

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_Y\DATA\VY110719\
 Data File : VY000578.D
 Acq On : 07 Nov 2019 14:21
 Operator : SY/MD
 Sample : K5723-09
 Misc : 7.46G/5ML/MSVOA_Y/SOIL
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 9-B

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	82	rBV2	14363	22190	1.58%	0.191%
2	4.724	478	490	500	rBV	31468	93840	6.67%	0.808%
3	5.761	647	660	672	rVB3	16156	50607	3.60%	0.436%
4	7.730	973	983	989	rBV	187975	447596	31.84%	3.854%
5	7.803	989	995	1009	rVB	320805	723555	51.47%	6.230%
6	8.157	1043	1053	1064	rVB	190902	429180	30.53%	3.695%
7	8.699	1133	1142	1153	rBV	531167	1036895	73.75%	8.928%
8	10.181	1377	1385	1393	rBV	834535	1405908	100.00%	12.106%
9	11.492	1592	1600	1610	rVB	760472	1232848	87.69%	10.615%
10	12.479	1754	1762	1769	rBV	613730	925583	65.84%	7.970%
11	13.302	1890	1897	1910	rBV2	115736	190842	13.57%	1.643%
12	13.424	1910	1917	1925	rBV	754658	1141348	81.18%	9.828%
13	13.528	1930	1934	1945	rVB2	31453	52941	3.77%	0.456%
14	14.052	2011	2020	2024	rBV2	7545	22215	1.58%	0.191%
15	14.211	2029	2046	2062	rVV4	204286	924523	65.76%	7.961%
16	15.265	2206	2219	2225	rBV	502255	936038	66.58%	8.060%
17	15.332	2225	2230	2237	rVB	381440	635566	45.21%	5.473%
18	15.418	2237	2244	2252	rBV	569701	1009717	71.82%	8.694%
19	15.509	2255	2259	2261	rBV4	10718	17621	1.25%	0.152%
20	15.887	2314	2321	2330	rBV4	9985	29927	2.13%	0.258%
21	16.009	2338	2341	2349	rVV4	18812	47276	3.36%	0.407%
22	16.088	2349	2354	2359	rVV6	11806	24494	1.74%	0.211%
23	16.149	2361	2364	2370	rVB2	18523	29154	2.07%	0.251%
24	16.289	2382	2387	2392	rBV4	15107	29954	2.13%	0.258%
25	16.363	2393	2399	2404	rBV	69707	126414	8.99%	1.088%
26	16.478	2413	2418	2422	rBV8	11739	27501	1.96%	0.237%

