

Data Path : Z:\VOASRV\HPCHEM1\MSVOA W\DATA\VW081318\
 Data File : VW004598.D
 Acq On : 10 Aug 2018 15:40
 Operator : SY/AP
 Sample : J4382-02
 Misc : 17.74G/5ML/MSVOA W/SOIL
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 JTY-SB-04-5-7

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 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_W\METHOD\82W080618S.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.752	18	27	29	rBV	25316	55244	1.24%	0.203%
2	1.813	29	37	56	rVB	2005663	4446252	100.00%	16.364%
3	2.319	114	120	129	rBV	100254	224449	5.05%	0.826%
4	4.129	408	417	433	rVB2	32404	96771	2.18%	0.356%
5	4.916	534	546	559	rBV2	30254	129447	2.91%	0.476%
6	5.208	581	594	615	rBV2	23902	106950	2.41%	0.394%
7	7.153	903	913	926	rBV	49035	156120	3.51%	0.575%
8	7.885	1023	1033	1038	rBV	455872	1071468	24.10%	3.943%
9	7.952	1038	1044	1063	rVB	915117	2018476	45.40%	7.429%
10	8.312	1090	1103	1115	rBV	468364	1048340	23.58%	3.858%
11	8.750	1166	1175	1182	rBV2	50284	105108	2.36%	0.387%
12	8.848	1182	1191	1206	rVB	1426929	2778658	62.49%	10.227%
13	10.329	1424	1434	1441	rBV	1641064	2847097	64.03%	10.479%
14	11.634	1640	1648	1657	rBV	1924553	3198399	71.93%	11.772%
15	12.622	1804	1810	1821	rVB	1126210	1809835	40.70%	6.661%
16	12.939	1853	1862	1869	rBV2	48074	85806	1.93%	0.316%
17	13.439	1938	1944	1950	rBV	436669	691624	15.56%	2.545%
18	13.567	1957	1965	1972	rVB	1956934	3122350	70.22%	11.492%
19	13.719	1985	1990	2001	rVB7	18299	59489	1.34%	0.219%
20	13.884	2012	2017	2022	rBV2	32751	49582	1.12%	0.182%
21	14.701	2136	2151	2163	rVV4	220230	872368	19.62%	3.211%
22	15.408	2259	2267	2273	rBV	273725	495533	11.14%	1.824%
23	15.481	2273	2279	2286	rVV	344492	643481	14.47%	2.368%
24	15.566	2286	2293	2302	rVB3	451431	887379	19.96%	3.266%
