

Data Path : Z:\VOASRV\HPCHEM1\MSVOA Y\DATA\VY110819\
 Data File : VY000627.D
 Acq On : 08 Nov 2019 18:54
 Operator : SY/MD
 Sample : K5723-15
 Misc : 3.96G/5ML/MSVOA Y/SOIL
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 10-D

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	83	rBV2	7576	15478	1.26%	0.193%
2	4.731	477	491	503	rBV3	24374	76839	6.24%	0.957%
3	5.761	649	660	670	rBV3	16644	48900	3.97%	0.609%
4	7.730	972	983	989	rBV2	164286	398131	32.33%	4.960%
5	7.803	989	995	1006	rVB	284942	638235	51.83%	7.952%
6	8.157	1043	1053	1064	rBV	172593	378990	30.78%	4.722%
7	8.699	1132	1142	1152	rBV	469855	912035	74.06%	11.363%
8	10.181	1377	1385	1394	rBV	717717	1231443	100.00%	15.343%
9	11.492	1592	1600	1609	rBV	691890	1111852	90.29%	13.853%
10	12.333	1733	1738	1745	rBV4	7956	14020	1.14%	0.175%
11	12.479	1755	1762	1771	rVB	532673	833233	67.66%	10.381%
12	13.302	1891	1897	1907	rBV2	37015	60000	4.87%	0.748%
13	13.424	1910	1917	1924	rBV	702238	1072515	87.09%	13.363%
14	14.211	2029	2046	2062	rBV6	77616	356323	28.94%	4.439%
15	15.265	2210	2219	2225	rBV2	166690	317742	25.80%	3.959%
16	15.332	2225	2230	2236	rVV2	109822	198890	16.15%	2.478%
17	15.418	2237	2244	2251	rVB2	177089	318042	25.83%	3.963%
18	15.875	2315	2319	2327	rVB6	9224	20310	1.65%	0.253%
19	16.283	2380	2386	2393	rVB4	10806	23242	1.89%	0.290%

