

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV062320\
 Data File : VV017037.D
 Acq On : 22 Jun 2020 23:21
 Operator : SY/MD
 Sample : L3067-19
 Misc : 25.0mL/MSVOA V/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BFXH6

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_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	2.132	311	324	346	rBV	7744770	11483890	3.60%	2.677%
2	3.212	640	660	683	rBV2	29393746	68987735	21.63%	16.081%
3	4.685	1078	1118	1171	rBV4	79835170	318876544	100.00%	74.329%
4	6.344	1618	1634	1660	rBV	1624629	3373164	1.06%	0.786%
5	9.755	2679	2695	2706	rBV	2351716	3803484	1.19%	0.887%
6	10.505	2916	2928	2941	rVB	9102681	15091909	4.73%	3.518%
7	11.556	3240	3255	3273	rBV	4631441	7390113	2.32%	1.723%

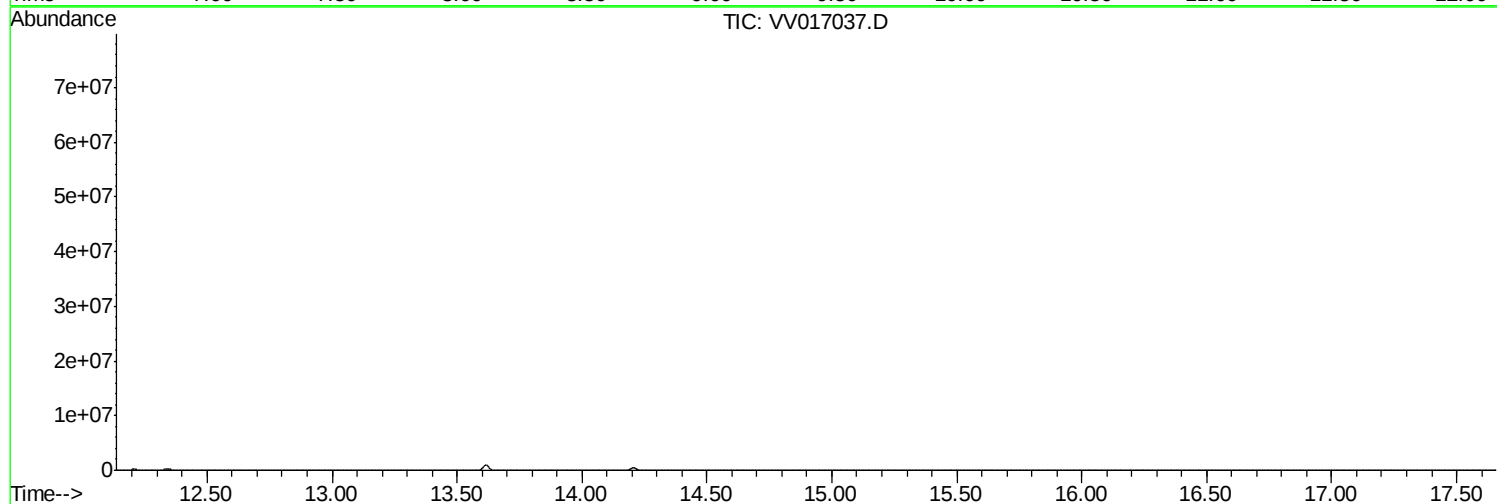
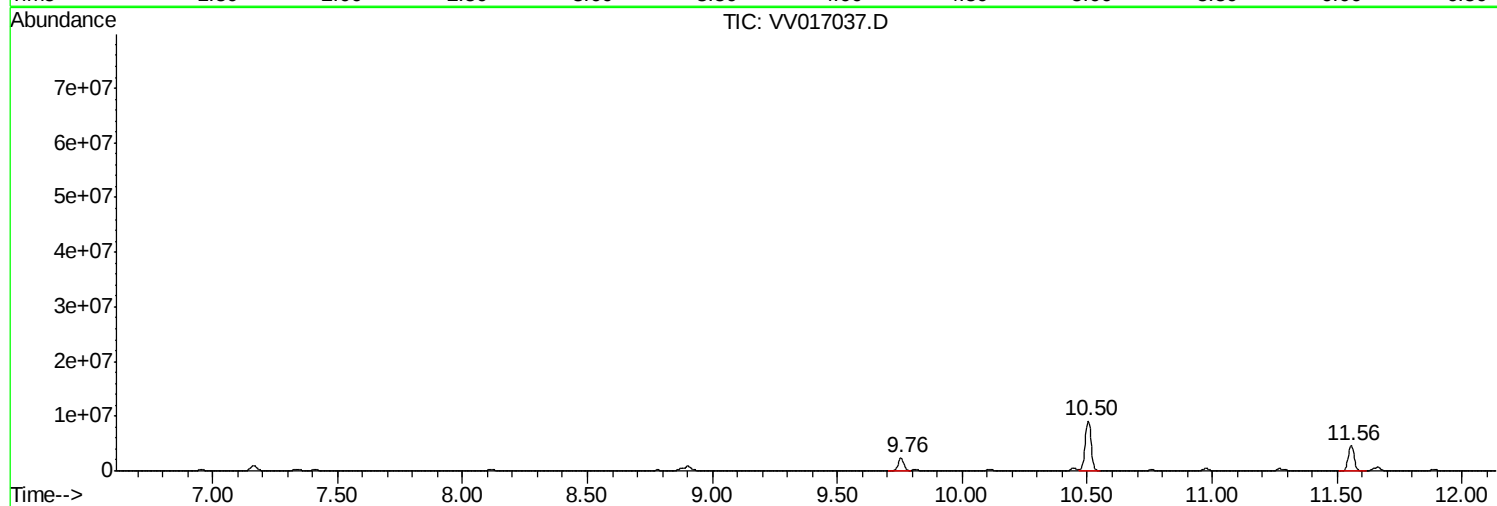
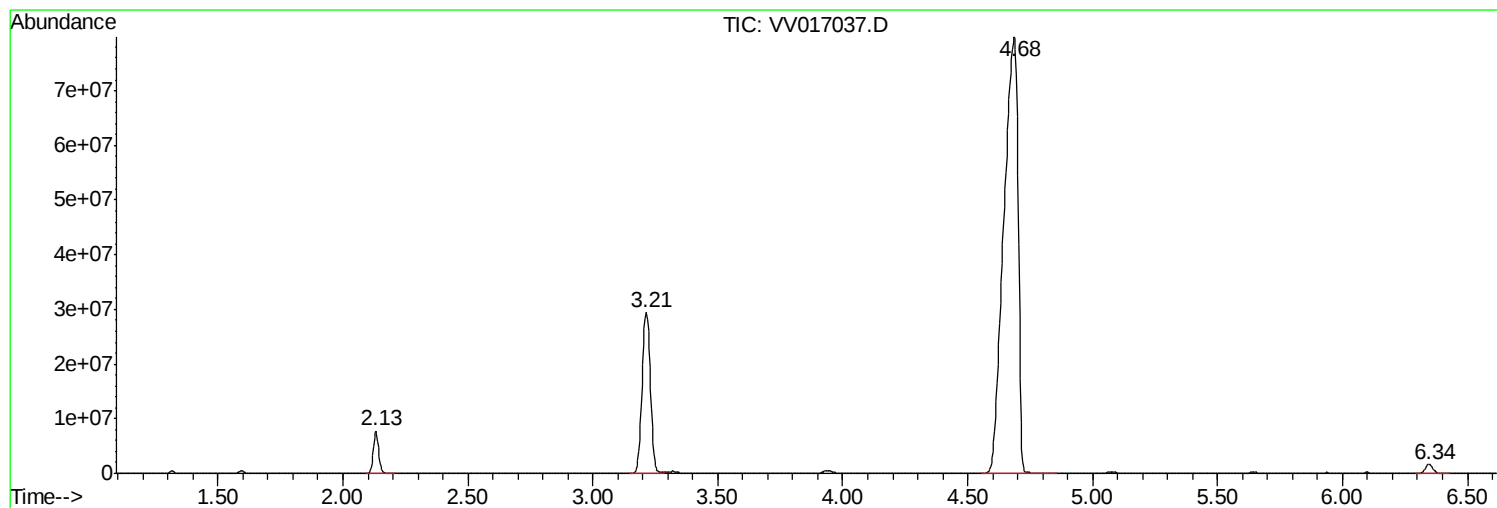
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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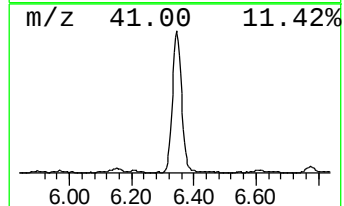
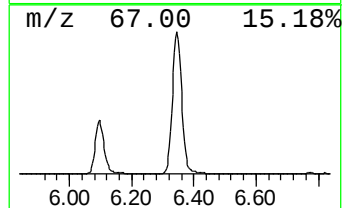
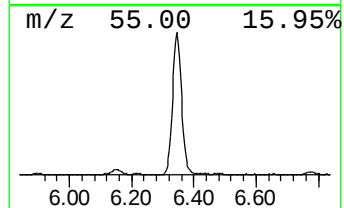
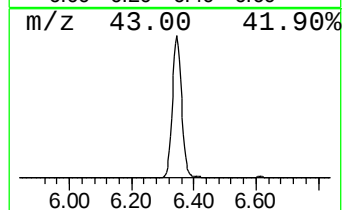
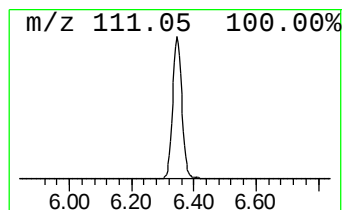
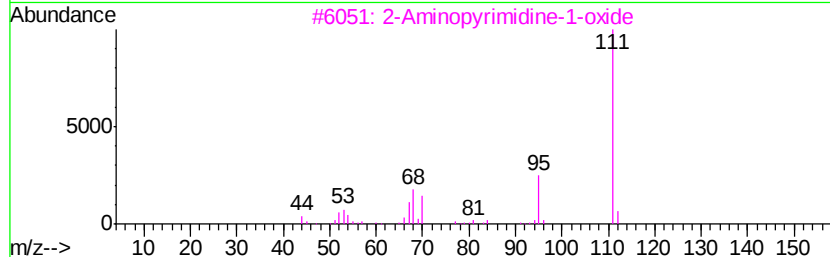
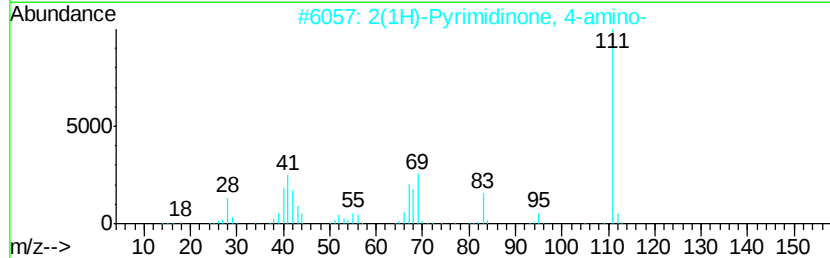
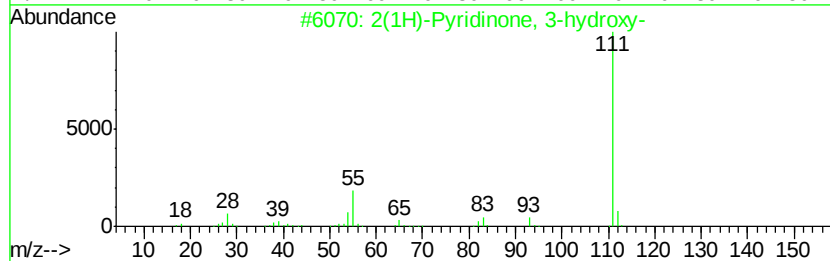
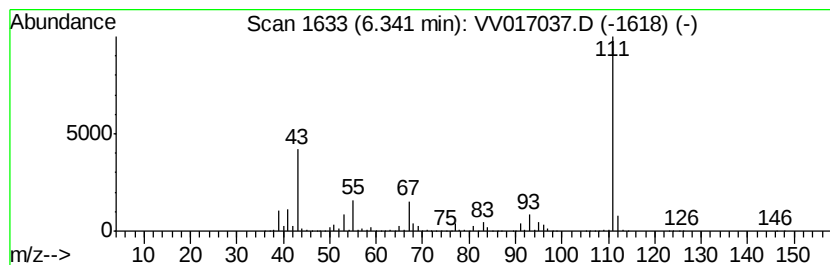