25	15.737	2313	2321	2331	rVB4	49559	170265	3.83%	0.627%

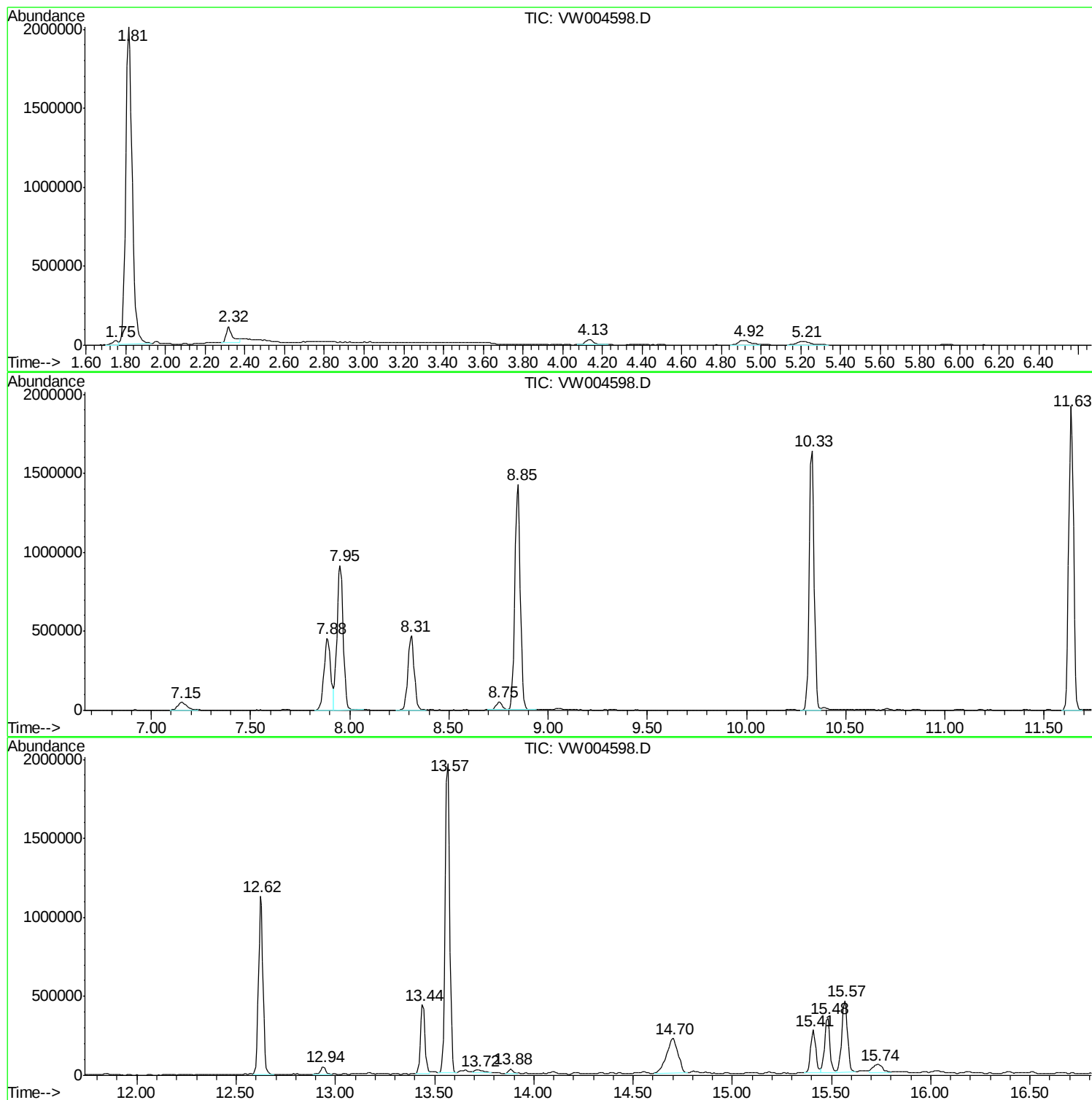
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Quant Title : SW846 8260

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



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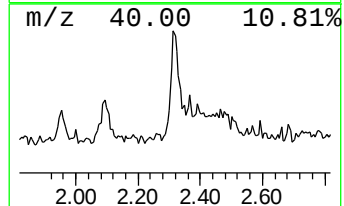
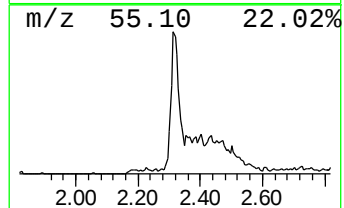
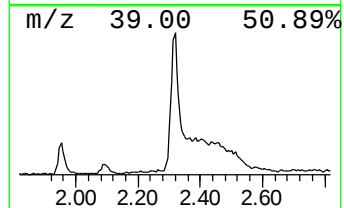
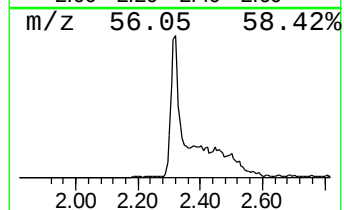
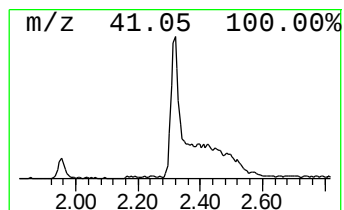
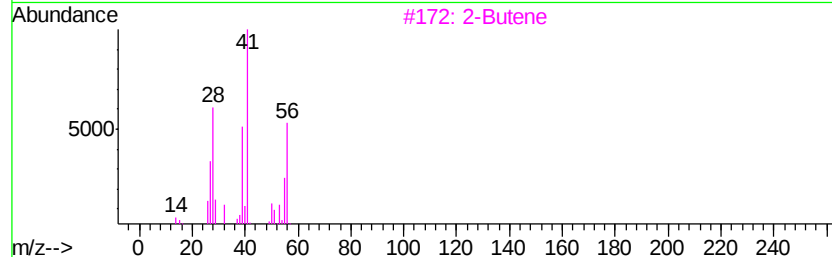
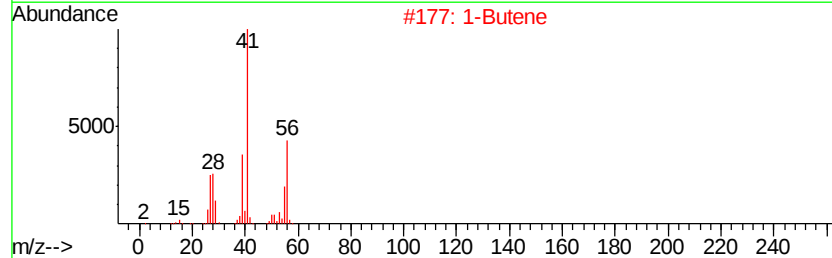
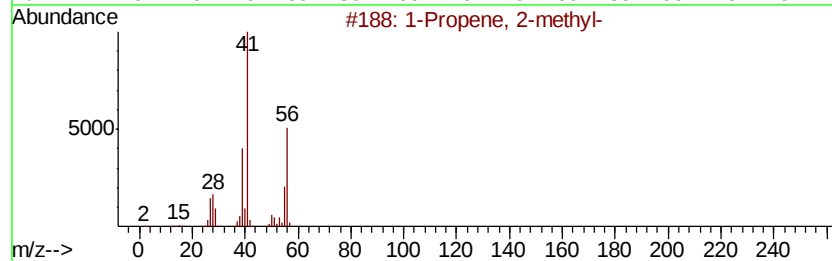
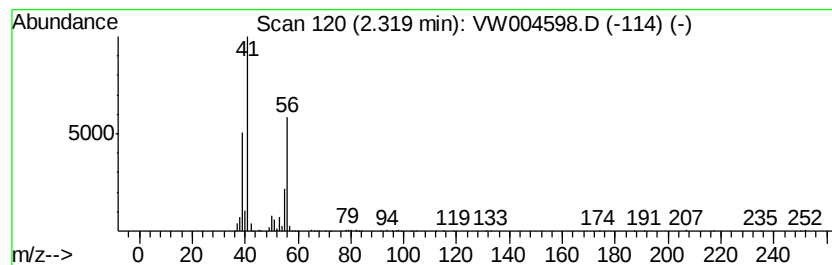
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_W\METHOD\82W080618S.M
Quant Title : SW846 8260

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

