

Data Path : Z:\VOASRV\HPCHEM1\MSVOA W\DATA\VW081318\
 Data File : VW004597.D
 Acq On : 10 Aug 2018 15:15
 Operator : SY/AP
 Sample : J4382-01
 Misc : 16.80G/5ML/MSVOA W/SOIL
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 JTY-SB-05-5-7

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	15	27	29	rBV	24202	55235	1.61%	0.196%
2	1.813	29	37	57	rVB	1461464	3421800	100.00%	12.161%
3	2.319	115	120	125	rBV	31467	58093	1.70%	0.206%
4	4.135	408	418	430	rBV	28927	90353	2.64%	0.321%
5	4.916	534	546	553	rBV2	30000	113323	3.31%	0.403%
6	5.007	553	561	578	rVV2	32553	129340	3.78%	0.460%
7	7.159	901	914	929	rBV2	58274	188003	5.49%	0.668%
8	7.885	1024	1033	1038	rBV2	479688	1129353	33.00%	4.014%
9	7.952	1038	1044	1057	rVB	972720	2132072	62.31%	7.577%
10	8.311	1092	1103	1114	rBV	466930	1026727	30.01%	3.649%
11	8.757	1167	1176	1182	rVB4	29597	63795	1.86%	0.227%
12	8.848	1182	1191	1210	rBV	1477444	2898539	84.71%	10.301%
13	10.329	1424	1434	1441	rBV	1887717	3304655	96.58%	11.744%