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	5.00 ug/L	3373160	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2(1H)-Pyridinone, 3-hydroxy-	111	C5H5N02	016867-04-2	64
2		2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	64
3		2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	50
4		2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	39
5		2(1H)-Pyridinone, 5-hydroxy-	111	C5H5N02	005154-01-8	38



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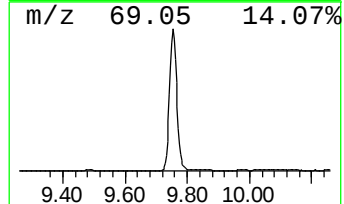
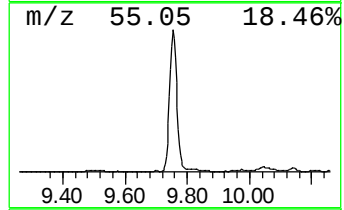
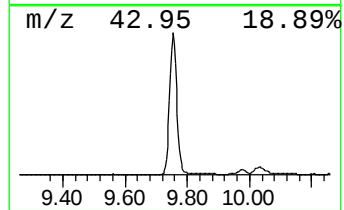
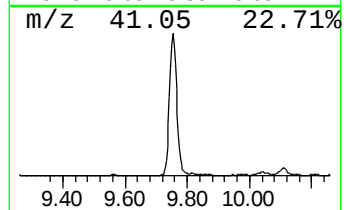
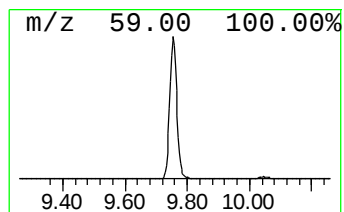