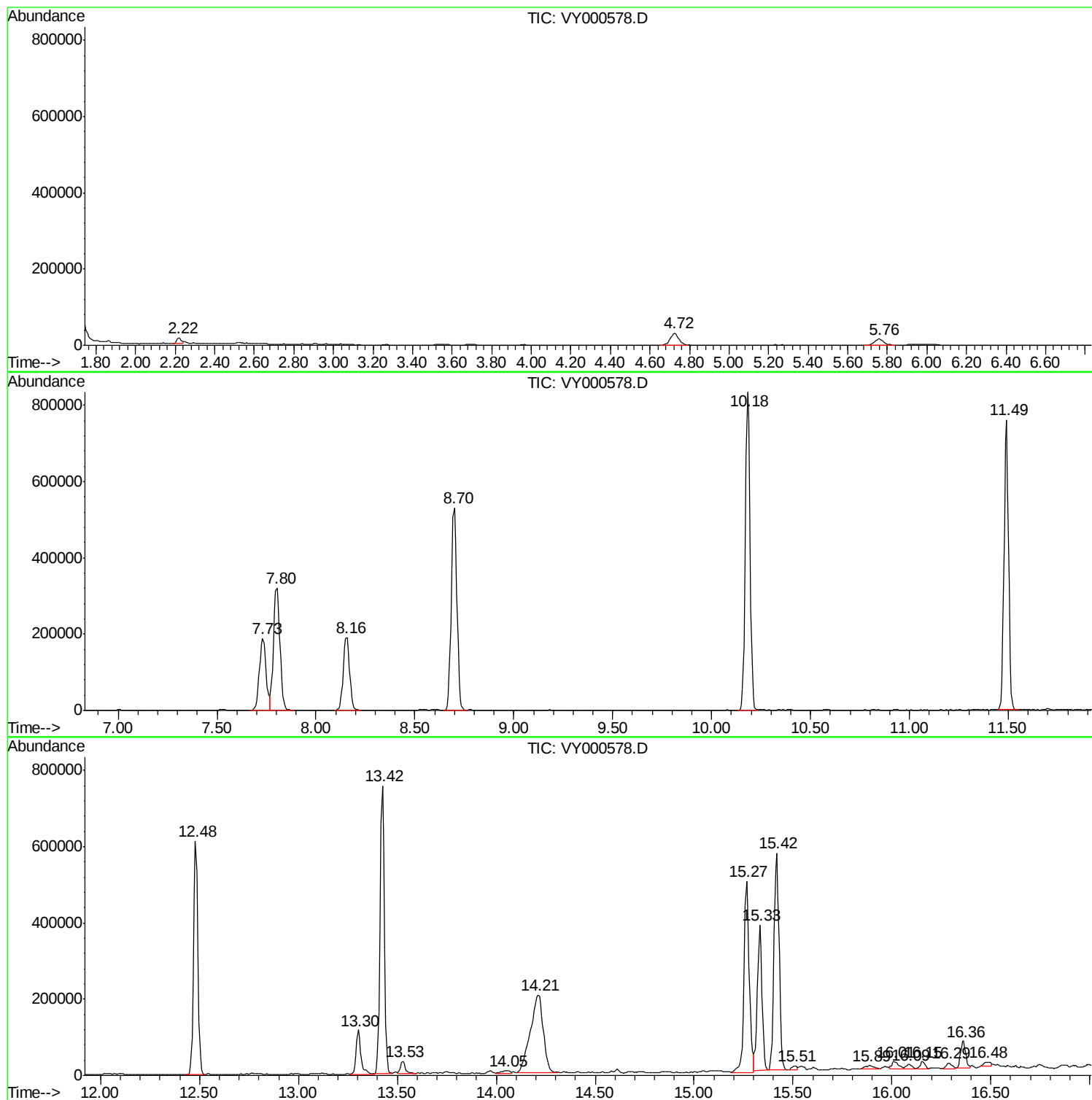
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Instrument :
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Quant Title : SW846 8260

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



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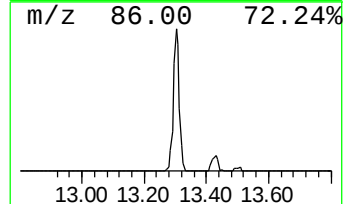
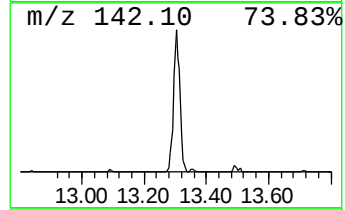
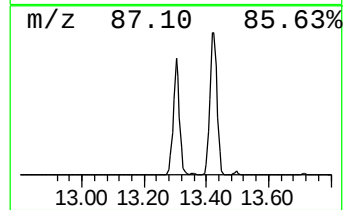
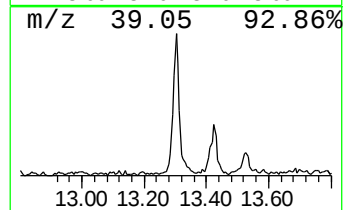
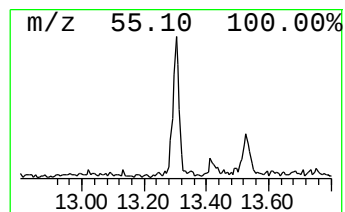
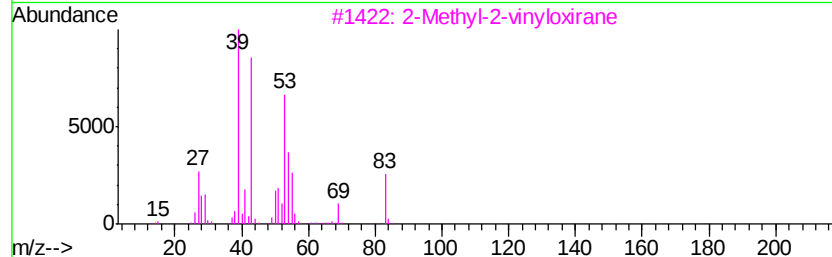
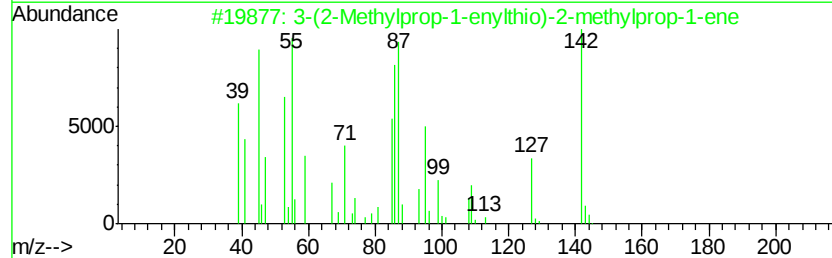
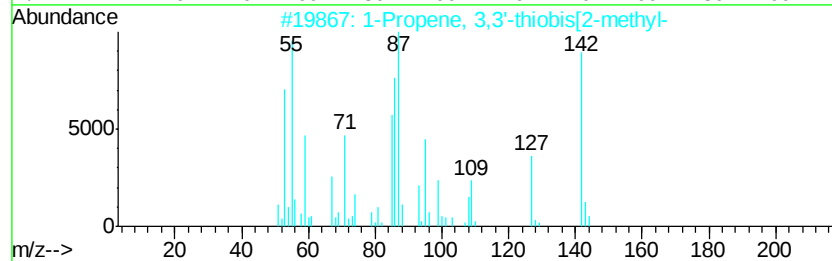
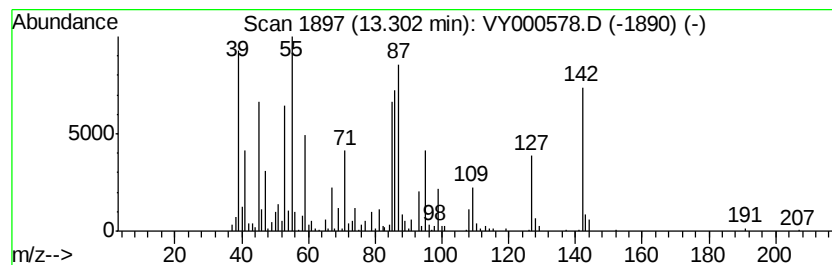
Instrument :
MSVOA_Y
ClientSampled :
9-B

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, 3,3'-thiobis[2-m... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.30	8.36 ug/l	190842	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 95