14	10.390	1441	1444	1451	rVB	20010	36371	1.06%	0.129%
15	11.634	1640	1648	1657	rBV	2022921	3391016	99.10%	12.051%
16	12.622	1804	1810	1820	rVB	1188201	1985473	58.02%	7.056%
17	12.939	1854	1862	1868	rBV4	53052	100934	2.95%	0.359%
18	13.176	1896	1901	1908	rVB3	23994	39811	1.16%	0.141%
19	13.439	1938	1944	1951	rBV	903801	1440144	42.09%	5.118%
20	13.567	1958	1965	1972	rVV	2096443	3359489	98.18%	11.939%
21	13.634	1972	1976	1984	rVB4	23073	59663	1.74%	0.212%
22	13.884	2012	2017	2021	rBV3	28173	47997	1.40%	0.171%
23	14.737	2152	2157	2163	rVB2	29441	46150	1.35%	0.164%
24	15.408	2258	2267	2273	rBV	460441	843462	24.65%	2.998%
25	15.481	2273	2279	2285	rVV	493858	928304	27.13%	3.299%
26	15.566	2285	2293	2301	rVV2	641714	1247918	36.47%	4.435%

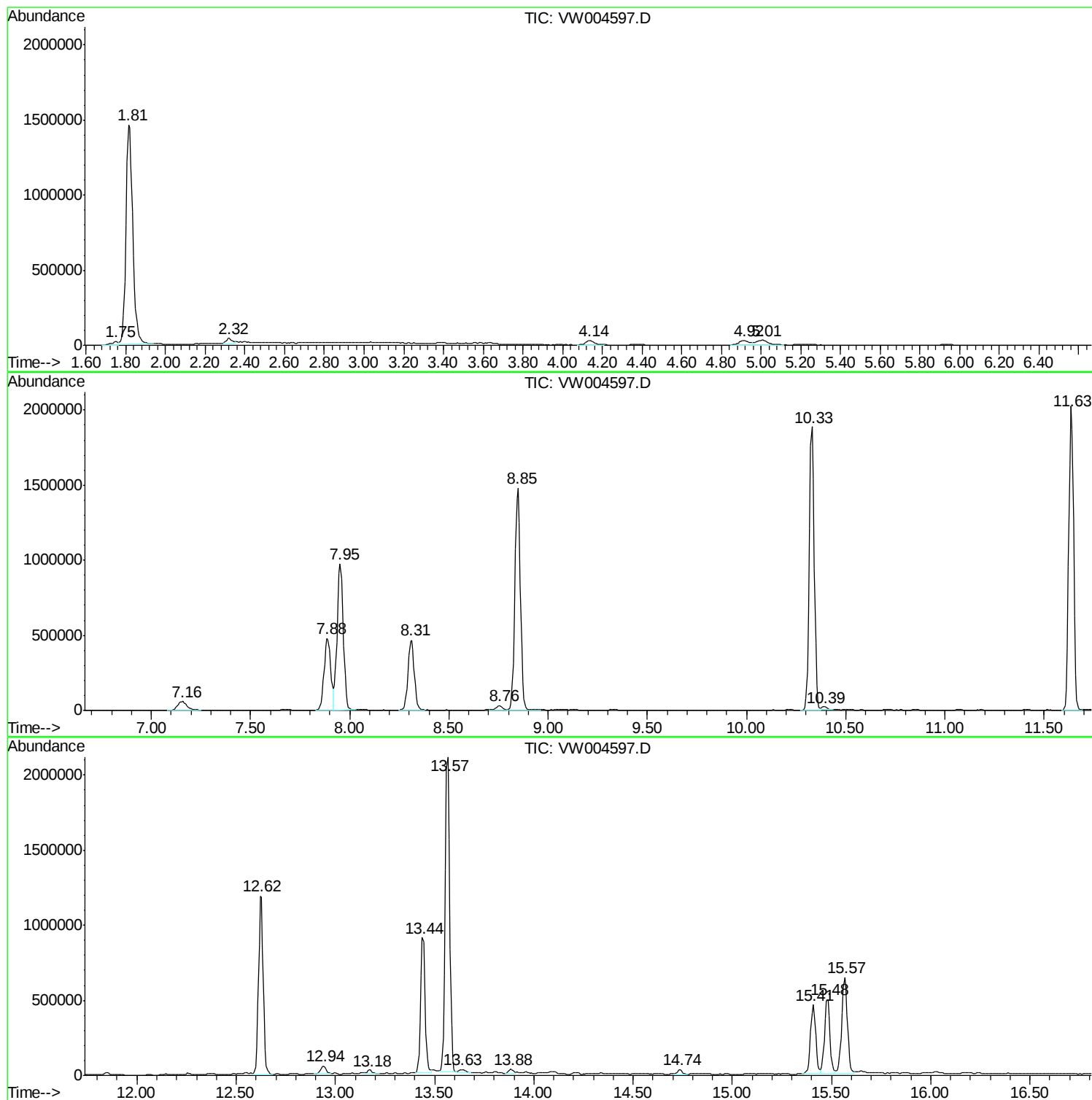
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Quant Title : SW846 8260

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



