

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_Y\DATA\VY110719\
 Data File : VY000577.D
 Acq On : 07 Nov 2019 13:58
 Operator : SY/MD
 Sample : K5723-08
 Misc : 7.27G/5ML/MSVOA_Y/SOIL
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 9-A

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_Y\METHODS\82Y103019S.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	2.219	74	79	92	rBV	90550	149992	10.54%	1.375%
2	4.724	477	490	504	rBV2	21847	70384	4.94%	0.645%
3	5.755	645	659	672	rBV4	15392	50652	3.56%	0.464%
4	7.730	970	983	989	rBV2	189426	454507	31.93%	4.168%
5	7.803	989	995	1007	rVB	330082	738717	51.89%	6.774%
6	8.151	1043	1052	1064	rBV	198348	438248	30.78%	4.019%
7	8.699	1133	1142	1153	rBV	546430	1057158	74.26%	9.694%
8	10.181	1377	1385	1393	rBV	832664	1423622	100.00%	13.054%
9	11.491	1592	1600	1608	rBV	773139	1242769	87.30%	11.396%
10	12.479	1754	1762	1771	rBV	610736	940667	66.08%	8.626%
11	13.302	1891	1897	1902	rBV2	167395	257678	18.10%	2.363%
12	13.424	1911	1917	1925	rBV	734479	1108035	77.83%	10.160%
13	13.528	1930	1934	1941	rVB2	27784	44242	3.11%	0.406%
14	13.961	2002	2005	2010	rVB2	10181	16344	1.15%	0.150%
15	14.613	2109	2112	2117	rVB5	11833	15531	1.09%	0.142%
16	14.674	2117	2122	2128	rBV9	6644	14617	1.03%	0.134%
17	15.265	2204	2219	2225	rBV	524466	921650	64.74%	8.451%
18	15.332	2225	2230	2237	rVV	414784	680726	47.82%	6.242%
19	15.418	2237	2244	2253	rVB2	608019	1085926	76.28%	9.958%
20	16.009	2336	2341	2351	rBV2	19168	45497	3.20%	0.417%
21	16.155	2361	2365	2371	rVB5	12958	22698	1.59%	0.208%
22	16.289	2382	2387	2391	rBV2	18565	32085	2.25%	0.294%
23	16.363	2394	2399	2404	rVB4	21622	37246	2.62%	0.342%
24	16.484	2411	2419	2423	rBV9	15063	39983	2.81%	0.367%
25	16.747	2458	2462	2472	rVB9	7556	16549	1.16%	0.152%

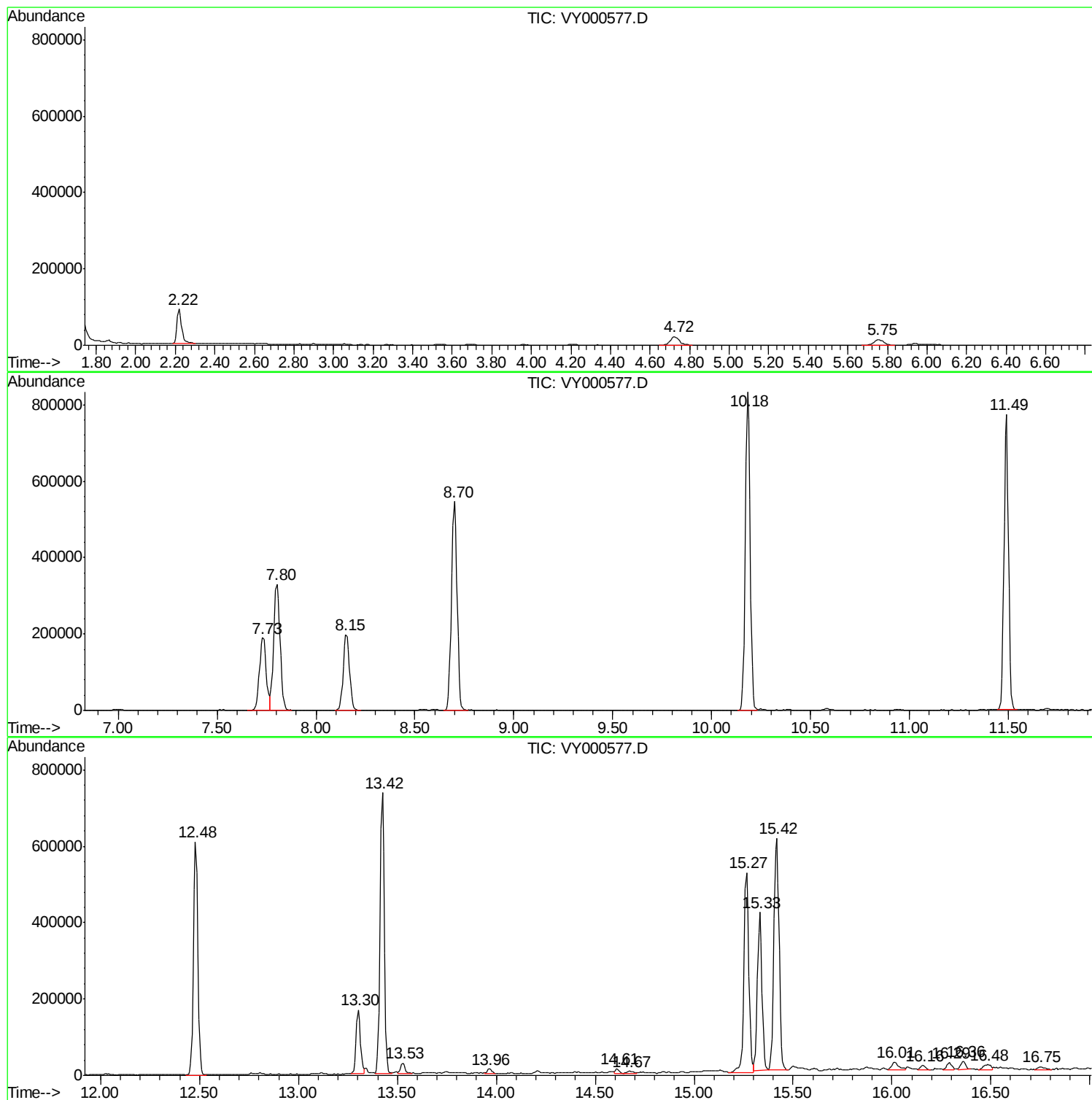