3		2-Methyl-2-vinylloxirane	84 C5H8O	001838-94-4 46
4		2-Ethylprop-1-ene (1-3)sultine	132 C5H8O2S	084735-13-7 28
5		Cyclobutene	54 C4H6	000822-35-5 25



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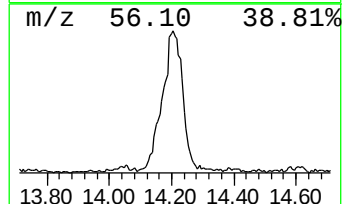
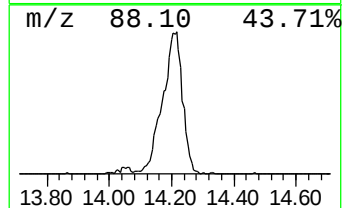
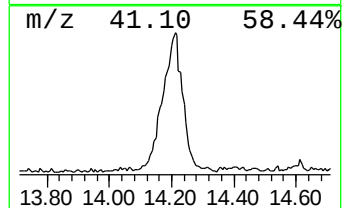
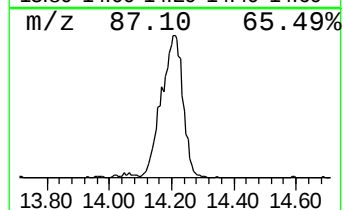
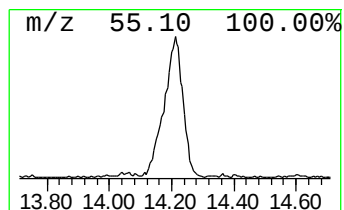
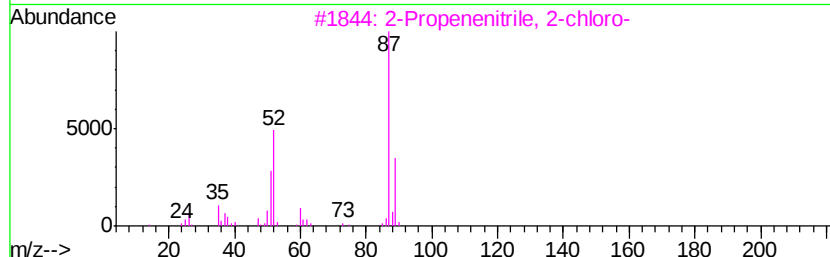
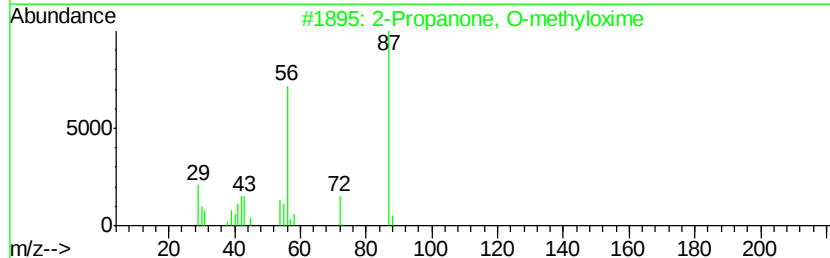
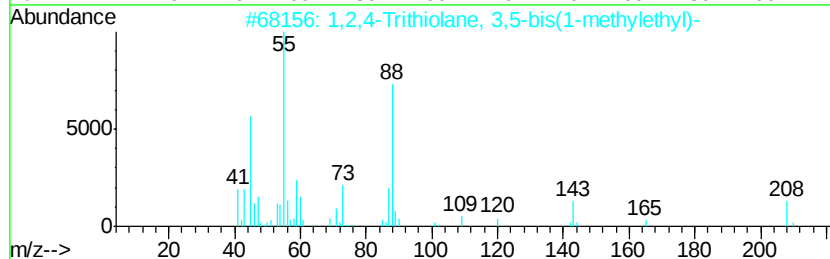
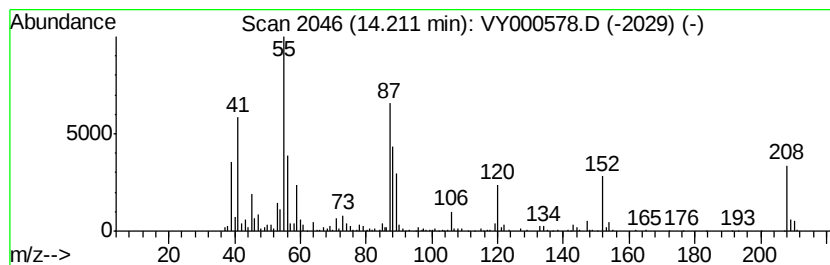
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TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown14.21 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.21	40.50 ug/l	924523	1,4-Dichlorobenzene-d4	13.