Peak Number 2 1-Propene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.32	5.56 ug/l	224449	Pentafluorobenzene	7.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Propene, 2-methyl-	56	C4H8	000115-11-7	90
2		1-Butene	56	C4H8	000106-98-9	86
3		2-Butene	56	C4H8	000107-01-7	80
4		2-Butene, (E)-	56	C4H8	000624-64-6	80
5		2-Butene, (Z)-	56	C4H8	000590-18-1	80



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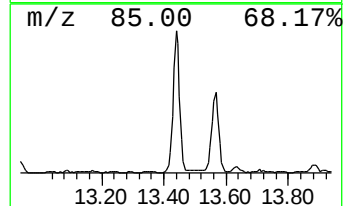
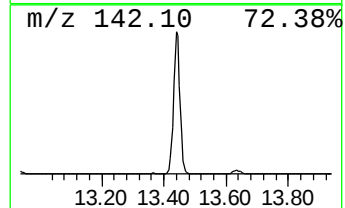
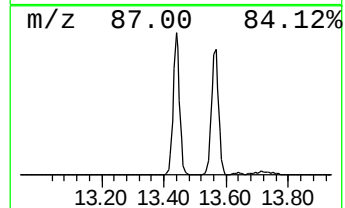
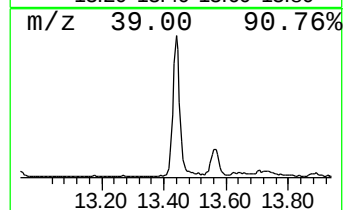
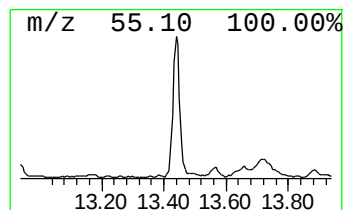
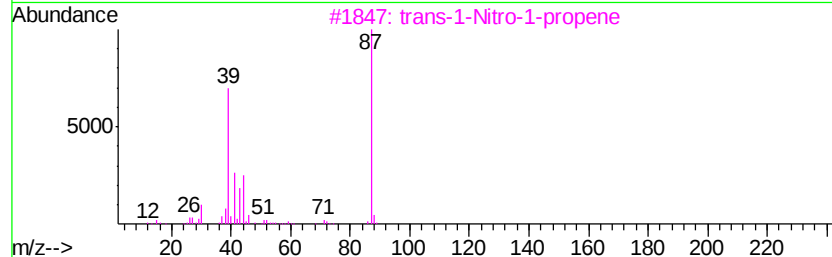
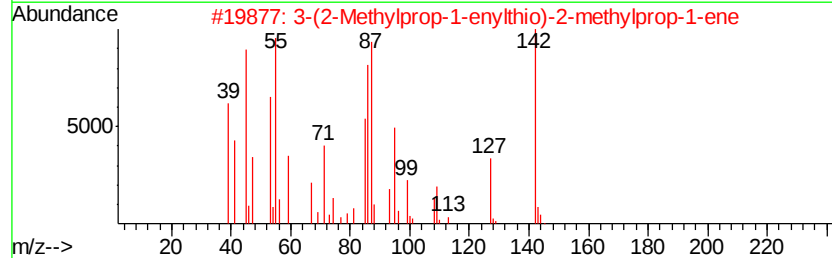
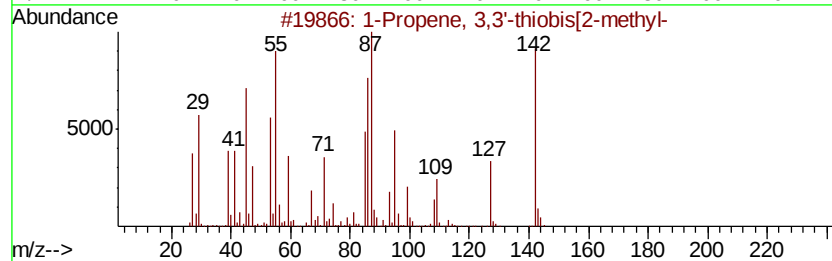
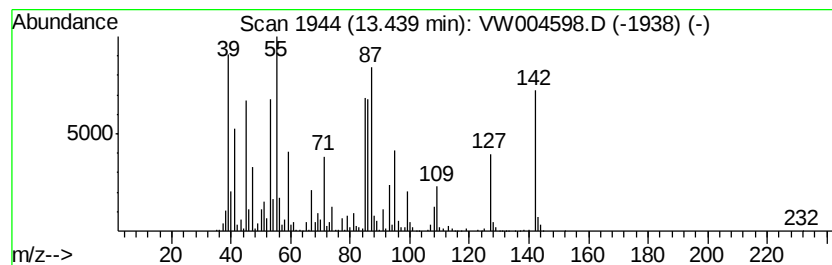
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Propene, 3,3'-thiobis[2-m... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.44	11.08 ug/l	691624	1,4-Dichlorobenzene-d4	13.57