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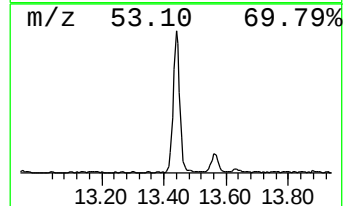
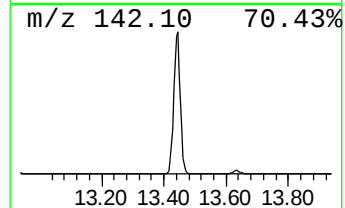
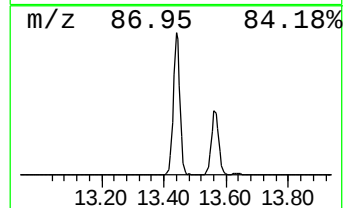
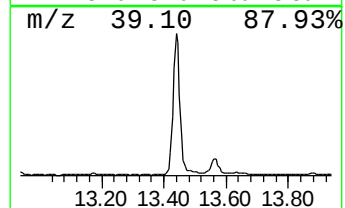
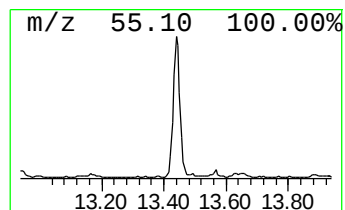
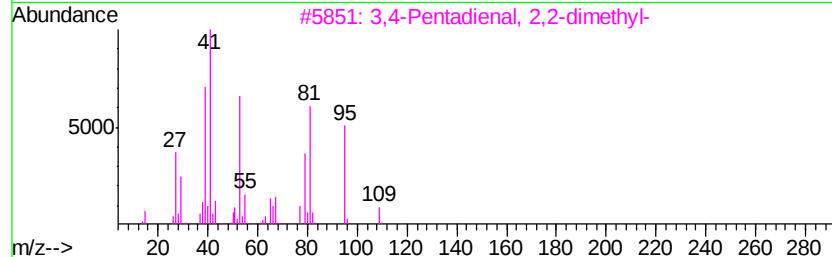
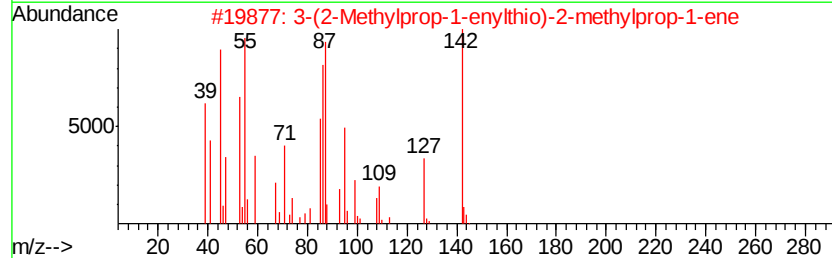
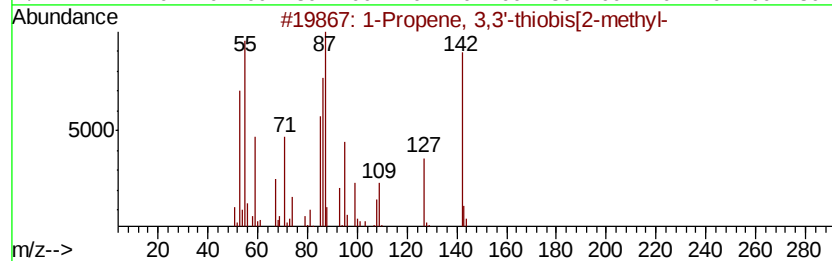
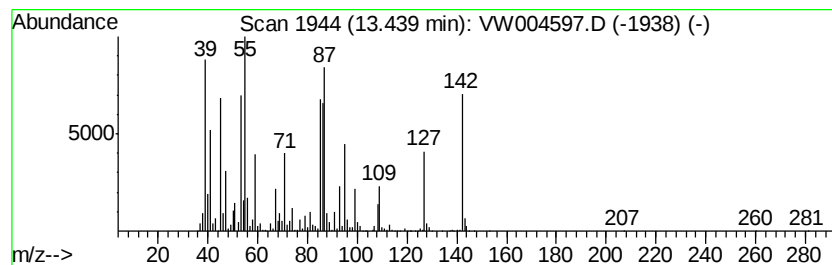
Instrument :
MSVOA_W
ClientSampleId :
JTY-SB-05-5-7

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, 3,3'-thiobis[2-m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.44	21.43 ug/l	1440140	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	3,4-Pentadienal, 2,2-dimethyl-	110 C7H10O	004058-51-9	38
4	2-Methyl-2-vinylloxirane	84 C5H8O	001838-94-4	37
5	2-Ethylprop-1-ene (1-3)sultine	132 C5H8O2S	084735-13-7	33



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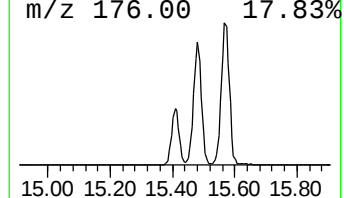
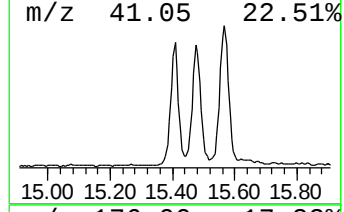
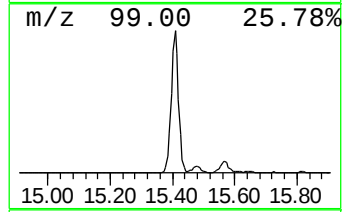