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Quant Method : Z:\V0ASRV\HPCHEM1\MSV0A_Y\METHODS\82Y103019S.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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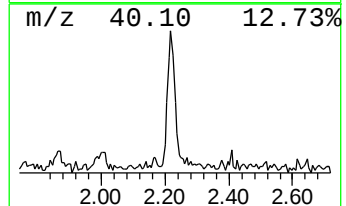
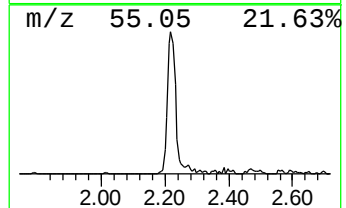
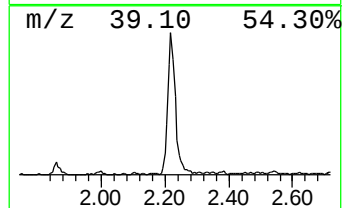
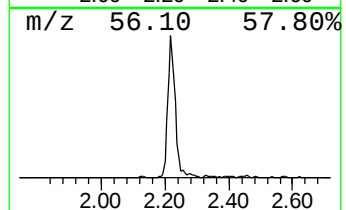
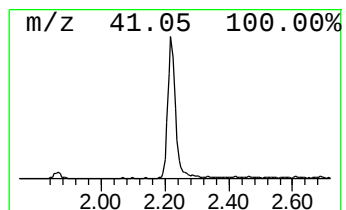
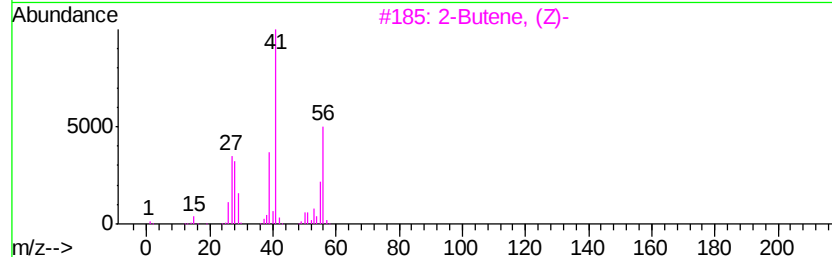
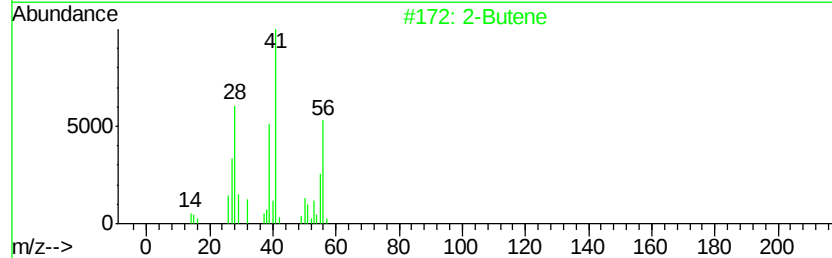
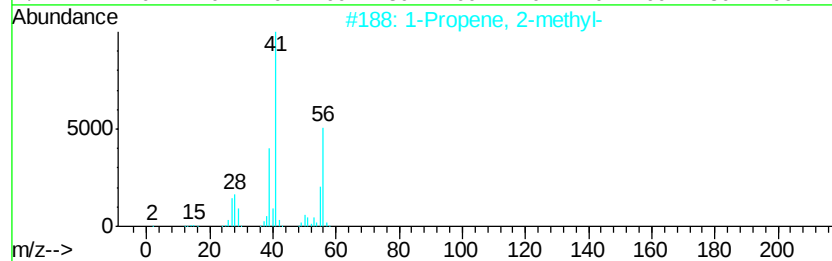
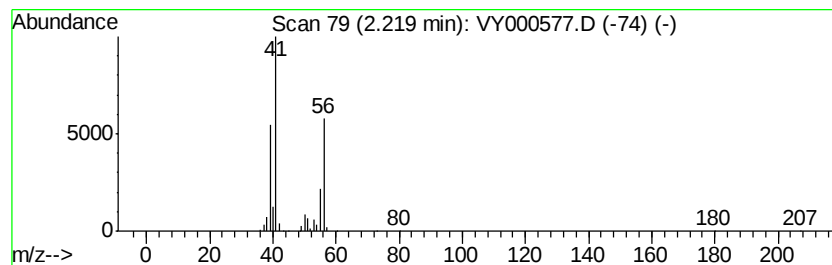
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_Y\METHODS\82Y103019S.M
Quant Title : SW846 8260

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

Peak Number 1 1-Propene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	10.15 ug/l	149992	Pentafluorobenzene	7.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Propene, 2-methyl-	56	C4H8	000115-11-7	90