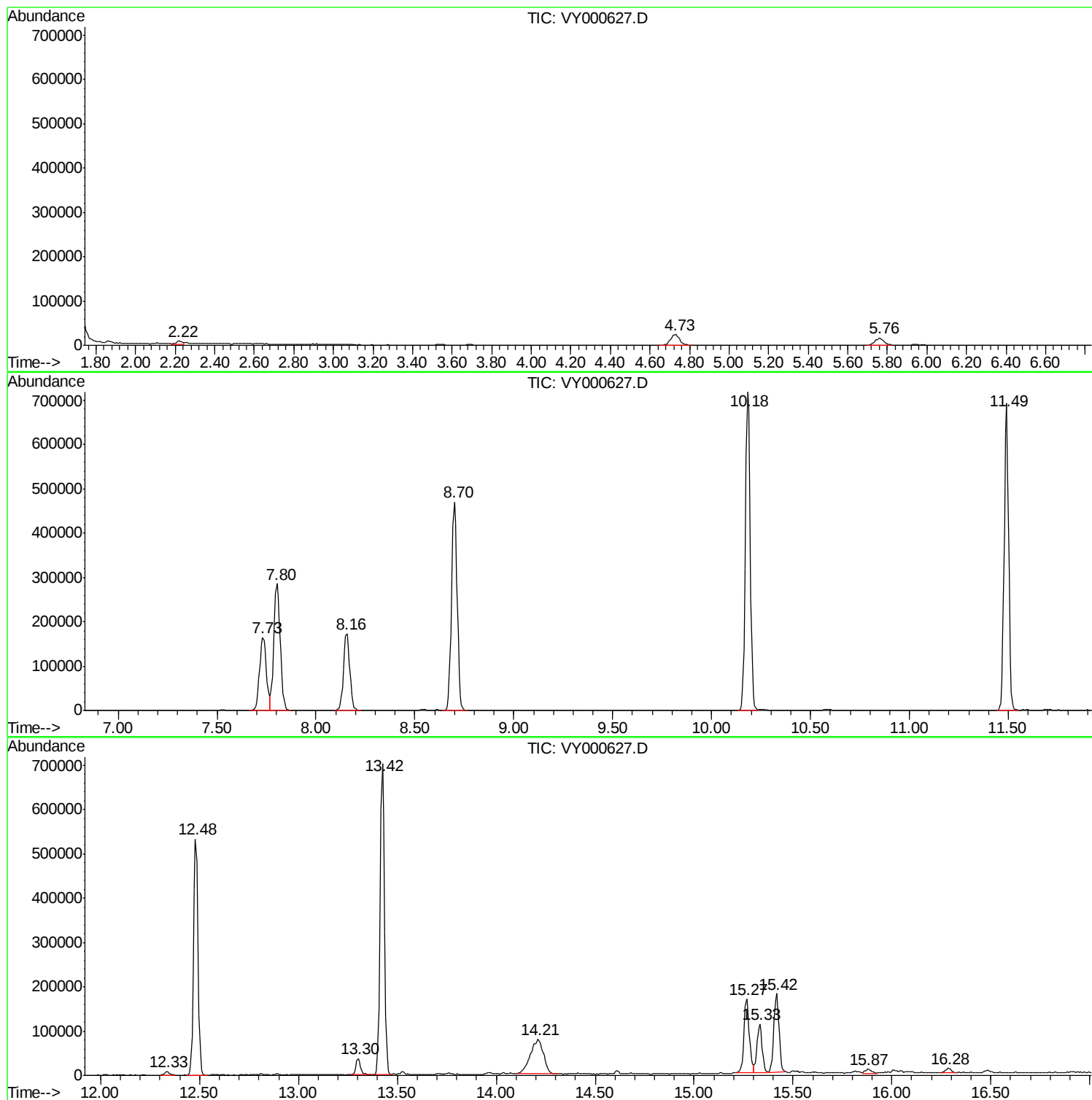
Sum of corrected areas: 8026220

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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



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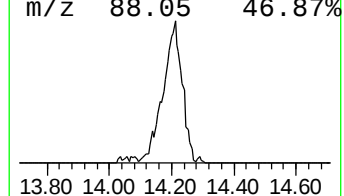
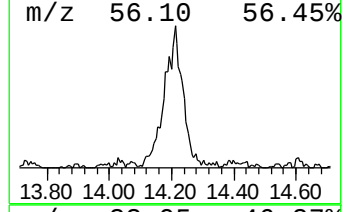