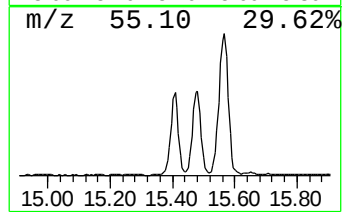
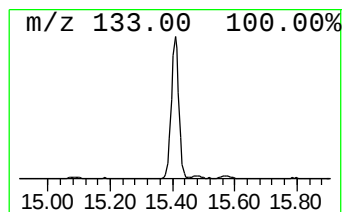
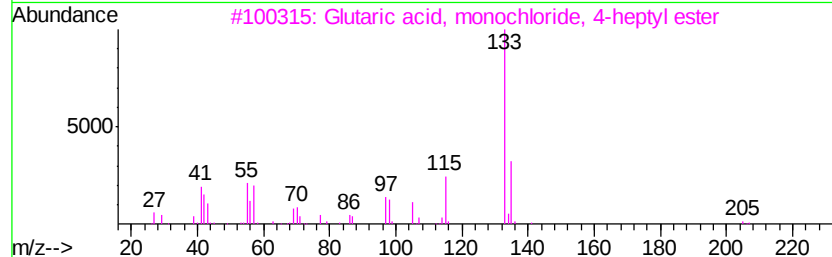
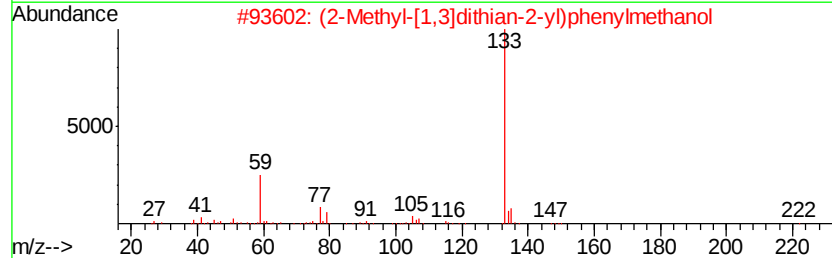
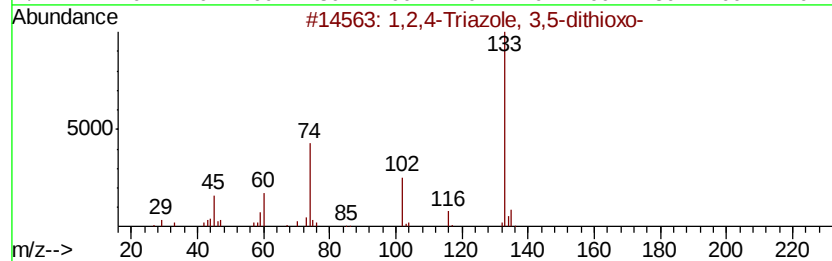
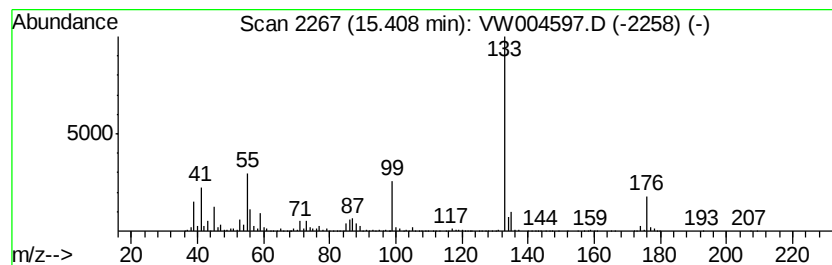
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 3 1,2,4-Triazole, 3,5-dithioxo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.41	12.55 ug/l	843462	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	50
2	(2-Methyl-[1,3]dithian-2-yl)phen...	240	C12H16OS2	078349-00-5	50
3	Glutaric acid, monochloride, 4-h...	248	C12H21ClO3	1000359-47-1	38
4	5-Aminoindazole	133	C7H7N3	019335-11-6	37
5	D-Alanine, N-(4-ethylbenzoyl)-, ...	319	C19H29NO3	1000354-08-9	28



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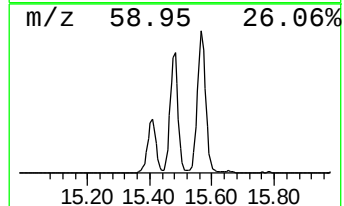
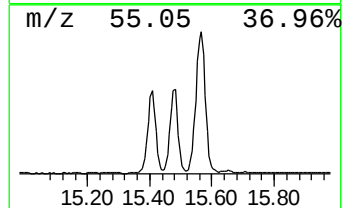
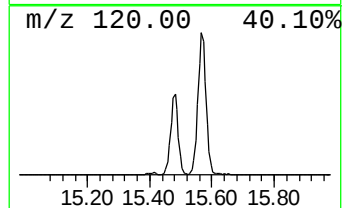
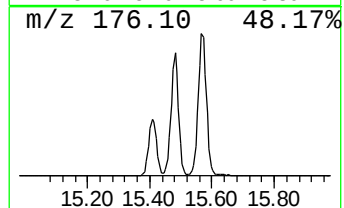
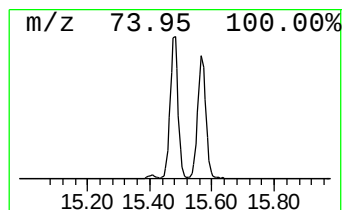