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2,4-Trithiolane, 3,5-bis(1-met...	208	C8H16S3	054934-99-5	10
2		2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	10
3		2-Propenenitrile, 2-chloro-	87	C3H2ClN	000920-37-6	10
4		2-[2-[2-[2-(2-Butoxyethoxy)ethox...	336	C16H32O7	1000351-94-0	10
5		2-Octen-1-ol, 7-ethoxy-3,7-dimet...	200	C12H24O2	1000132-19-5	10



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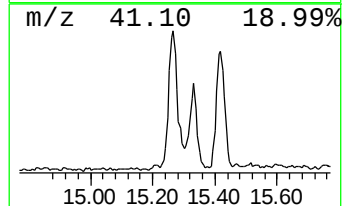
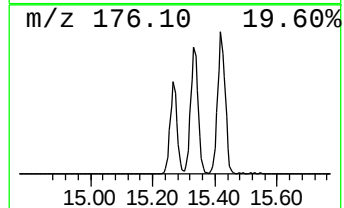
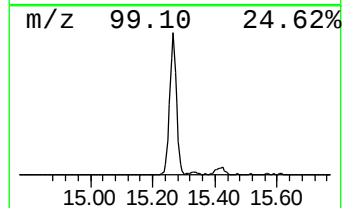
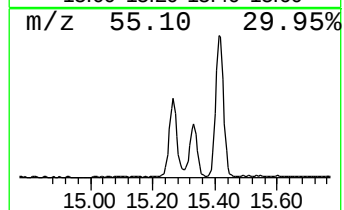
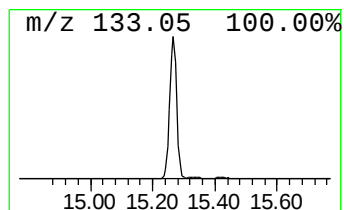
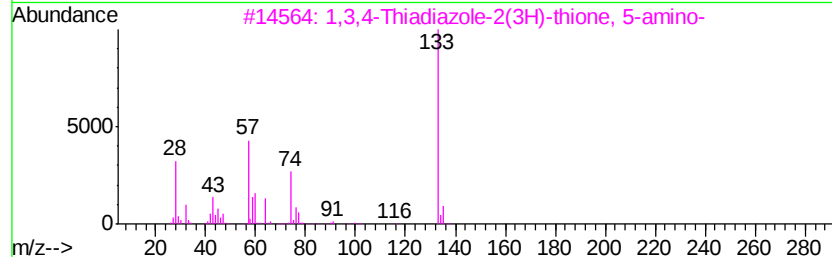
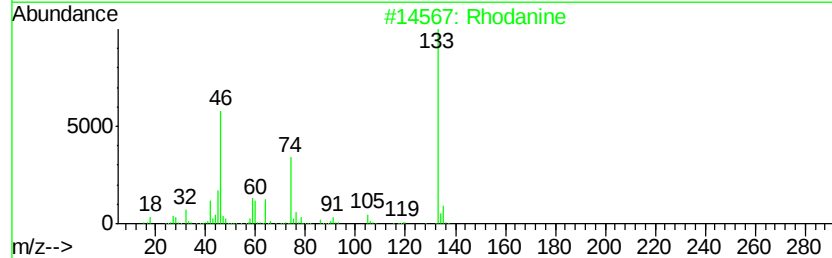
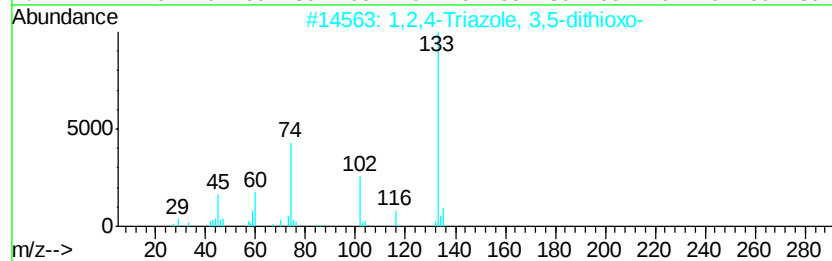
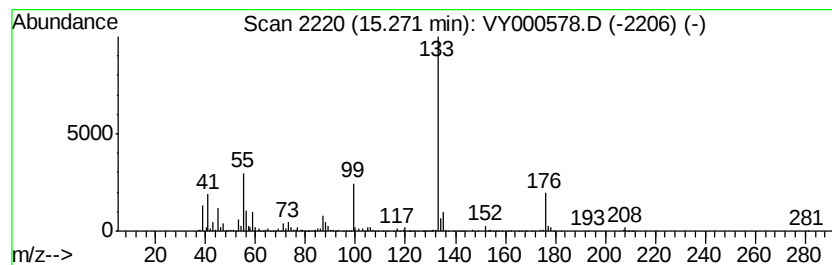
Instrument :