2		2-Butene	56	C4H8	000107-01-7	50
3		2-Butene, (Z)-	56	C4H8	000590-18-1	49
4		1-Butene	56	C4H8	000106-98-9	49
5		Cyclobutane	56	C4H8	000287-23-0	49



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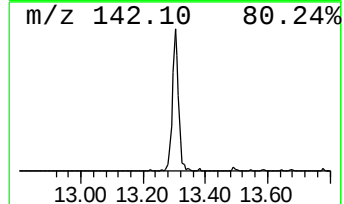
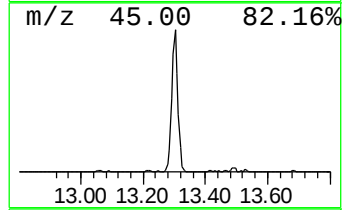
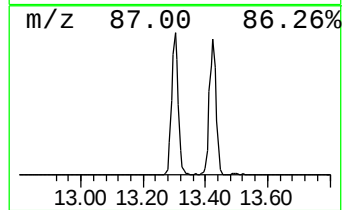
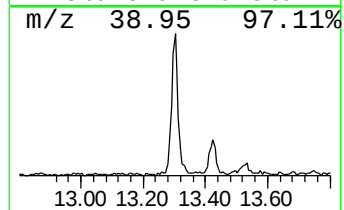
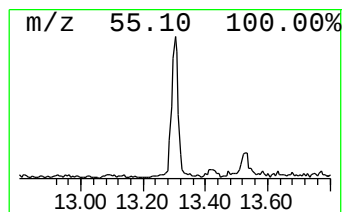
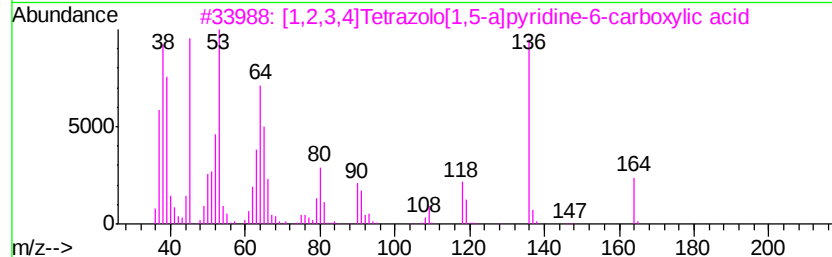
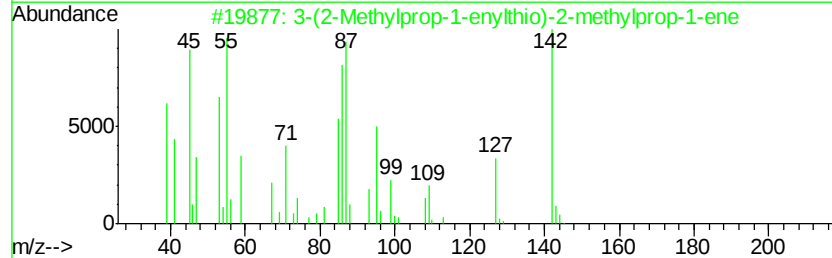
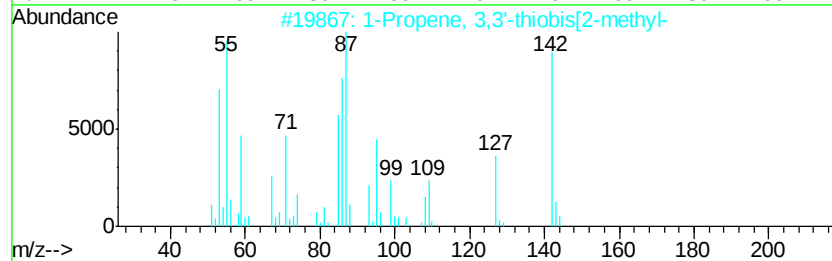
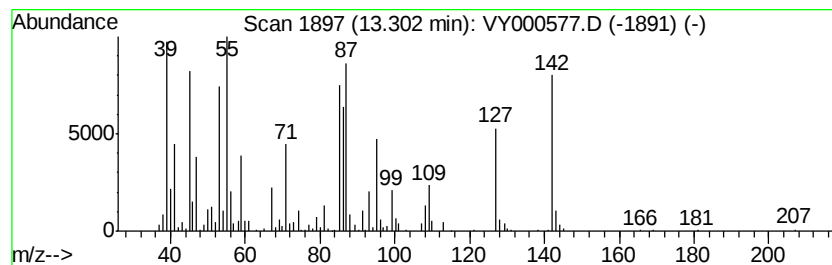
Instrument :
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ClientSampleId :
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Peak Number 2 1-Propene, 3,3'-thiobis[2-m... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.30	11.63 ug/l	257678	1,4-Dichlorobenzene-d4	13.42		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 3,3'-thiobis[2-methyl-	142	C8H14S	023973-54-8	98	