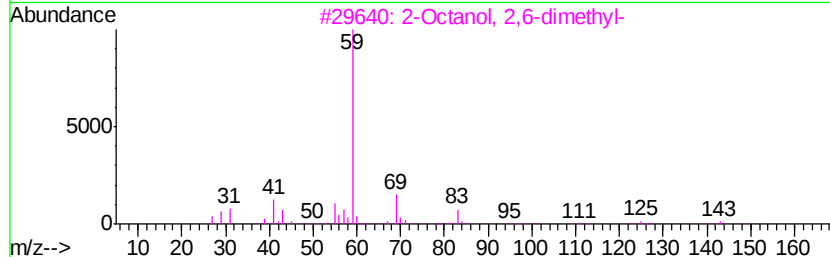
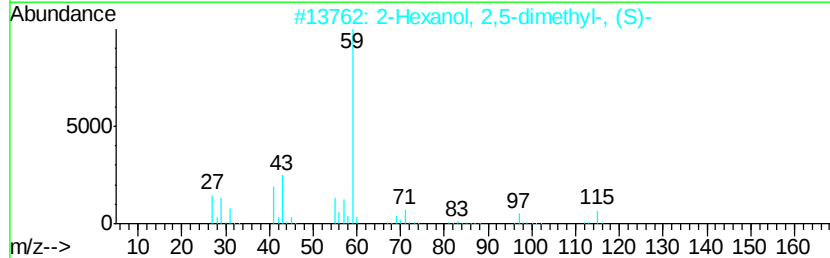
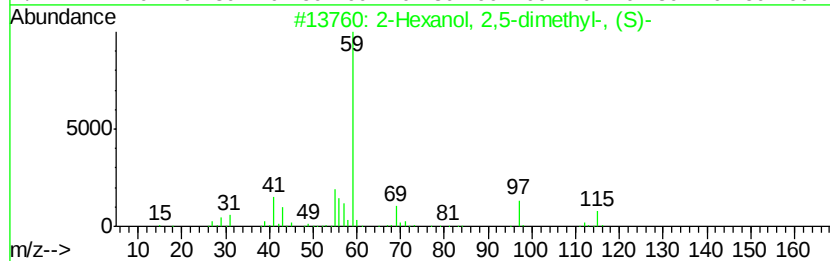
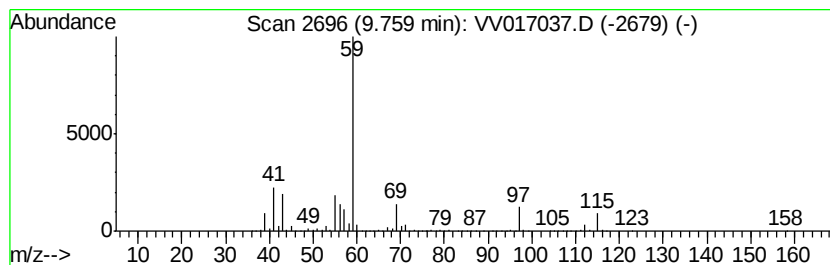
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.76	5.00 ug/L	3803480	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	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	64	
4	2-Hydroxy-2,4-dimethyl-3-pentanone	130	C7H14O2	003212-67-7	59	
5	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	40	



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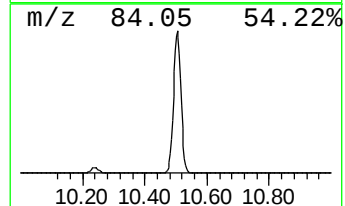
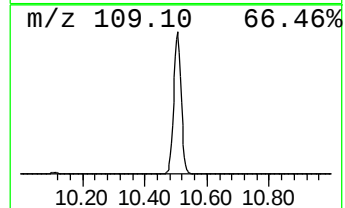
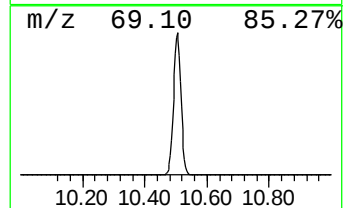