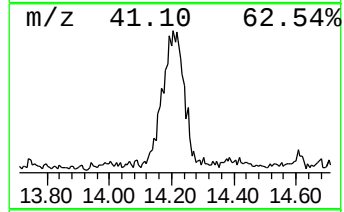
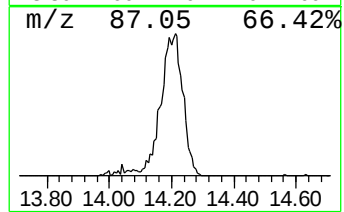
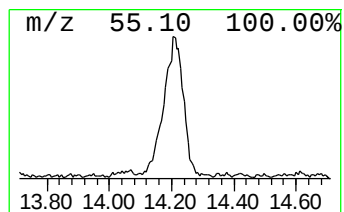
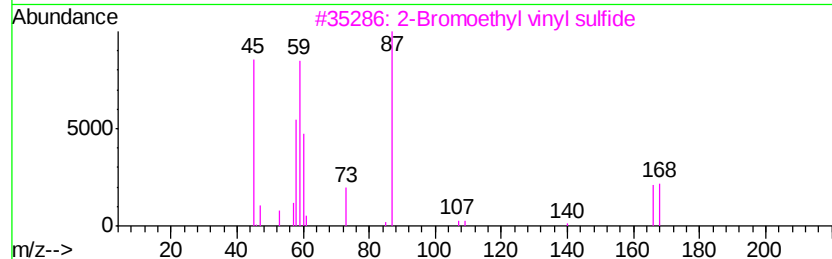
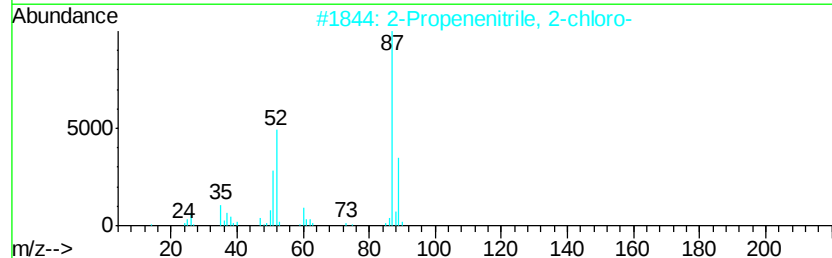
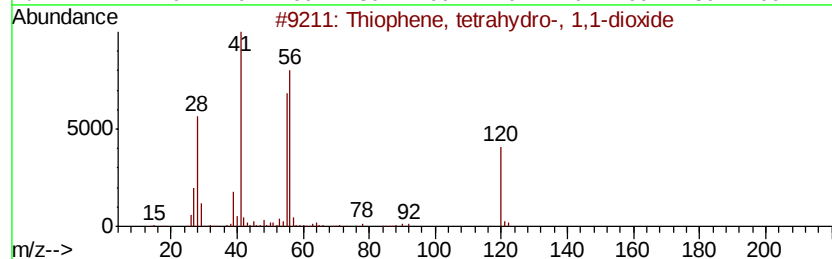
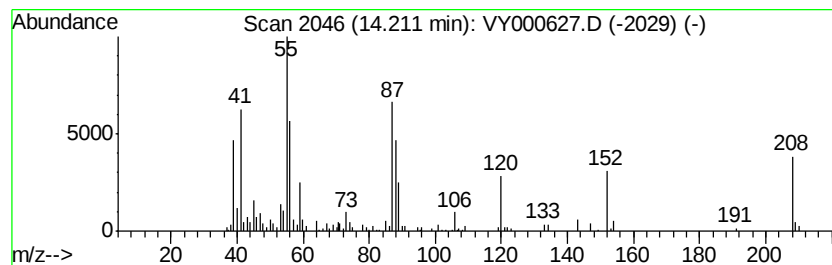
Instrument :
MSVOA_Y
ClientSampled :
10-D