2	3-(2-Methylprop-1-enylthio)-2-me...	142	C8H14S	1000122-39-8	98	
3	[1,2,3,4]Tetrazolo[1,5-a]pyridin...	164	C6H4N4O2	1000362-60-7	35	
4	2-Ethylprop-1-ene (1-3)sultine	132	C5H8O2S	084735-13-7	33	
5	5.alpha.-Androstan-16-one, cycli...	350	C21H34S2	002759-86-6	23	



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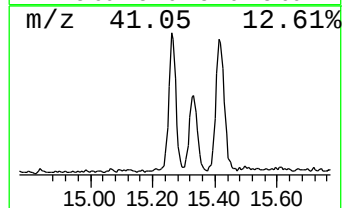
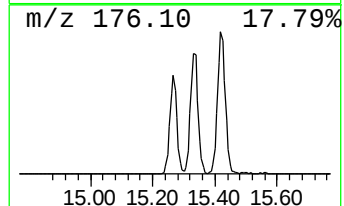
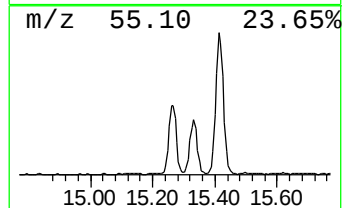
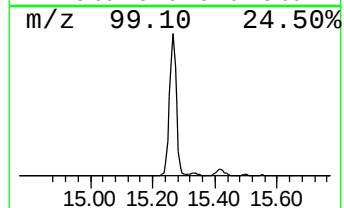
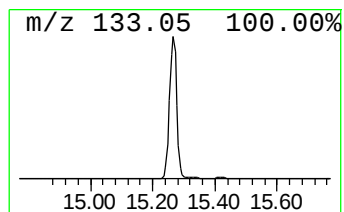
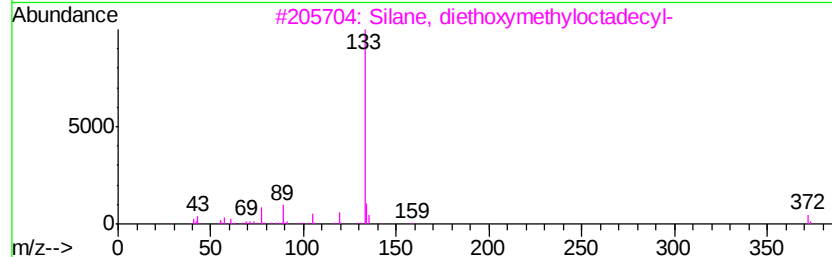
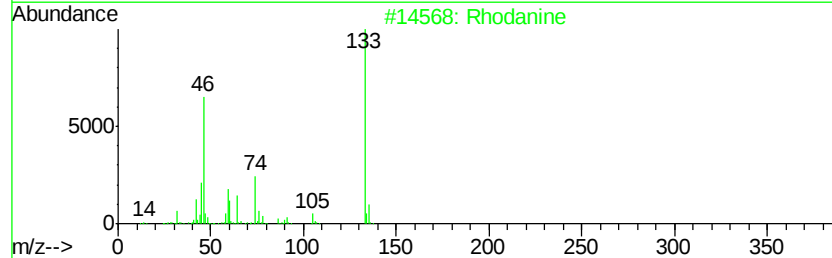
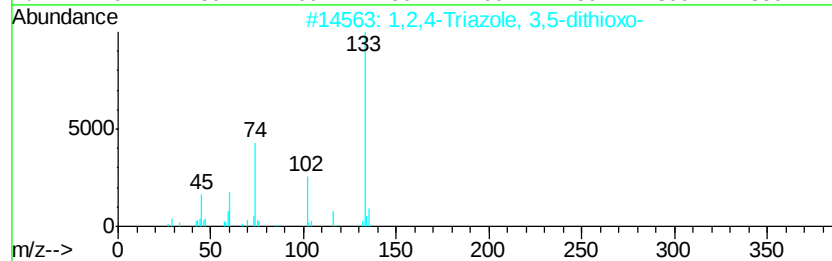
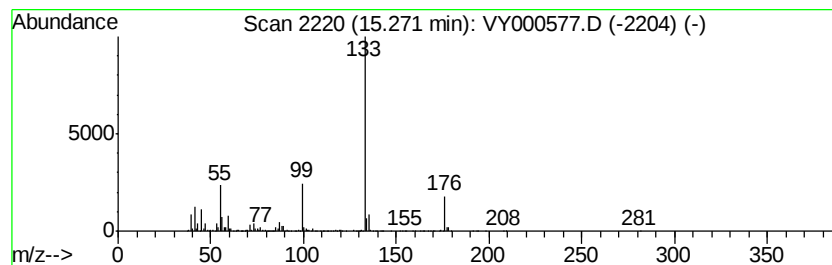
Instrument :
MSV0A_Y
ClientSampleId :