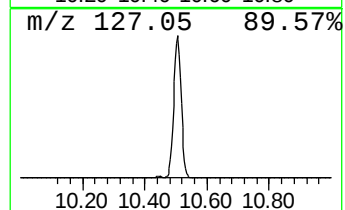
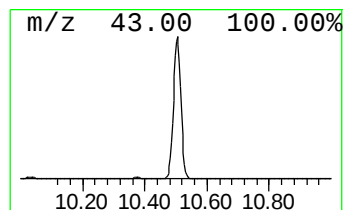
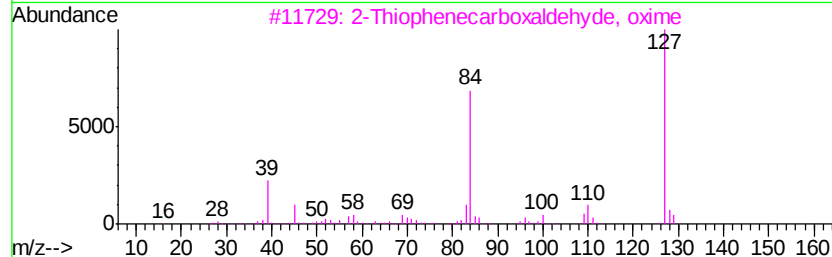
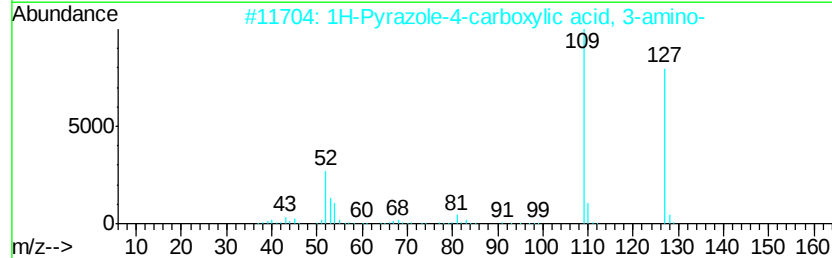
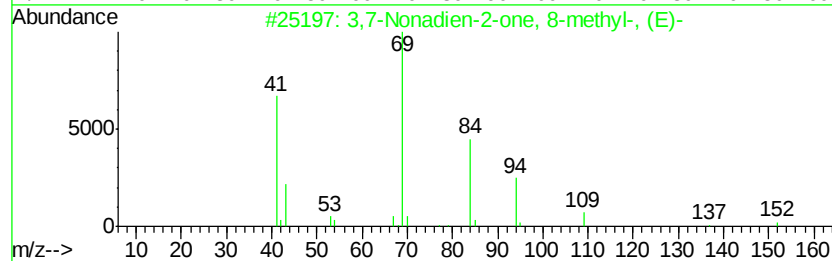
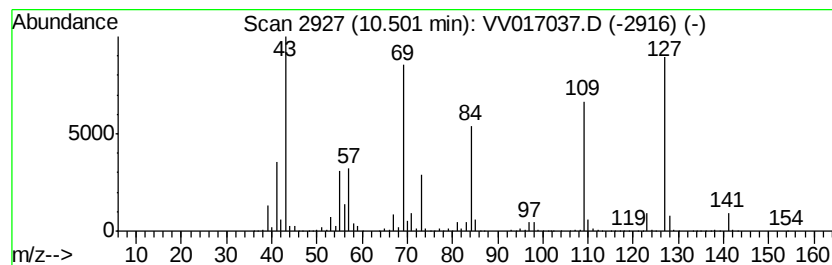
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.50	10.21 ug/L	15091900	1,4-Dichlorobenzene-d4	11.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,7-Nonadien-2-one, 8-methyl-, (E)-	152	C10H16O	035408-14-1	35
2		1H-Pyrazole-4-carboxylic acid, 3-amino-	127	C4H5N3O2	041680-34-6	35
3		2-Thiophenecarboxaldehyde, oxime	127	C5H5NOS	029683-84-9	35
4		Pentane, 3-methylene-	84	C6H12	000760-21-4	27
