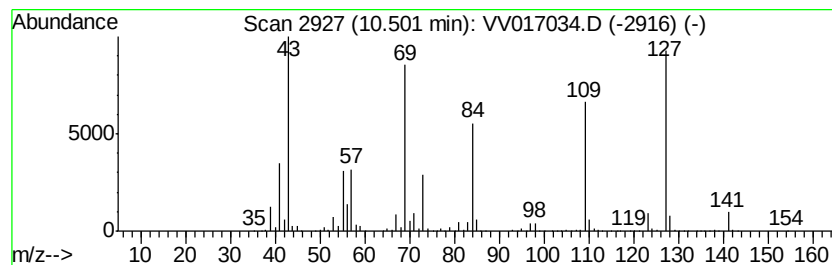
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Peak Number 3 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.50	22.66 ug/L	2739080	1,4-Dichlorobenzene-d4	11.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Thiophenecarboxaldehyde, oxime	127	C5H5NOS	029683-84-9	35
2		1H-Pyrazole-4-carboxylic acid, 3...	127	C4H5N3O2	041680-34-6	35
3		Cyclopropane, (1,2-dimethylpropyl)-	112	C8H16	006976-27-8	27
4		2-Pentene, 4-methyl-, (Z)-	84	C6H12	000691-38-3	27
5		2-Nonen-4-one	140	C9H16O	032064-72-5	27



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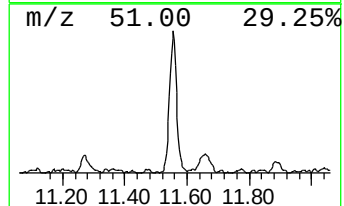
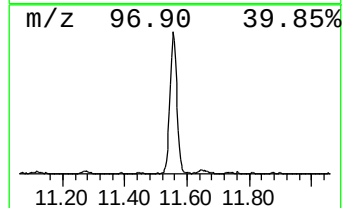
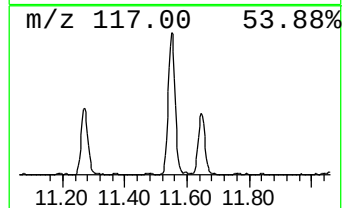
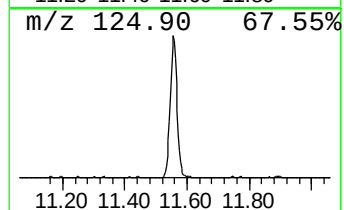
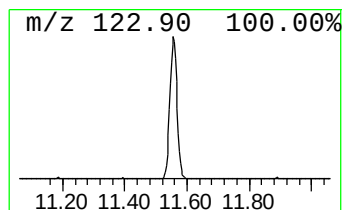
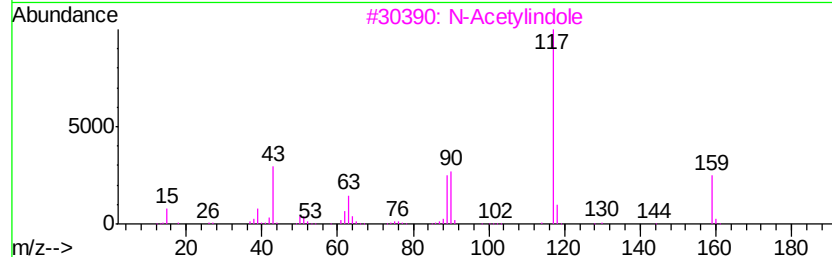
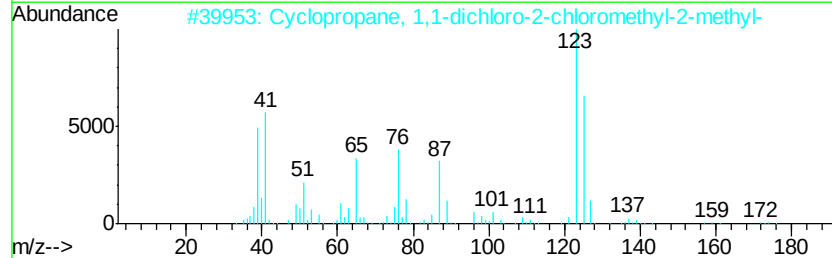
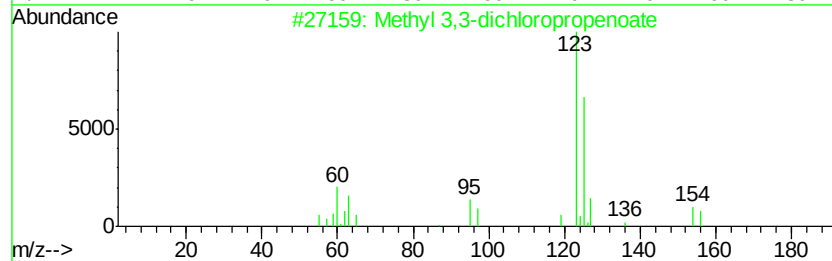
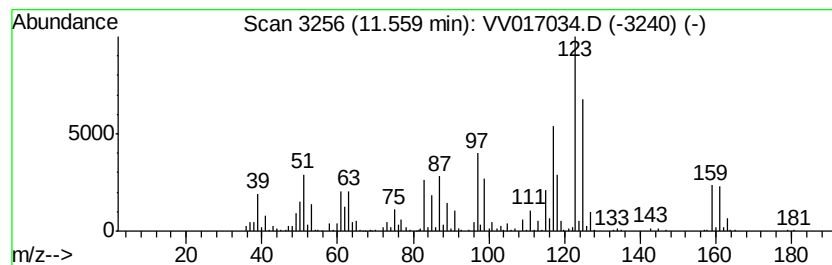
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Peak Number 4 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.56	4.05 ug/L	489977	1,4-Dichlorobenzene-d4	11.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methyl 3,3-dichloropropenoate	154	C4H4Cl2O2	002257-46-7	22
2		Cyclopropane, 1,1-dichloro-2-chl...	172	C5H7Cl3	015997-19-0	16
3		N-Acetylindole	159	C10H9NO	000576-15-8	14
4		Phenol, 4-nitroso-	123	C6H5NO2	000104-91-6	12
5		1-Propene, 3,3,3-trichloro-2-met...	158	C4H5Cl3	004749-27-3	12



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2(1H)-Pyrimidinon...	6.34	4.5	ug/L	403996	1	5.64	444475	5.0
2-Hexanol, 2,5-di...	9.75	4.6	ug/L	644396	2	8.87	701936	5.0
unknown-01	10.50	22.7	ug/L	2739080	3	11.27	604389	5.0
unknown-02	11.56	4.0	ug/L	489977	3	11.27	604389	5.0