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Peak Number 3 1,2,4-Triazole, 3,5-dithioxo- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.27	41.59 ug/l	921650	1,4-Dichlorobenzene-d4	13.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Triazole, 3,5-dithioxo-	133	C2H3N3S2	005650-03-3	58
2	Rhodanine	133	C3H3NOS2	000141-84-4	47
3	Silane, diethoxymethyloctadecyl-	386	C23H50O2Si	067859-75-0	38
4	Dipropyl chlorothiophosphate	216	C6H14ClO2PS	1000370-34-3	33
5	4-Ethylbenzoic acid, 2-formyl-4,...	322	C16H12Cl2O3	1000331-31-6	28



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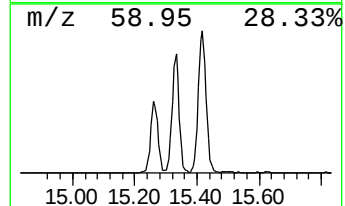
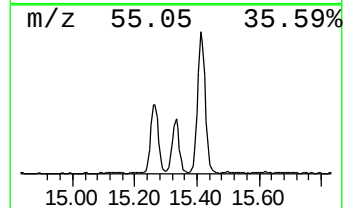
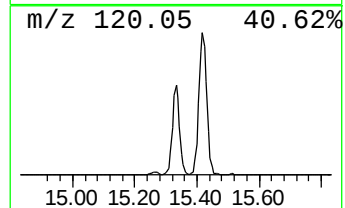
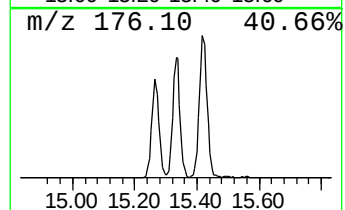
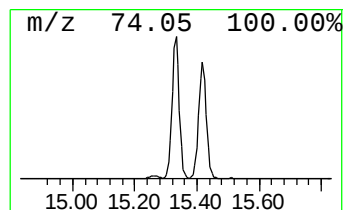
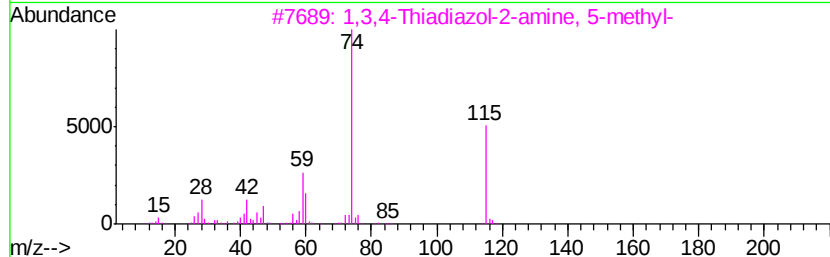
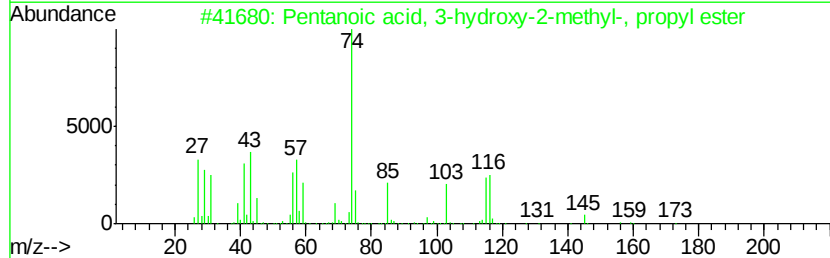
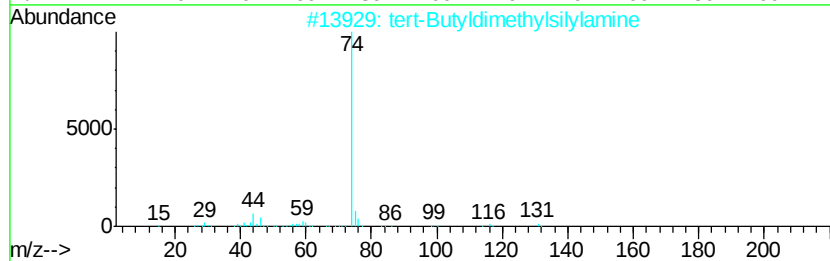
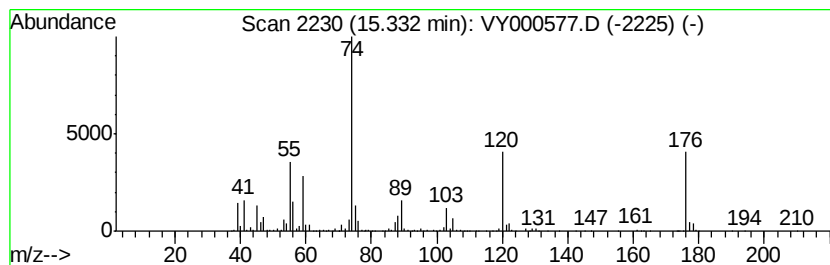