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-Propene, 3,3'-thiobis[2-methyl-	142 C8H14S	023973-54-8 96
2		3-(2-Methylprop-1-enylthio)-2-me...	142 C8H14S	1000122-39-8 95
3		trans-1-Nitro-1-propene	87 C3H5NO2	017082-05-2 43
4		Tetrazole-5-thiole, 1-allyl-	142 C4H6N4S	007624-33-1 35
5		2-Ethylprop-1-ene (1-3)sultine	132 C5H8O2S	084735-13-7 33



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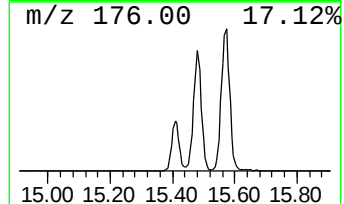
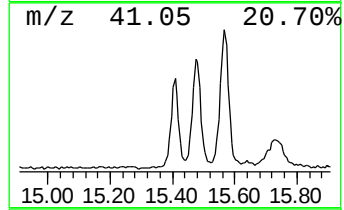
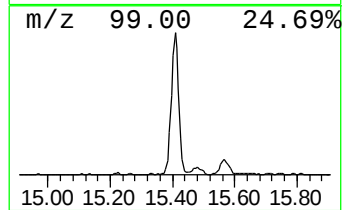
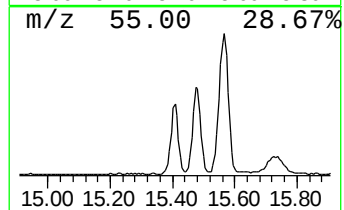
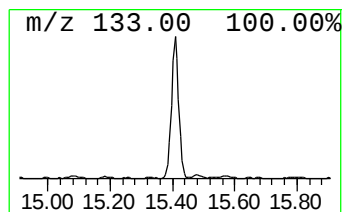
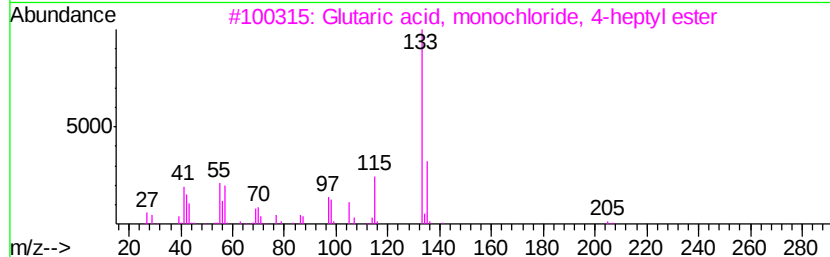
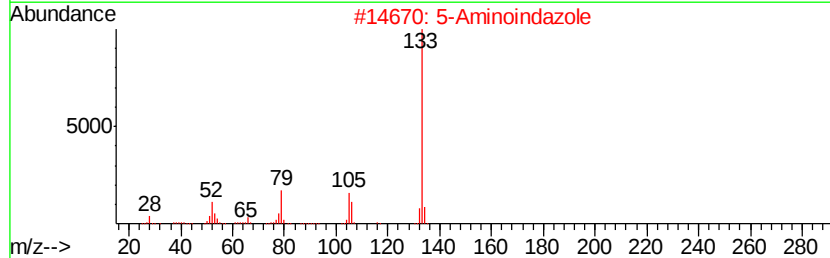
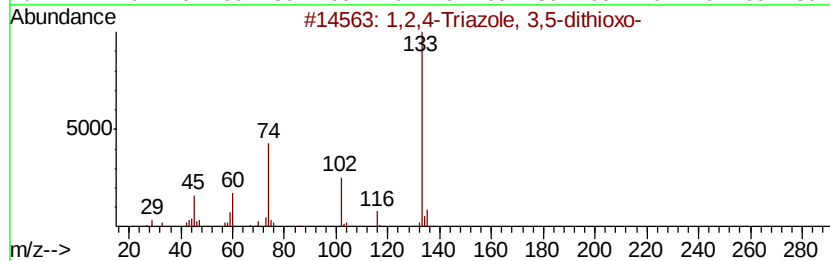
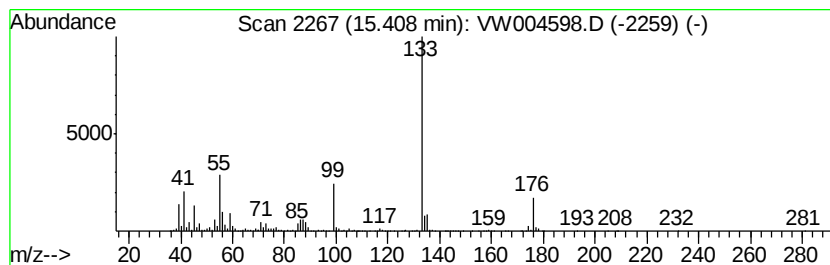
