

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_Y\DATA\VY110719\
 Data File : VY000593.D
 Acq On : 07 Nov 2019 19:54
 Operator : SY/MD
 Sample : K5723-10
 Misc : 6.70G/5ML/MSVOA_Y/SOIL
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 9-C

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 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_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	73	79	88	rBV3	24184	47027	3.97%	0.501%
2	4.725	480	490	500	rBV3	14957	46499	3.92%	0.495%
3	5.755	648	659	671	rBV3	25247	76021	6.42%	0.809%
4	7.730	972	983	989	rBV	157340	365997	30.89%	3.896%
5	7.803	989	995	1007	rVB	262637	589713	49.77%	6.278%
6	8.157	1043	1053	1066	rBV	153752	350898	29.61%	3.735%
7	8.699	1133	1142	1153	rBV	431971	843129	71.15%	8.975%
8	10.181	1377	1385	1392	rBV	666895	1127165	95.12%	11.999%
9	11.492	1591	1600	1611	rBV	608719	979743	82.68%	10.430%
10	12.479	1755	1762	1773	rVB	461635	720396	60.80%	7.669%
11	13.302	1887	1897	1905	rBV	200170	312834	26.40%	3.330%
12	13.424	1909	1917	1924	rVV	547972	839011	70.81%	8.931%
13	13.528	1929	1934	1944	rVB	37634	62658	5.29%	0.667%
14	13.967	2000	2006	2014	rBV4	8580	18003	1.52%	0.192%
15	14.583	2101	2107	2110	rBV6	11448	22015	1.86%	0.234%
16	14.613	2110	2112	2117	rVB4	11890	13657	1.15%	0.145%
17	15.265	2210	2219	2224	rBV	501539	827385	69.83%	8.808%
18	15.332	2224	2230	2237	rVV	449126	752562	63.51%	8.011%
19	15.418	2237	2244	2254	rVB2	674262	1184937	100.00%	12.614%
20	15.503	2254	2258	2261	rBV6	9097	13042	1.10%	0.139%
21	15.881	2315	2320	2327	rBV10	8236	15818	1.33%	0.168%
22	16.009	2336	2341	2349	rBV2	22831	44607	3.76%	0.475%
23	16.082	2351	2353	2359	rVB7	7702	12103	1.02%	0.129%
24	16.155	2361	2365	2370	rBV7	7403	13459	1.14%	0.143%
25	16.283	2382	2386	2392	rVB4	14626	27179	2.29%	0.289%
26	16.357	2393	2398	2403	rBV2	25036	44248	3.73%	0.471%