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 unknown15.33 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.33	30.72 ug/l	680726	1,4-Dichlorobenzene-d4	13.42

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	23
3		1,3,4-Thiadiazol-2-amine, 5-methyl-	115	C3H5N3S	000108-33-8	17
4		Heptanoic acid, methyl ester	144	C8H16O2	000106-73-0	17
5		Phenylalanine	165	C9H11NO2	000063-91-2	17



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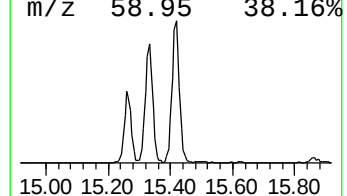
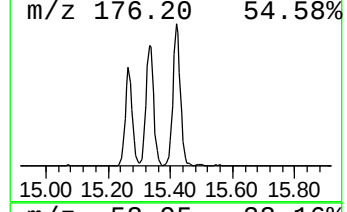
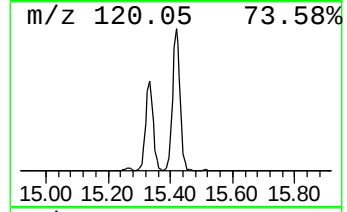
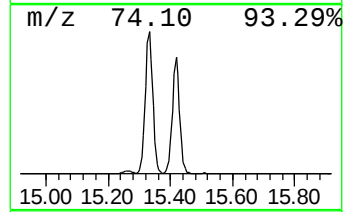
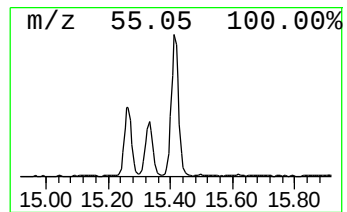
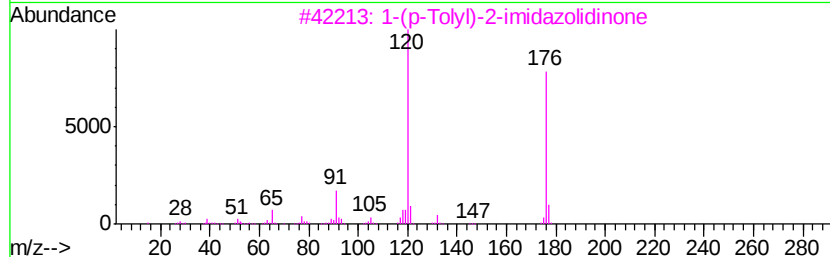
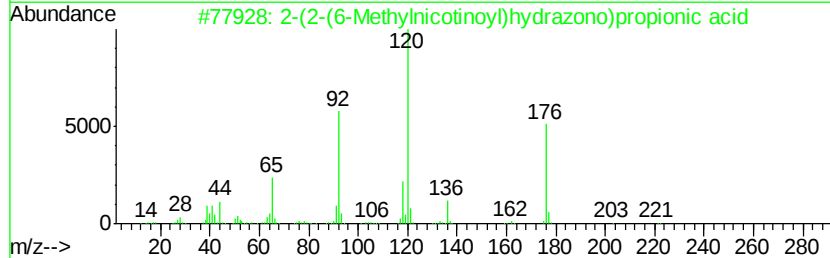
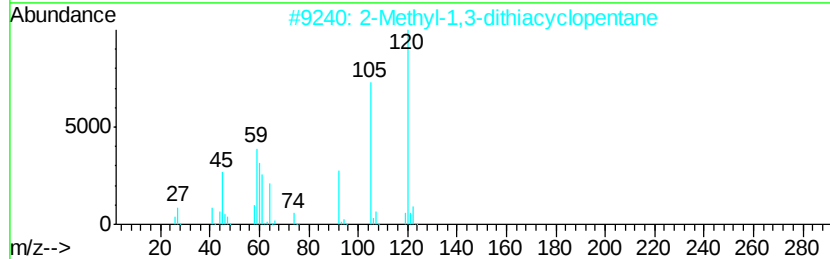
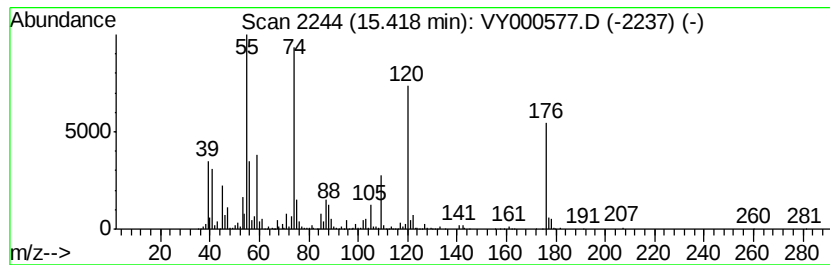
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ClientSampled :
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Quant Title : SW846 8260

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

Peak Number 5 2-Methyl-1,3-dithiacyclopentane... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.42	49.00 ug/l	1085930	1,4-Dichlorobenzene-d4	13.42
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Methyl-1,3-dithiacyclopentane	120 C4H8S2	005616-51-3	25
2	2-(2-(6-Methylnicotinoyl)hydrazono...	221 C10H11N3O3	1000244-73-4	22
3	1-(p-Tolyl)-2-imidazolidinone	176 C10H12N2O	090917-76-3	22
4	1,3-Dithiane	120 C4H8S2	000505-23-7	18
5	1,3,4-Thiadiazol-2-amine, 5-methyl-	115 C3H5N3S	000108-33-8	14



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Propene, 2-methyl-	2.22	10.2	ug/l	149992	1	7.80	738717	50.0
1-Propene, 3,3'-t...	13.30	11.6	ug/l	257678	4	13.42	1108040	50.0
1,2,4-Triazole, 3...	15.27	41.6	ug/l	921650	4	13.42	1108040	50.0
unknown15.33	15.33	30.7	ug/l	680726	4	13.42	1108040	50.0
2-Methyl-1,3-dith...	15.42	49.0	ug/l	1085930	4	13.42	1108040	50.0