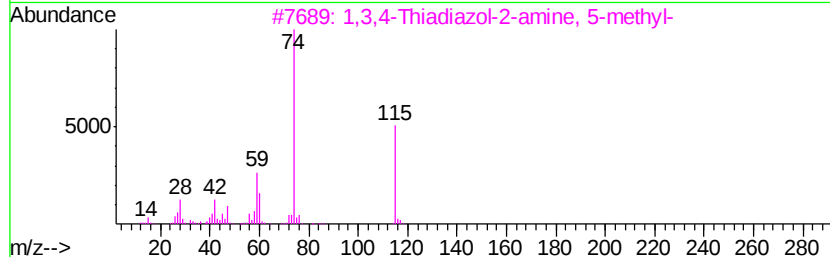
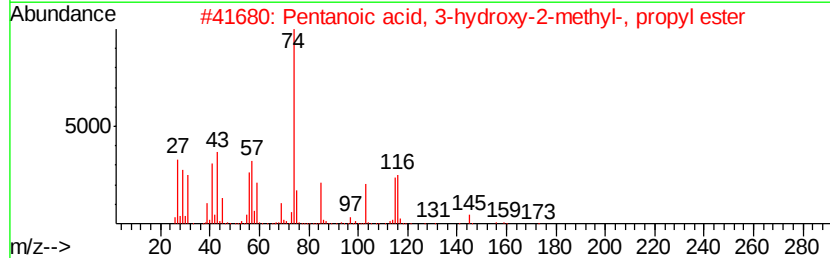
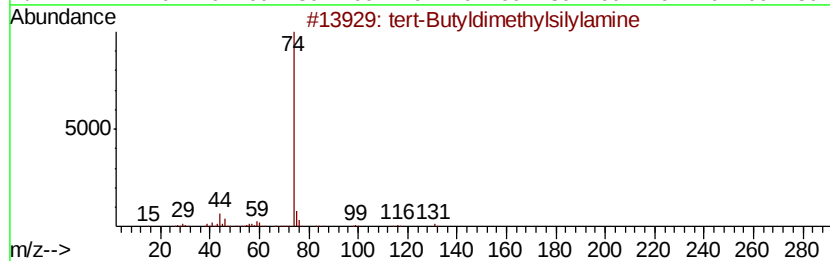
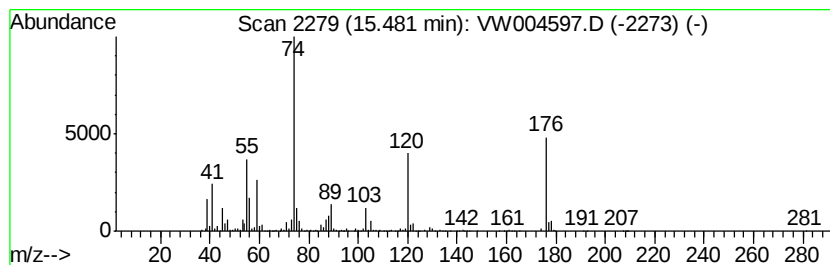
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown15.48 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.48	13.82 ug/l	928304	1,4-Dichlorobenzene-d4	13.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	tert-Butyldimethylsilylamine	131	C6H17NSi	1000366-62-1	27
2		Pentanoic acid, 3-hydroxy-2-meth...	174	C9H18O3	1000151-17-3	25
3		1,3,4-Thiadiazol-2-amine, 5-methyl-	115	C3H5N3S	000108-33-8	25
4		.alpha.-D-Glucopyranosiduronic a...	236	C9H16O7	031506-20-4	17
5		4,4,5-Trimethyl-6,8-dioxa-3-thia...	174	C8H14O2S	069697-53-6	17



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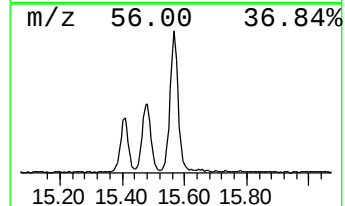
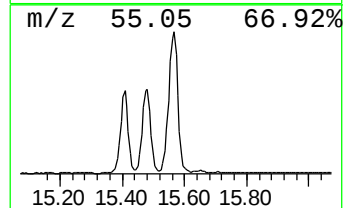
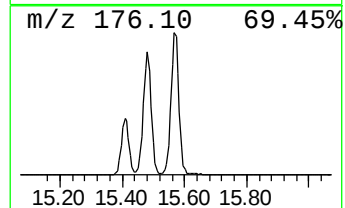
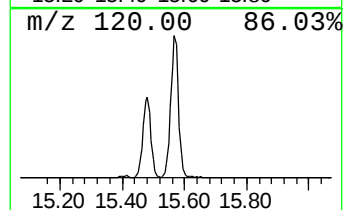
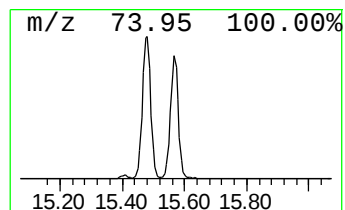