27	16.479	2410	2418	2433	rBV2	12487	43744	3.69%	0.466%

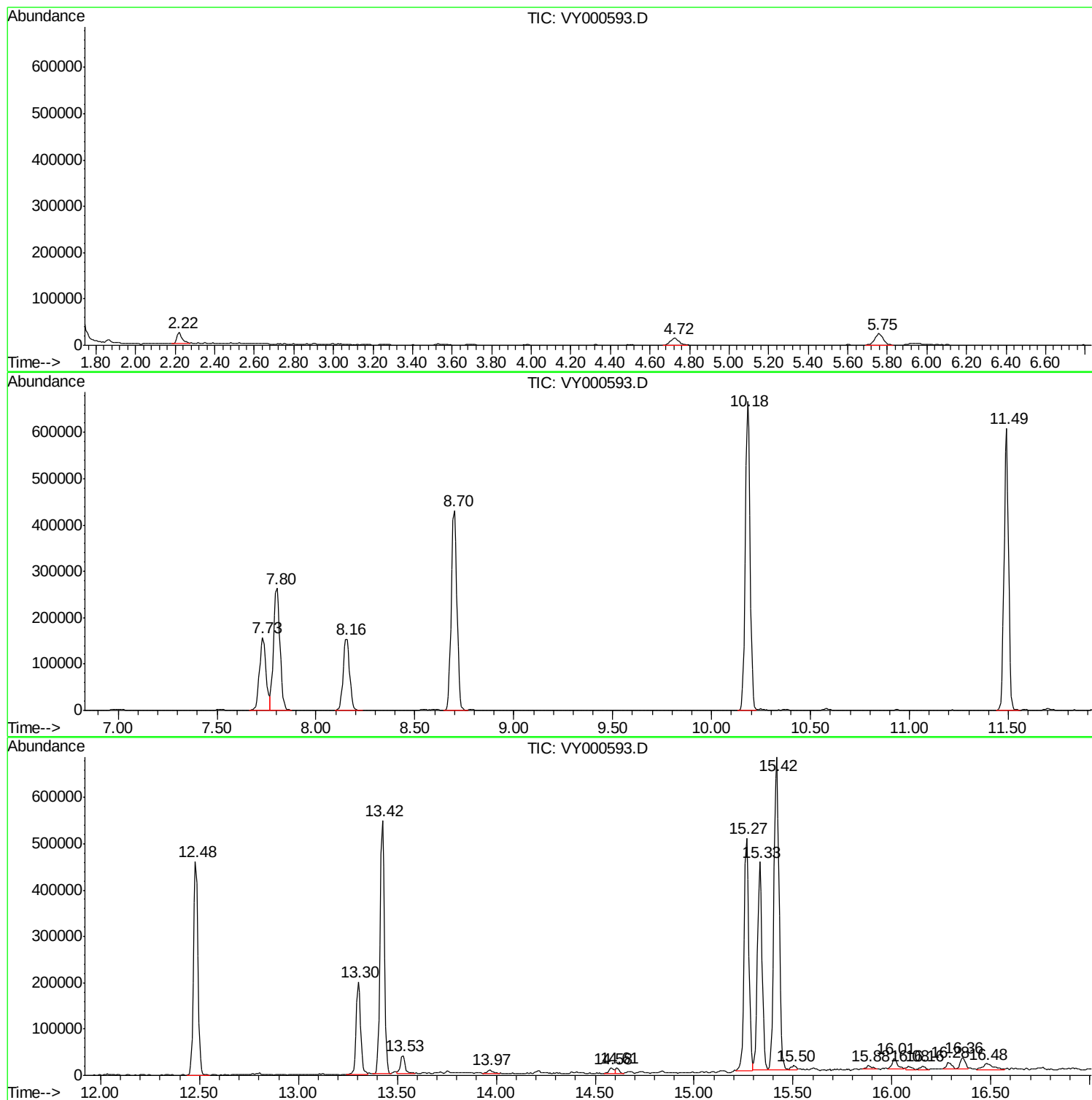
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Quant Method : Z:\V0ASRV\HPCHEM1\MSV0A_Y\METHODS\82Y103019S.M
Quant Title : SW846 8260

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



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Instrument :
MSV0A_Y
ClientSampled :
9-C

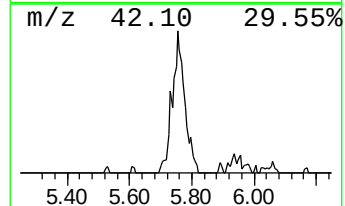
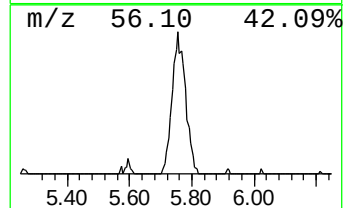
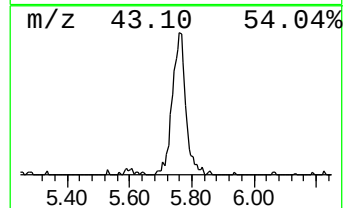
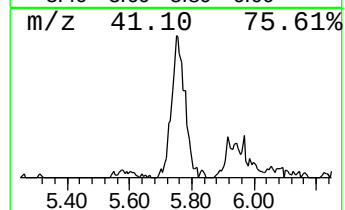
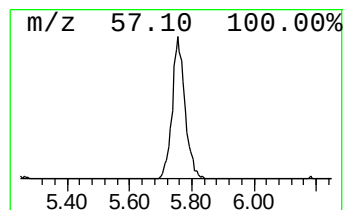
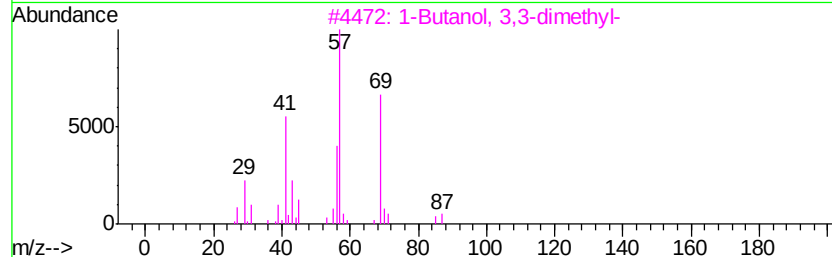
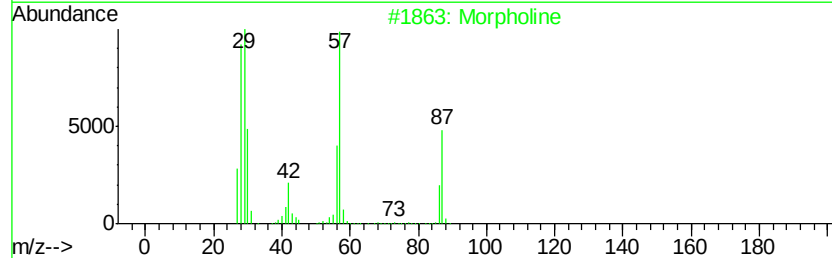
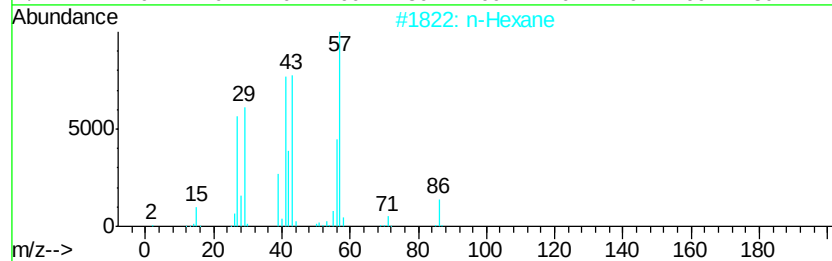
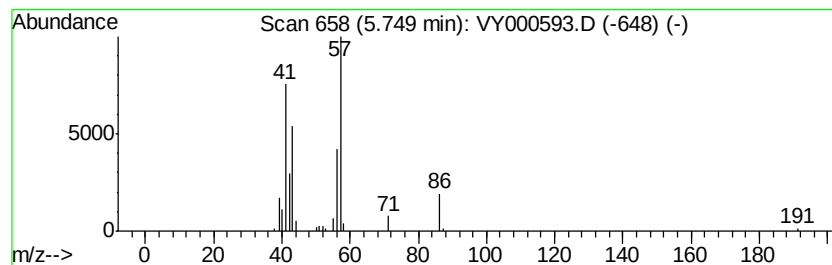
Quant Method : Z:\V0ASRV\HPCHEM1\MSV0A_Y\METHODS\82Y103019S.M
Quant Title : SW846 8260

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