5		Cyclopropane, (1,2-dimethylpropyl)-	112	C8H16	006976-27-8	27



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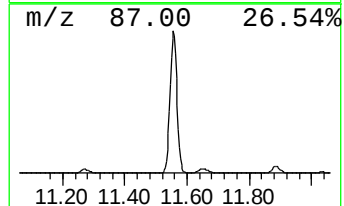
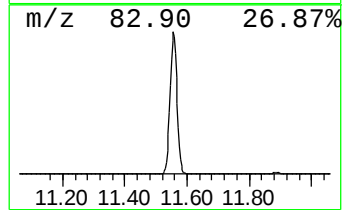
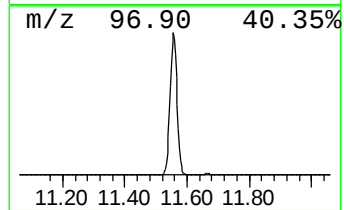
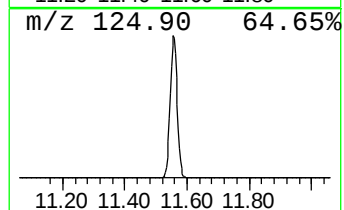
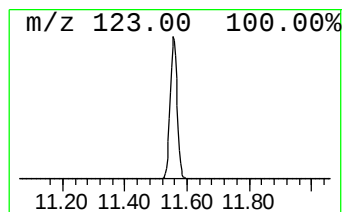
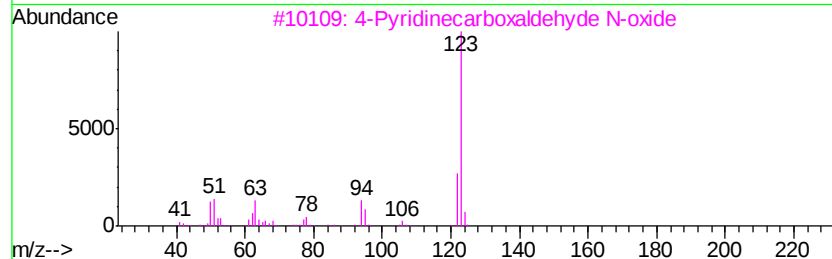
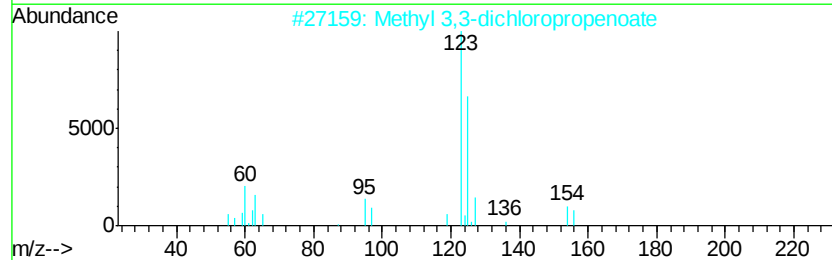
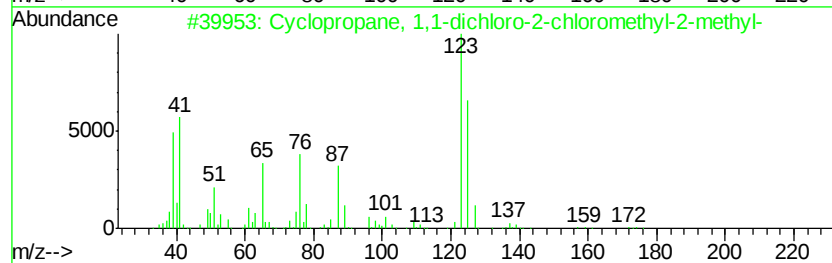
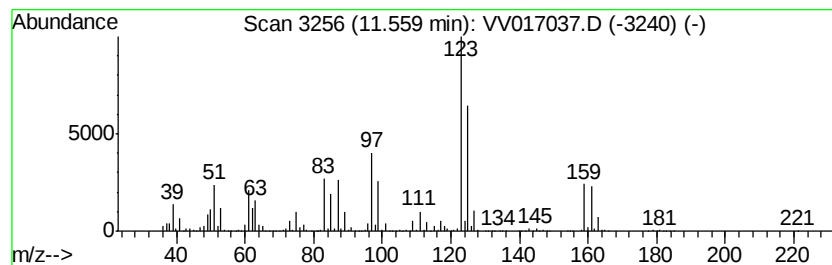
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Peak Number 5 unknown-02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.56	5.00 ug/L	7390110	1,4-Dichlorobenzene-d4	11.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopropane, 1,1-dichloro-2-chl...	172	C5H7Cl3	015997-19-0	35
2		Methyl 3,3-dichloropropenoate	154	C4H4Cl2O2	002257-46-7	27
3		4-Pyridinecarboxaldehyde N-oxide	123	C6H5NO2	007216-42-4	22
4		2,2-Dichloroethyl ethyl carbonate	186	C5H8Cl2O3	1000373-78-3	16
5		1-Propene, 3,3,3-trichloro-2-met...	158	C4H5Cl3	004749-27-3	16



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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(1H)-Pyridinone,...	6.34	5.0	ug/L	3373160	1	5.64	3373160	5.0
2-Hexanol, 2,5-di...	9.76	5.0	ug/L	3803480	2	8.87	3803480	5.0
unknown-01	10.50	10.2	ug/L	15091900	3	11.27	7390110	5.0
unknown-02	11.56	5.0	ug/L	7390110	3	11.27	7390110	5.0