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 unknown14.21 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.21	16.61 ug/l	356323	1,4-Dichlorobenzene-d4	13.42
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Thiophene, tetrahydro-, 1,1-dioxide	120 C4H8O2S	000126-33-0 11
2		2-Propenenitrile, 2-chloro-	87 C3H2ClN	000920-37-6 11
3		2-Bromoethyl vinyl sulfide	166 C4H7BrS	1000226-90-6 10
4		1,2,4-Trithiolane, 3,5-bis(1-met...	208 C8H16S3	054934-99-5 10
5		1,3-Dioxolane, 2-butyl-4-methyl-	144 C8H16O2	074094-60-3 10



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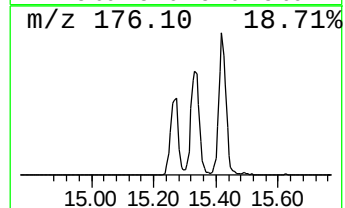
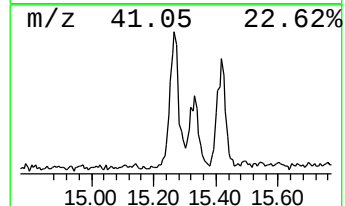
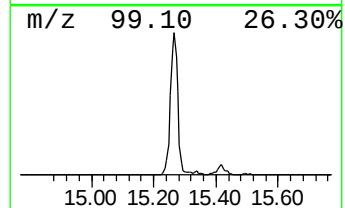
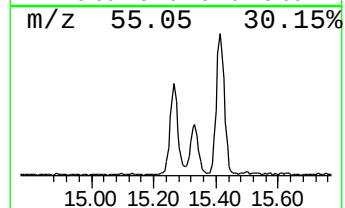
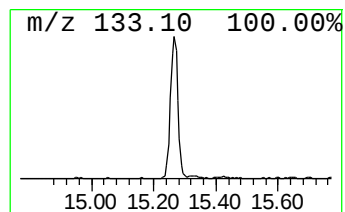
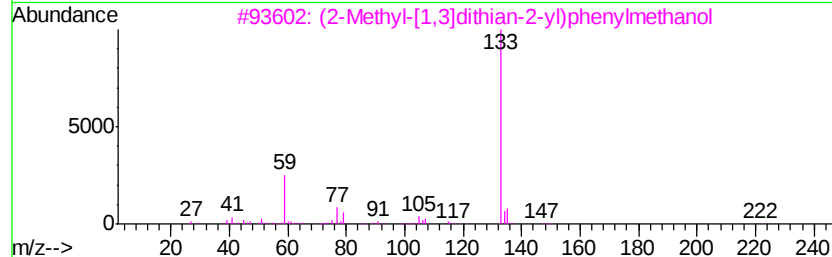
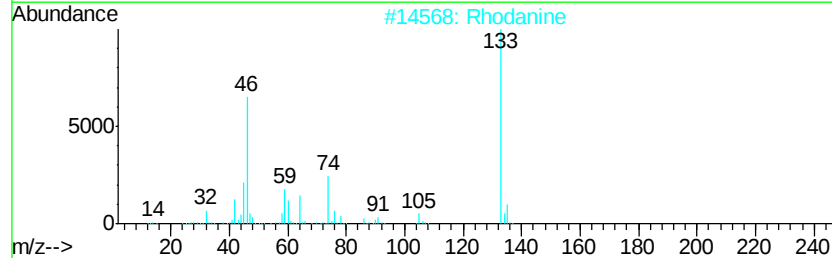
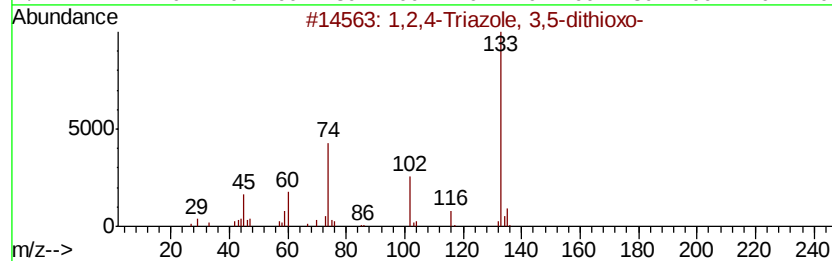
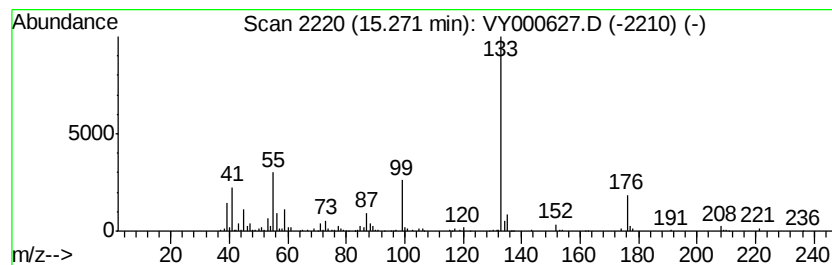
Instrument :
MSVOA_Y
ClientSampleId :
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Quant Title : SW846 8260

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

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.27	14.81 ug/l	317742	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	58	
3	(2-Methyl-[1,3]dithian-2-yl)phen...	240	C12H16OS2	078349-00-5	50	
4	1,3,4-Thiadiazole-2(3H)-thione, ...	133	C2H3N3S2	002349-67-9	38	
5	D-Alanine, N-(4-ethylbenzoyl)-, ...	319	C19H29NO3	1000354-08-9	38	