Peak Number 1 n-Hexane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.75	6.45 ug/l	76021	Pentafluorobenzene	7.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexane	86	C6H14	000110-54-3	78
2		Morpholine	87	C4H9NO	000110-91-8	36
3		1-Butanol, 3,3-dimethyl-	102	C6H14O	000624-95-3	33
4		Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	28
5		Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	27



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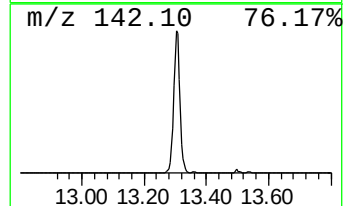
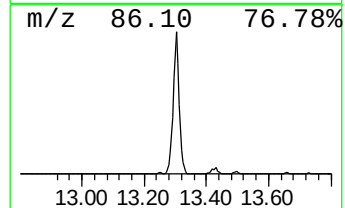
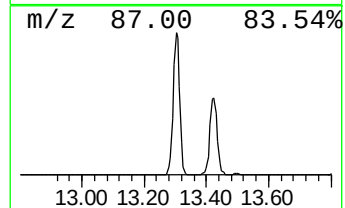
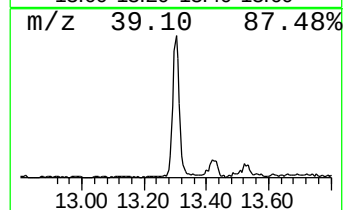
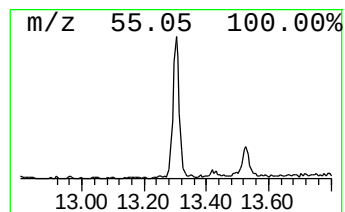
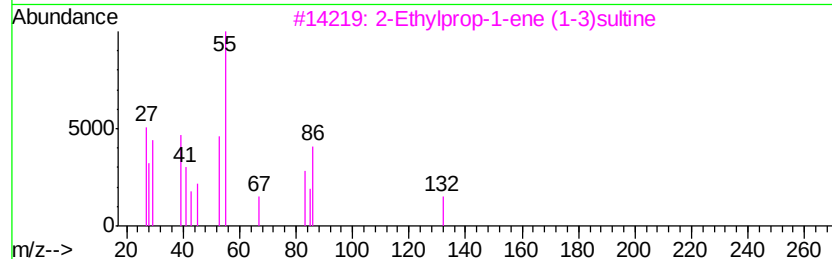
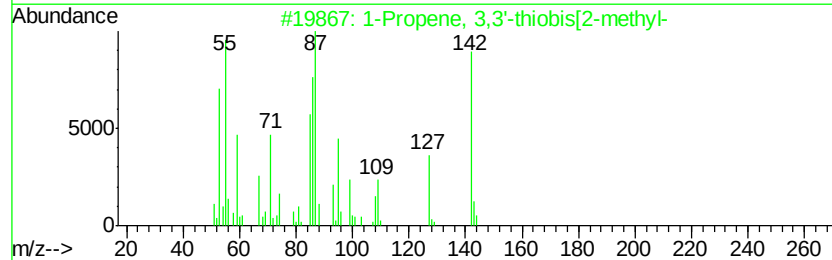
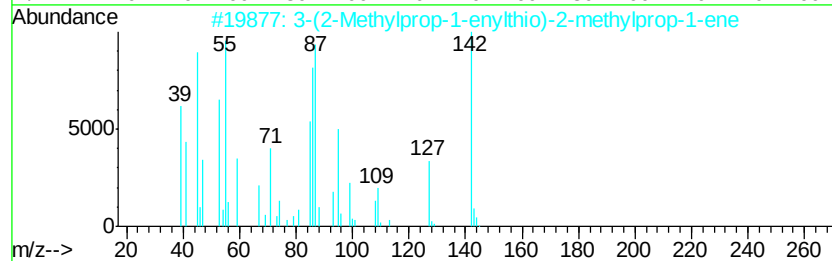
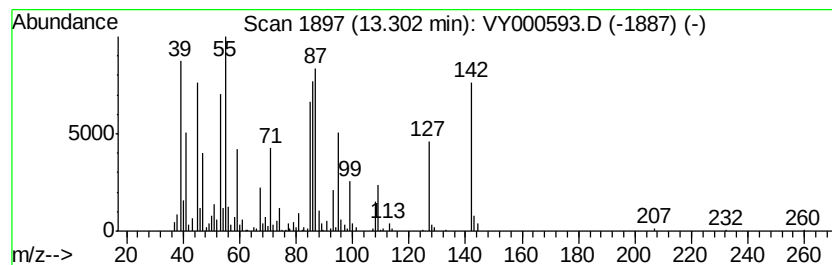
Instrument :
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ClientSampleId :