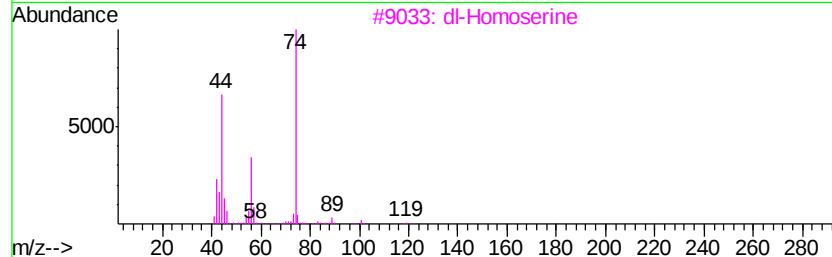
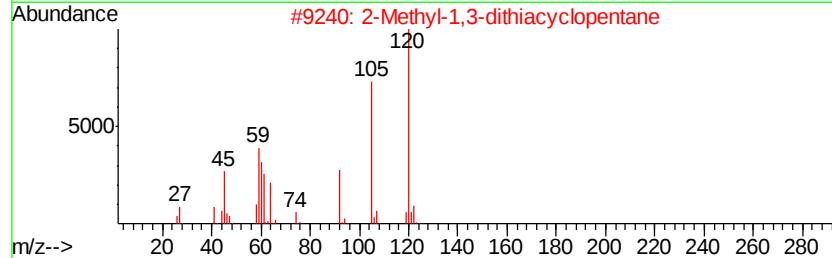
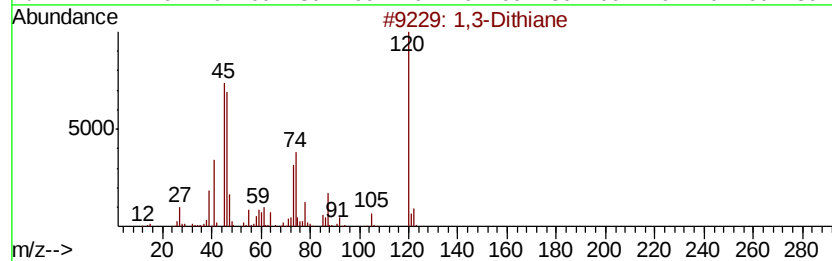
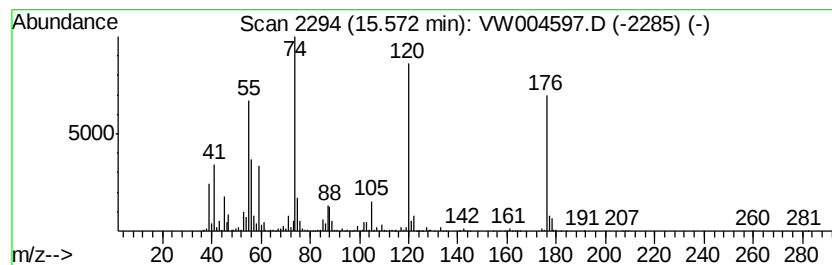
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Peak Number 5 unknown15.57 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.57	18.57 ug/l	1247920	1,4-Dichlorobenzene-d4	13.57	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dithiane	120	C4H8S2	000505-23-7	27
2	2-Methyl-1,3-dithiacyclopentane	120	C4H8S2	005616-51-3	22
3	dl-Homoserine	119	C4H9NO3	001927-25-9	16
4	N-Formyl-N'-methylsemithiocarbazide	133	C3H7N3OS	058064-52-1	14
5	1,3,4-Thiadiazol-2-amine, 5-methyl-	115	C3H5N3S	000108-33-8	12



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Propene, 3,3'-t...	13.44	21.4	ug/l	1440140	4	13.57	3359490	50.0
1,2,4-Triazole, 3...	15.41	12.6	ug/l	843462	4	13.57	3359490	50.0
unknown15.48	15.48	13.8	ug/l	928304	4	13.57	3359490	50.0
unknown15.57	15.57	18.6	ug/l	1247920	4	13.57	3359490	50.0