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ClientSampleId :
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	41.01 ug/l	936038	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		1,3,4-Thiadiazole-2(3H)-thione, ...	133 C2H3N3S2	002349-67-9 42
4		(2-Methyl-[1,3]dithian-2-yl)phen...	240 C12H16OS2	078349-00-5 40
5		Thiophene, 2,2'-(1,1,2,2,3,3,4,4...	416 C13H6F10S2	024014-44-6 28



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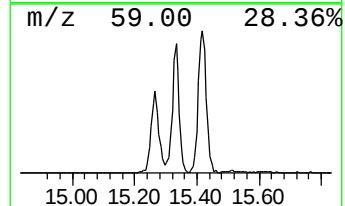
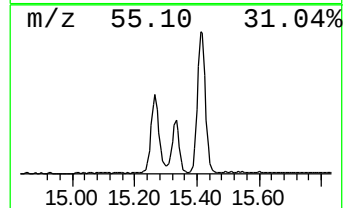
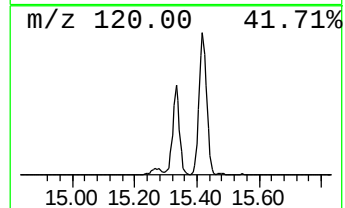
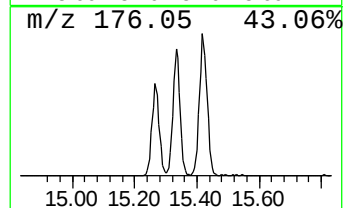
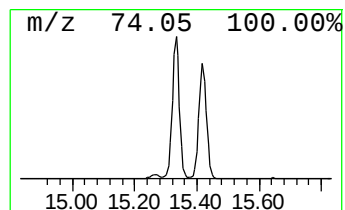
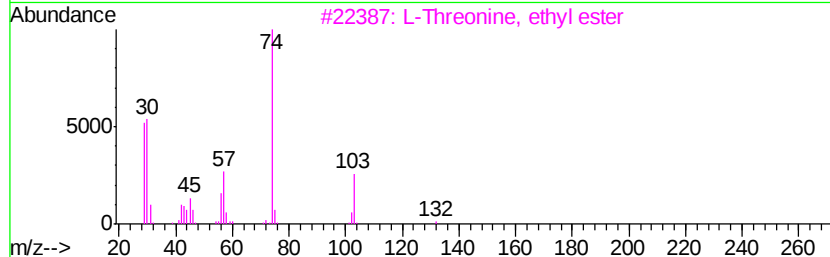
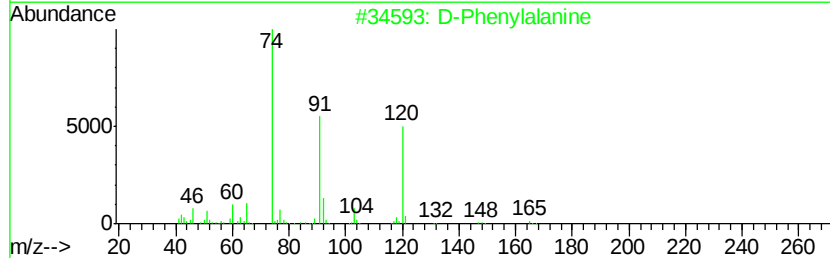
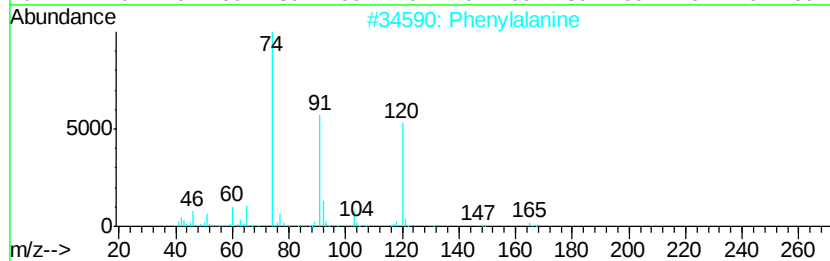
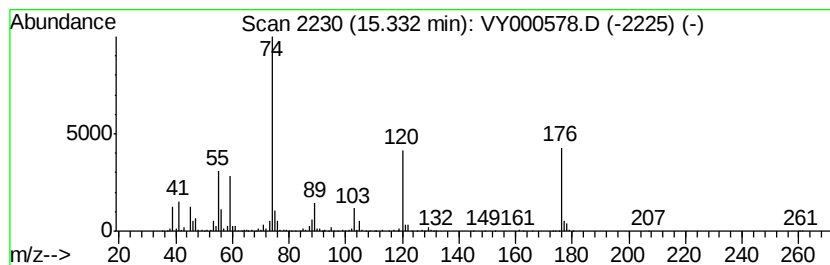