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Peak Number 2 3-(2-Methylprop-1-enylthio)... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.30	18.64 ug/l	312834	1,4-Dichlorobenzene-d4	13.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(2-Methylprop-1-enylthio)-2-me...	142	C8H14S	1000122-39-8	95
2	1-Propene, 3,3'-thiobis[2-methyl-	142	C8H14S	023973-54-8	95
3	2-Ethylprop-1-ene (1-3)sultine	132	C5H8O2S	084735-13-7	28
4	Tetrazole-5-thiole, 1-allyl-	142	C4H6N4S	007624-33-1	25
5	5-Hexenoic acid, 5-bromo-, methy...	206	C7H11BrO2	279214-92-5	25



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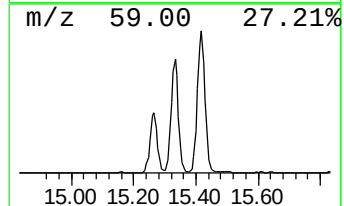
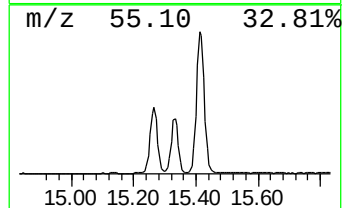
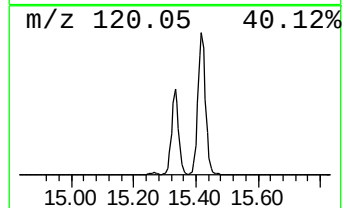
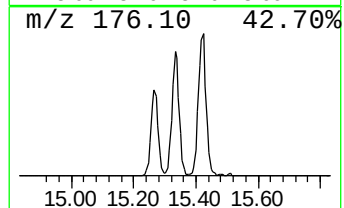
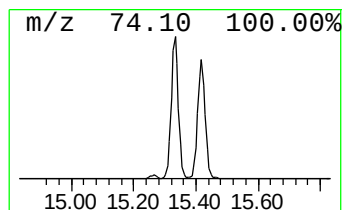
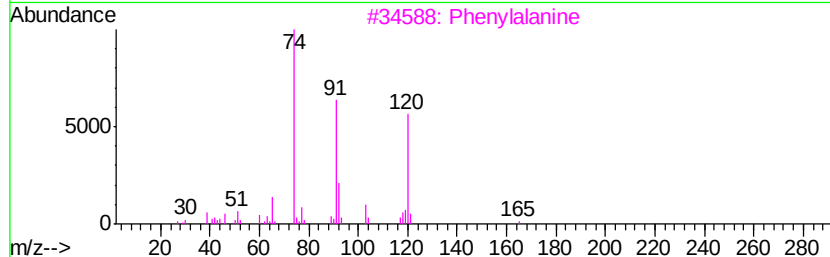
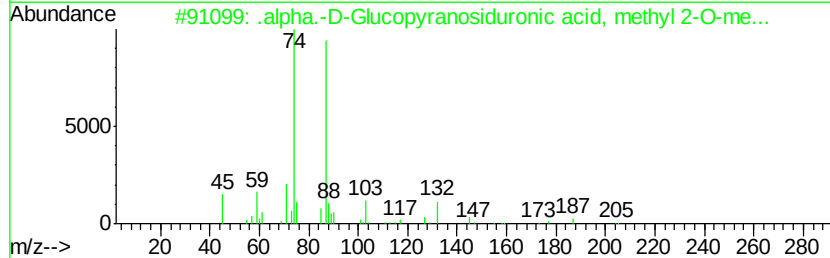