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TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown15.41 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.41	7.94 ug/l	495533	1,4-Dichlorobenzene-d4	13.57	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Triazole, 3,5-dithioxo-	133	C2H3N3S2	005650-03-3	40
2	5-Aminoindazole	133	C7H7N3	019335-11-6	37
3	Glutaric acid, monochloride, 4-h...	248	C12H21ClO3	1000359-47-1	33
4	Thiophene, 2,2'-(1,1,2,2,3,3,4,4...	416	C13H6F10S2	024014-44-6	28
5	(2-Methyl[1,3]dithian-2-yl)methanol	164	C6H12OS2	1000191-37-4	28



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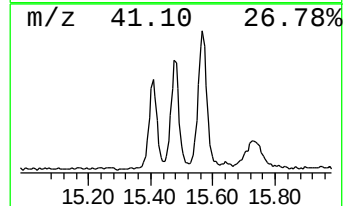
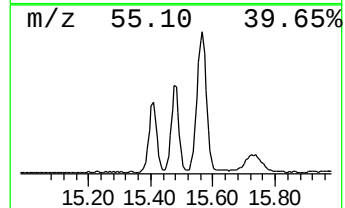
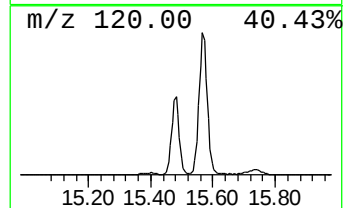
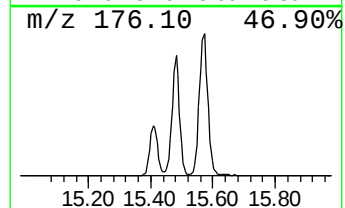
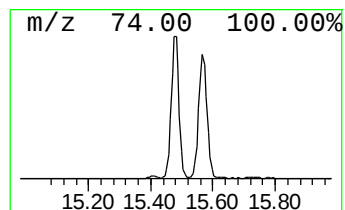
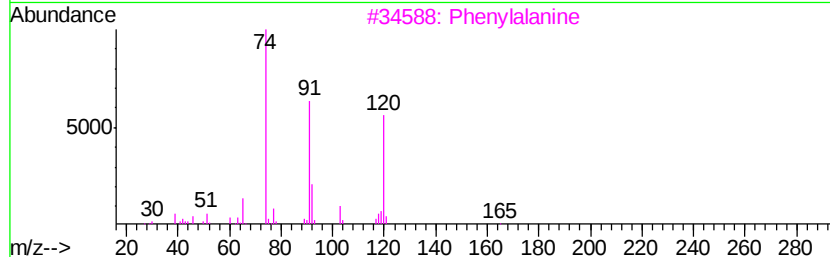
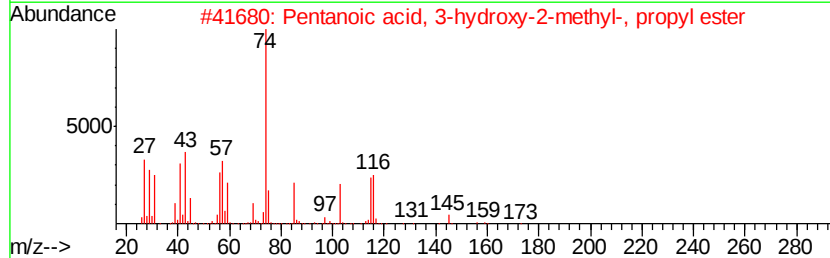
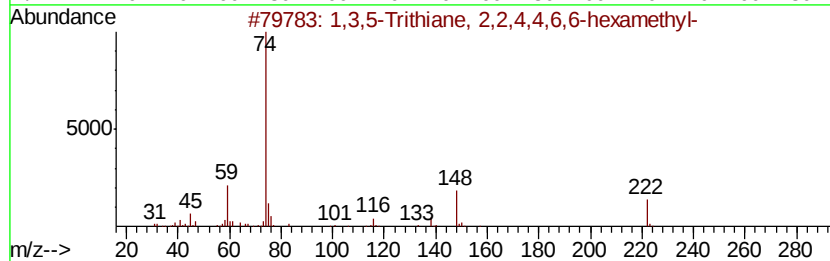
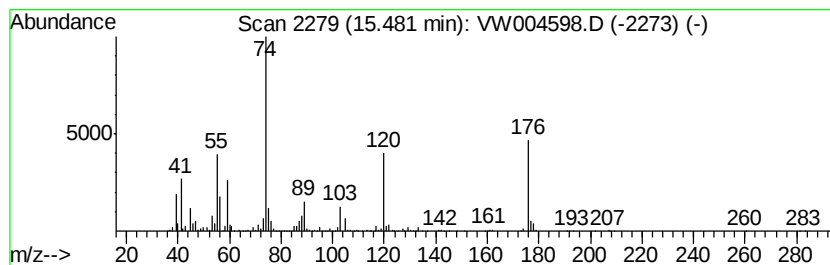