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TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown15.33 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.33	27.84 ug/l	635566	1,4-Dichlorobenzene-d4	13.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenylalanine	165	C9H11NO2	000063-91-2	28
2		D-Phenylalanine	165	C9H11NO2	000673-06-3	28
3		L-Threonine, ethyl ester	147	C6H13NO3	023926-51-4	27
4		1,3,4-Thiadiazol-2-amine, 5-methyl-	115	C3H5N3S	000108-33-8	25
5		1,3,2-Oxathioborolane, 2-ethyl-5...	130	C5H11BOS	1000163-05-5	16



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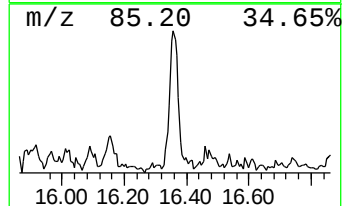
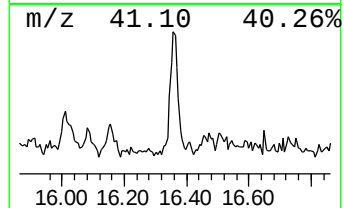
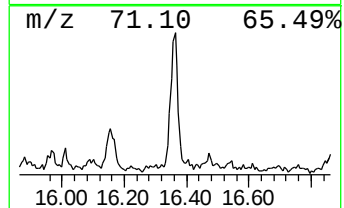
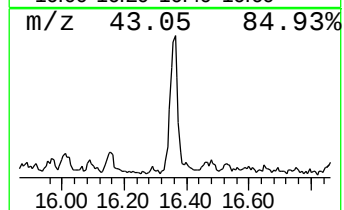
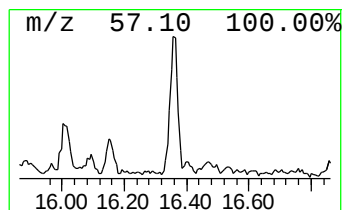
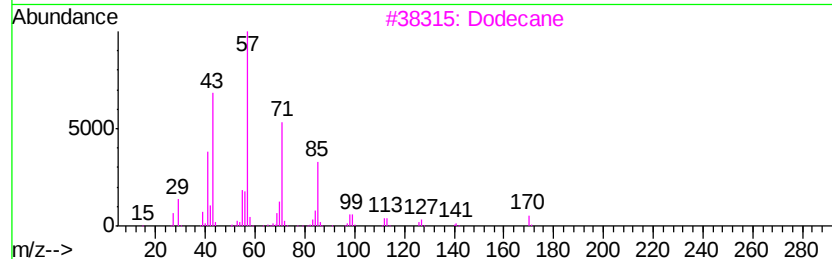
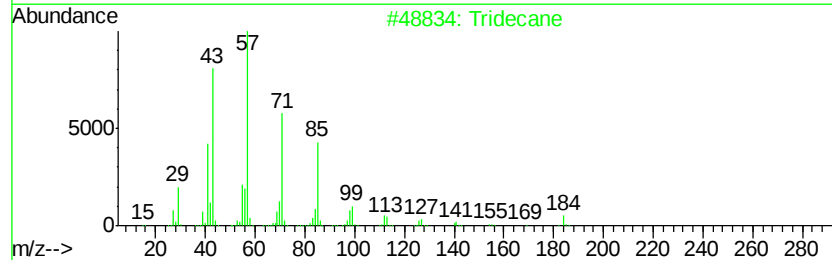