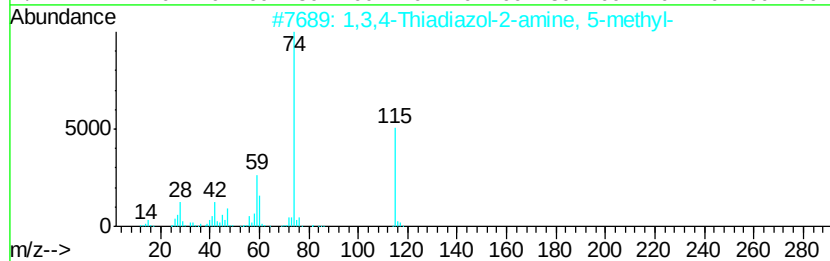
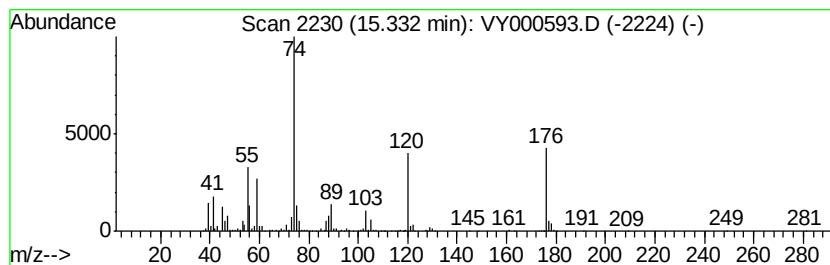
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Peak Number 3 unknown15.33 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.33	44.85 ug/l	752562	1,4-Dichlorobenzene-d4	13.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,4-Thiadiazol-2-amine, 5-methyl-	115	C3H5N3S	000108-33-8	25
2		.alpha.-D-Glucopyranosiduronic a...	236	C9H16O7	031506-20-4	17
3		Phenylalanine	165	C9H11NO2	000063-91-2	17
4		Heptanoic acid, methyl ester	144	C8H16O2	000106-73-0	17
5		1,3,2-Oxathioborolane, 2-ethyl-5...	130	C5H11BO5	1000163-05-5	16



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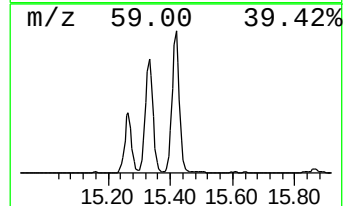
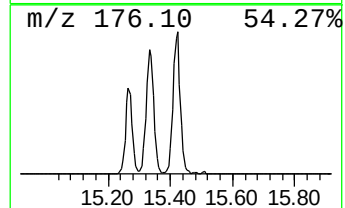
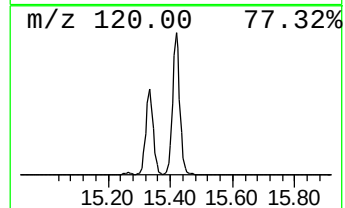
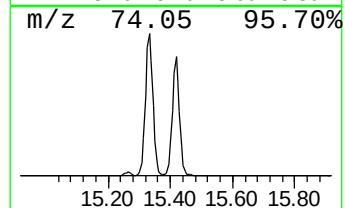
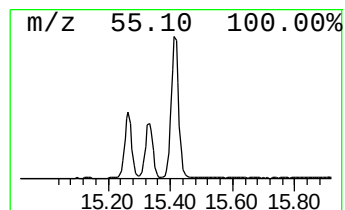