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 unknown15.48 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.48	10.30 ug/l	643481	1,4-Dichlorobenzene-d4	13.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,5-Trithiane, 2,2,4,4,6,6-hex...	222	C9H18S3	000828-26-2	25
2		Pentanoic acid, 3-hydroxy-2-meth...	174	C9H18O3	1000151-17-3	25
3		Phenvlalanine	165	C9H11NO2	000063-91-2	25
4		1,3,4-Thiadiazol-2-amine, 5-methyl-	115	C3H5N3S	000108-33-8	17
5		Pentanoic acid, 3-methyl-, methy...	130	C7H14O2	002177-78-8	17



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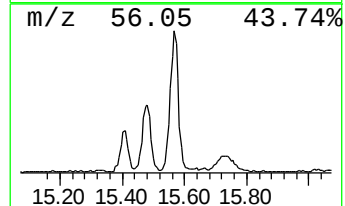
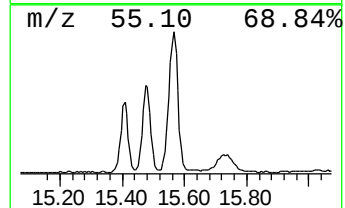
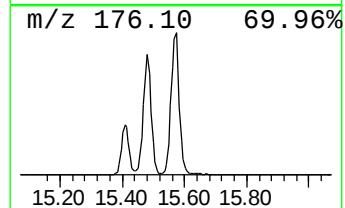
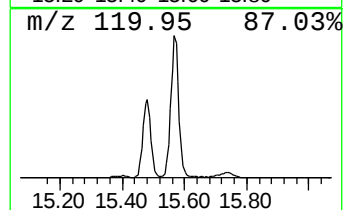
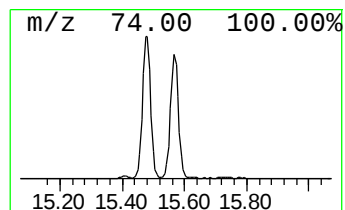
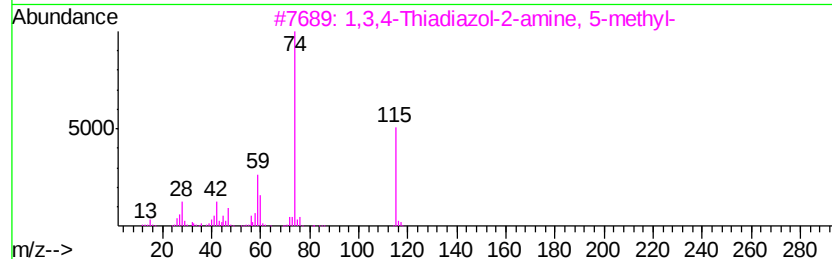
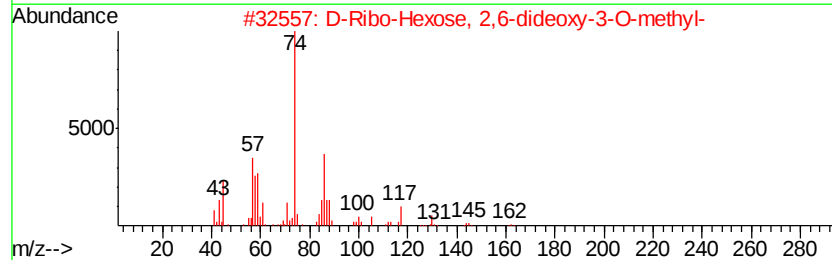
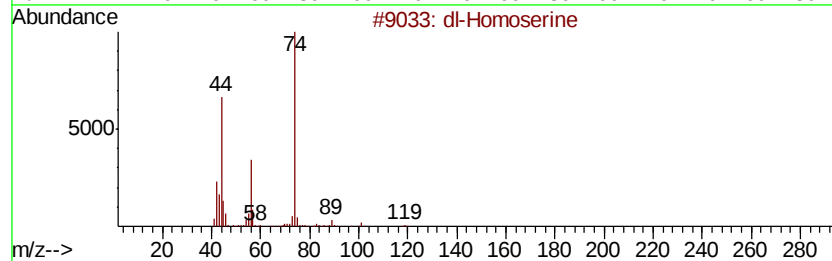