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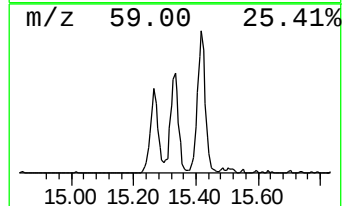
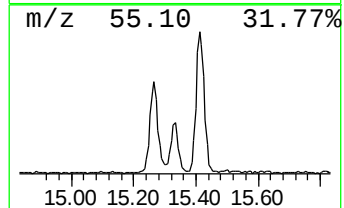
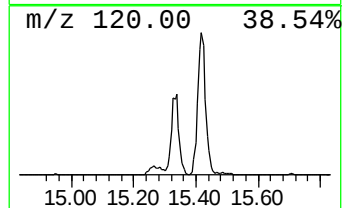
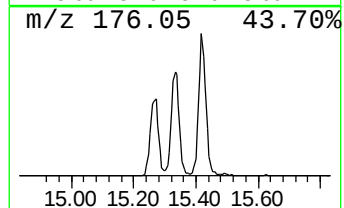
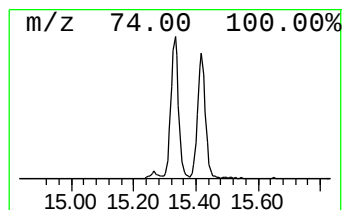
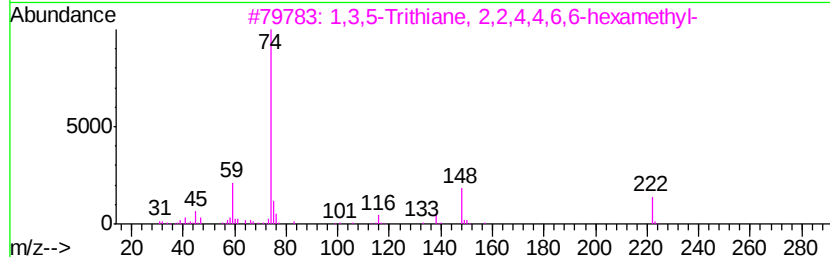
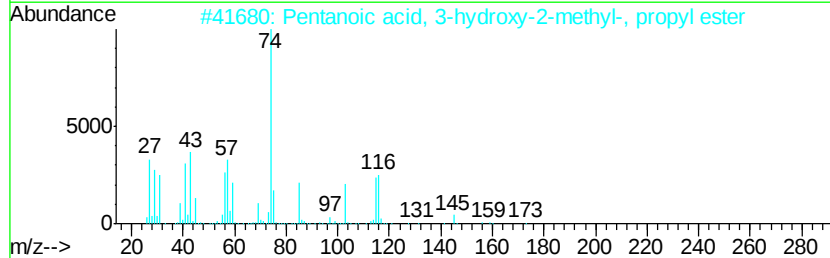
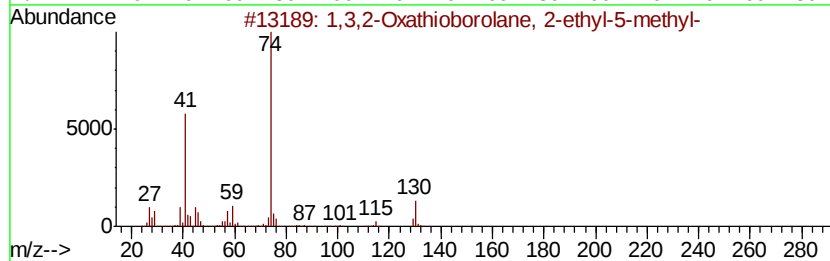
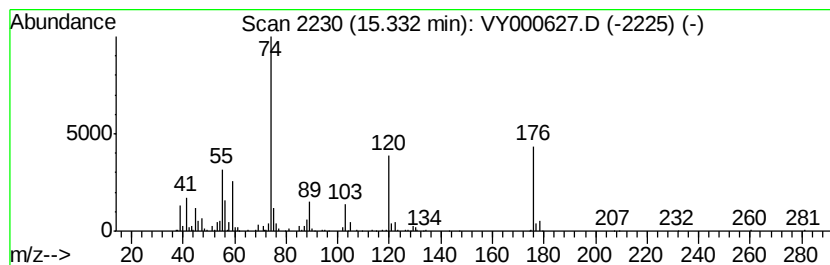
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Quant Title : SW846 8260

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Peak Number 3 unknown15.33 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.33	9.27 ug/l	198890	1,4-Dichlorobenzene-d4	13.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,2-Oxathioborolane, 2-ethyl-5...	130	C5H11BOS	1000163-05-5	27
2		Pentanoic acid, 3-hydroxy-2-meth...	174	C9H18O3	1000151-17-3	25
3		1,3,5-Trithiane, 2,2,4,4,6,6-hex...	222	C9H18S3	000828-26-2	17
4		Propanoic acid	74	C3H6O2	000079-09-4	16
5		dl-Homoserine	119	C4H9NO3	001927-25-9	16