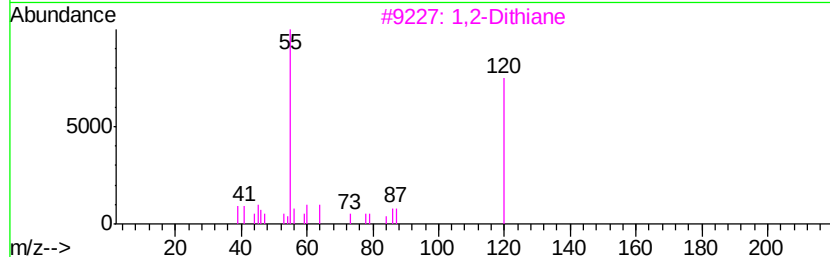
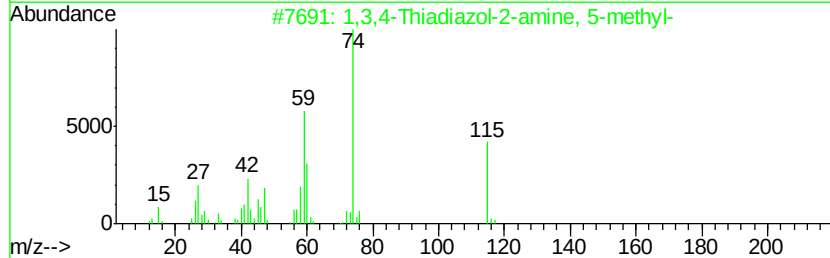
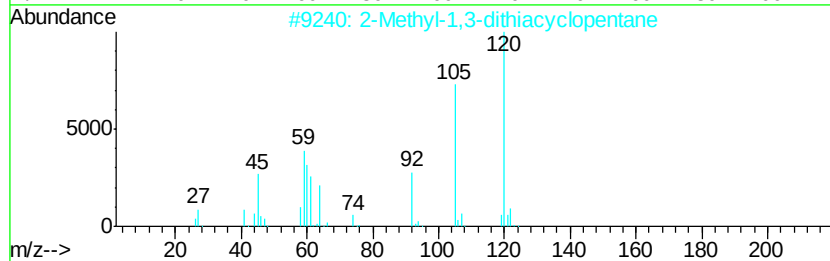
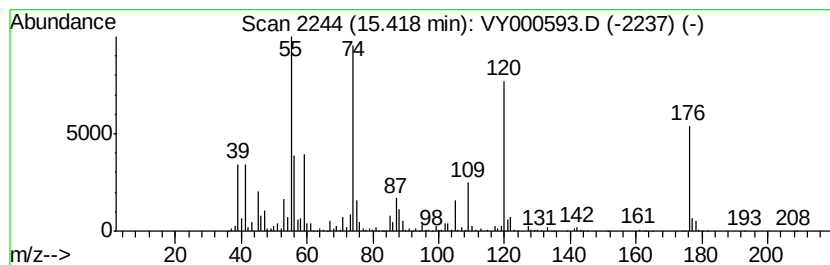
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Peak Number 4 unknown15.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.42	70.62 ug/l	1184940	1,4-Dichlorobenzene-d4	13.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyl-1,3-dithiacyclopentane	120	C4H8S2	005616-51-3	25	
2	1,3,4-Thiadiazol-2-amine, 5-methyl-	115	C3H5N3S	000108-33-8	22	
3	1,2-Dithiane	120	C4H8S2	000505-20-4	22	
4	1,3-Dithiane	120	C4H8S2	000505-23-7	22	
5	Phenylalanine	165	C9H11NO2	000063-91-2	17	



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexane	5.75	6.5	ug/l	76021	1	7.80	589713	50.0
3-(2-Methylprop-1...	13.30	18.6	ug/l	312834	4	13.42	839011	50.0
unknown15.33	15.33	44.9	ug/l	752562	4	13.42	839011	50.0
unknown15.42	15.42	70.6	ug/l	1184940	4	13.42	839011	50.0