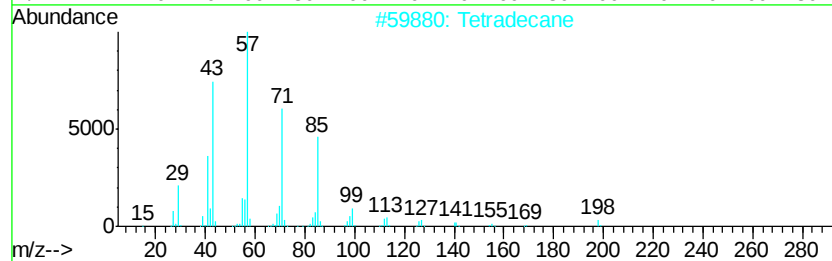
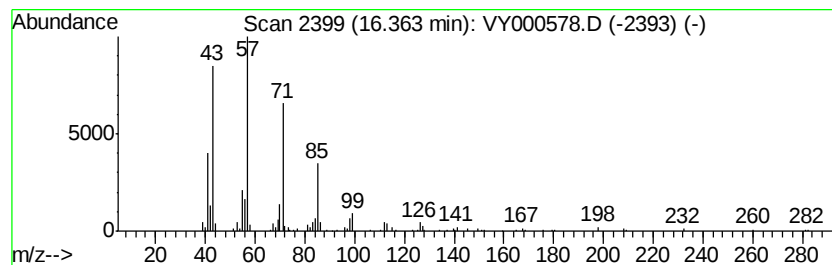
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 6 Tetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.36	5.54 ug/l	126414	1,4-Dichlorobenzene-d4	13.42

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane	198	C14H30	000629-59-4	94
2		Tridecane	184	C13H28	000629-50-5	87
3		Dodecane	170	C12H26	000112-40-3	86
4		Tetradecane, 1-chloro-	232	C14H29Cl	002425-54-9	80
5		Hexadecane	226	C16H34	000544-76-3	80



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Propene, 3,3'-t...	13.30	8.4	ug/l	190842	4	13.42	1141350	50.0
unknown14.21	14.21	40.5	ug/l	924523	4	13.42	1141350	50.0
1,2,4-Triazole, 3...	15.27	41.0	ug/l	936038	4	13.42	1141350	50.0
unknown15.33	15.33	27.8	ug/l	635566	4	13.42	1141350	50.0
Tetradecane	16.36	5.5	ug/l	126414	4	13.42	1141350	50.0