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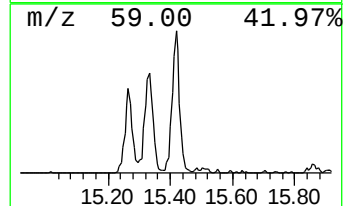
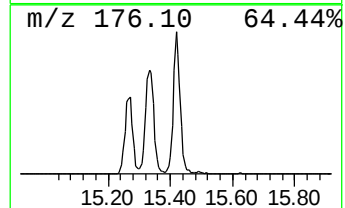
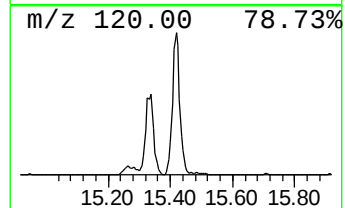
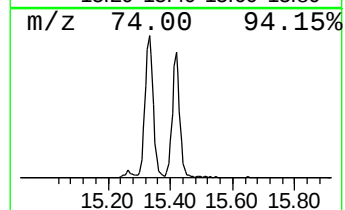
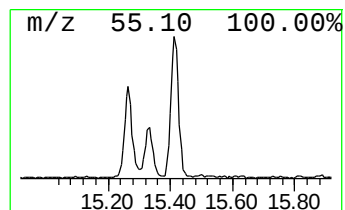
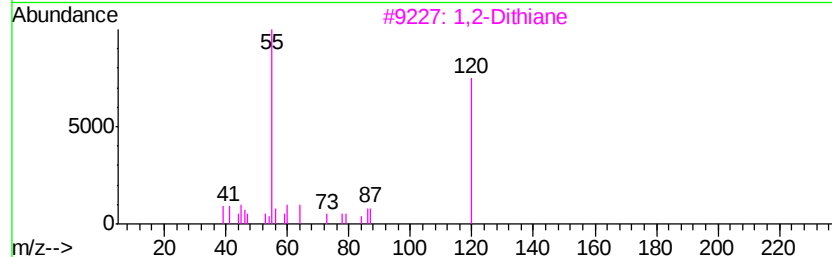
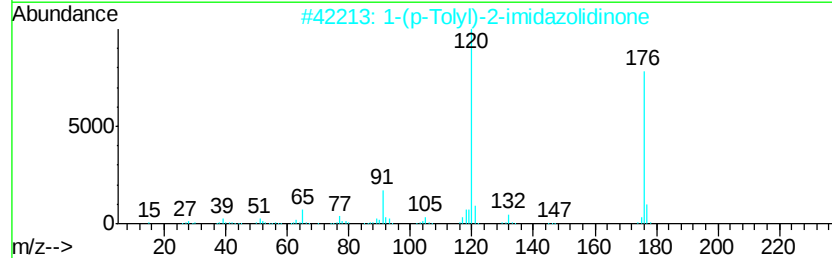
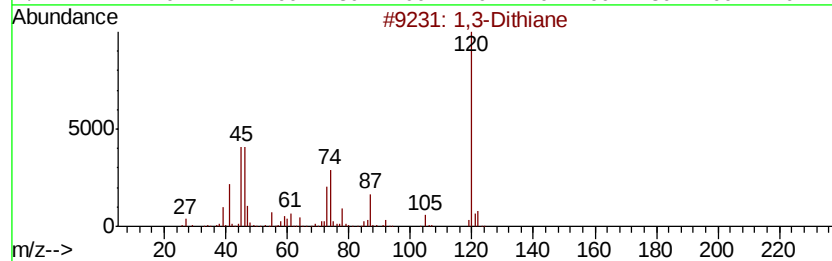
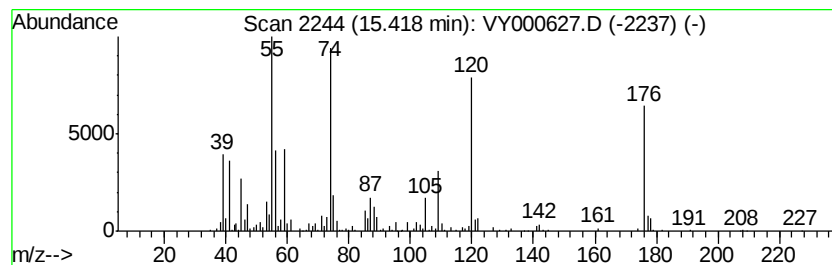
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TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown15.42 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.42	14.83 ug/l	318042	1,4-Dichlorobenzene-d4	13.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dithiane	120	C4H8S2	000505-23-7	25
2		1-(p-Tolyl)-2-imidazolidinone	176	C10H12N2O	090917-76-3	22
3		1,2-Dithiane	120	C4H8S2	000505-20-4	14
4		7-Methoxy-1-tetralone	176	C11H12O2	006836-19-7	12
5		5,6-Dihydro-2-methyl-1,4-dithiin...	176	C6H8O2S2	035756-29-7	11



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown14.21	14.21	16.6	ug/l	356323	4	13.42	1072520	50.0
1,2,4-Triazole, 3...	15.27	14.8	ug/l	317742	4	13.42	1072520	50.0
unknown15.33	15.33	9.3	ug/l	198890	4	13.42	1072520	50.0
unknown15.42	15.42	14.8	ug/l	318042	4	13.42	1072520	50.0