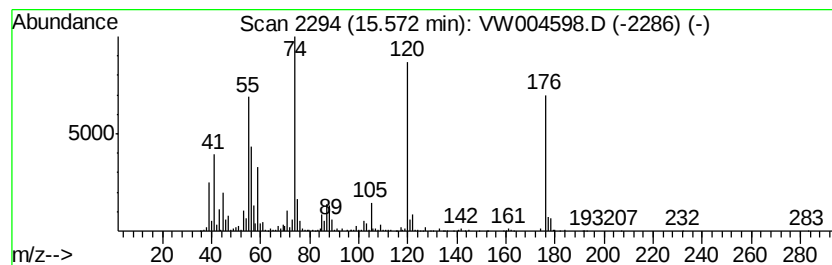
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown15.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.57	14.21 ug/l	887379	1,4-Dichlorobenzene-d4	13.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	dl-Homoserine	119	C4H9NO3	001927-25-9	27
2		D-Ribo-Hexose, 2,6-dideoxy-3-O-m...	162	C7H14O4	013089-76-4	16
3		1,3,4-Thiadiazol-2-amine, 5-methyl-	115	C3H5N3S	000108-33-8	14
4		.alpha.-D-Glucopyranosiduronic a...	236	C9H16O7	031506-20-4	12
5		1,3-Dithiane	120	C4H8S2	000505-23-7	12



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Propene, 2-methyl-	2.32	5.6	ug/l	224449	1	7.95	2018480	50.0
1-Propene, 3,3'-t...	13.44	11.1	ug/l	691624	4	13.57	3122350	50.0
unknown15.41	15.41	7.9	ug/l	495533	4	13.57	3122350	50.0
unknown15.48	15.48	10.3	ug/l	643481	4	13.57	3122350	50.0
unknown15.57	15.57	14.2	ug/l	887379	4	13.57	3122350	50.0