

Data Path : Z:\VOASRV\HPCHEM1\MSVOA Y\DATA\VY052220\
 Data File : VY002752.D
 Acq On : 22 May 2020 14:11
 Operator : SY/MD
 Sample : L2748-01
 Misc : 8.36G/5ML/MSVOA Y/SOIL
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 L-DRUM-COMP

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\82Y051520S.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	2.224	74	80	93	rBV	41648	82129	5.37%	0.782%
2	4.724	479	490	502	rBV3	16584	53159	3.47%	0.506%
3	7.723	971	982	987	rBV	195608	464648	30.37%	4.422%
4	7.797	987	994	1006	rVB	382044	868522	56.77%	8.266%
5	8.144	1041	1051	1063	rBV	179341	404120	26.41%	3.846%
6	8.693	1131	1141	1154	rBV	531052	1037012	67.78%	9.870%
7	10.180	1377	1385	1392	rBV	888483	1529946	100.00%	14.561%
8	10.241	1392	1395	1400	rVV	26300	48715	3.18%	0.464%
9	10.290	1400	1403	1409	rVB4	10926	16961	1.11%	0.161%
10	10.369	1409	1416	1423	rBV9	7207	17023	1.11%	0.162%
11	10.583	1445	1451	1455	rBV	7264	16760	1.10%	0.160%
12	11.491	1590	1600	1610	rBV	780553	1257416	82.19%	11.967%
13	11.595	1610	1617	1620	rBV2	9193	16288	1.06%	0.155%
14	11.704	1630	1635	1644	rVB4	19721	49736	3.25%	0.473%
15	12.028	1686	1688	1695	rVB4	12635	19451	1.27%	0.185%
16	12.393	1741	1748	1755	rBV2	17104	32255	2.11%	0.307%
17	12.479	1755	1762	1772	rVB	604475	977263	63.88%	9.301%
18	12.735	1800	1804	1806	rBV3	12579	15613	1.02%	0.149%
19	12.808	1812	1816	1821	rVB3	28666	46854	3.06%	0.446%
20	13.119	1862	1867	1872	rBV	29751	43224	2.83%	0.411%
21	13.302	1891	1897	1904	rVB3	149826	248842	16.26%	2.368%
22	13.424	1910	1917	1924	rBV	704840	1097538	71.74%	10.446%
23	13.527	1931	1934	1942	rVB5	13690	20815	1.36%	0.198%
24	13.625	1946	1950	1955	rBV5	17532	37081	2.42%	0.353%
25	13.747	1966	1970	1975	rVB2	30478	46272	3.02%	0.440%
26	13.966	2001	2006	2013	rVB4	23552	39747	2.60%	0.378%
27	14.076	2020	2024	2029	rBV5	17871	31680	2.07%	0.302%
28	14.131	2029	2033	2041	rBV9	8624	19913	1.30%	0.190%
29	14.204	2041	2045	2050	rBV6	12126	23252	1.52%	0.221%
30	14.253	2050	2053	2057	rBV3	22331	39063	2.55%	0.372%
31	14.405	2070	2078	2085	rBV	316602	524905	34.31%	4.996%
32	14.478	2085	2090	2095	rVB8	15170	26793	1.75%	0.255%
33	14.582	2101	2107	2110	rBV2	64368	89951	5.88%	0.856%
34	14.613	2110	2112	2116	rVV3	24805	28253	1.85%	0.269%

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ALS Vial : 7 Sample Multiplier: 1

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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 >
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35	14.667	2116	2121	2128	rVV3	30613	77950	5.09%	0.742%
36	14.734	2128	2132	2136	rVB4	20493	32304	2.11%	0.307%
37	14.838	2144	2149	2154	rBV3	39808	69769	4.56%	0.664%
38	14.942	2162	2166	2170	rVB6	15143	24299	1.59%	0.231%
39	14.997	2170	2175	2178	rBV7	10922	19800	1.29%	0.188%
40	15.094	2188	2191	2195	rVB2	13104	17737	1.16%	0.169%
41	15.216	2205	2211	2213	rBV7	10391	20794	1.36%	0.198%
42	15.271	2215	2220	2226	rVV2	71269	151828	9.92%	1.445%
43	15.338	2226	2231	2238	rVV	69965	157089	10.27%	1.495%
44	15.423	2240	2245	2252	rVB4	86284	171956	11.24%	1.637%
45	15.728	2291	2295	2302	rVB5	25700	47341	3.09%	0.451%
46	16.015	2336	2342	2351	rVB	183001	372795	24.37%	3.548%
47	16.234	2372	2378	2384	rBV	23395	49557	3.24%	0.472%
48	16.295	2384	2388	2393	rVV2	12170	22617	1.48%	0.215%

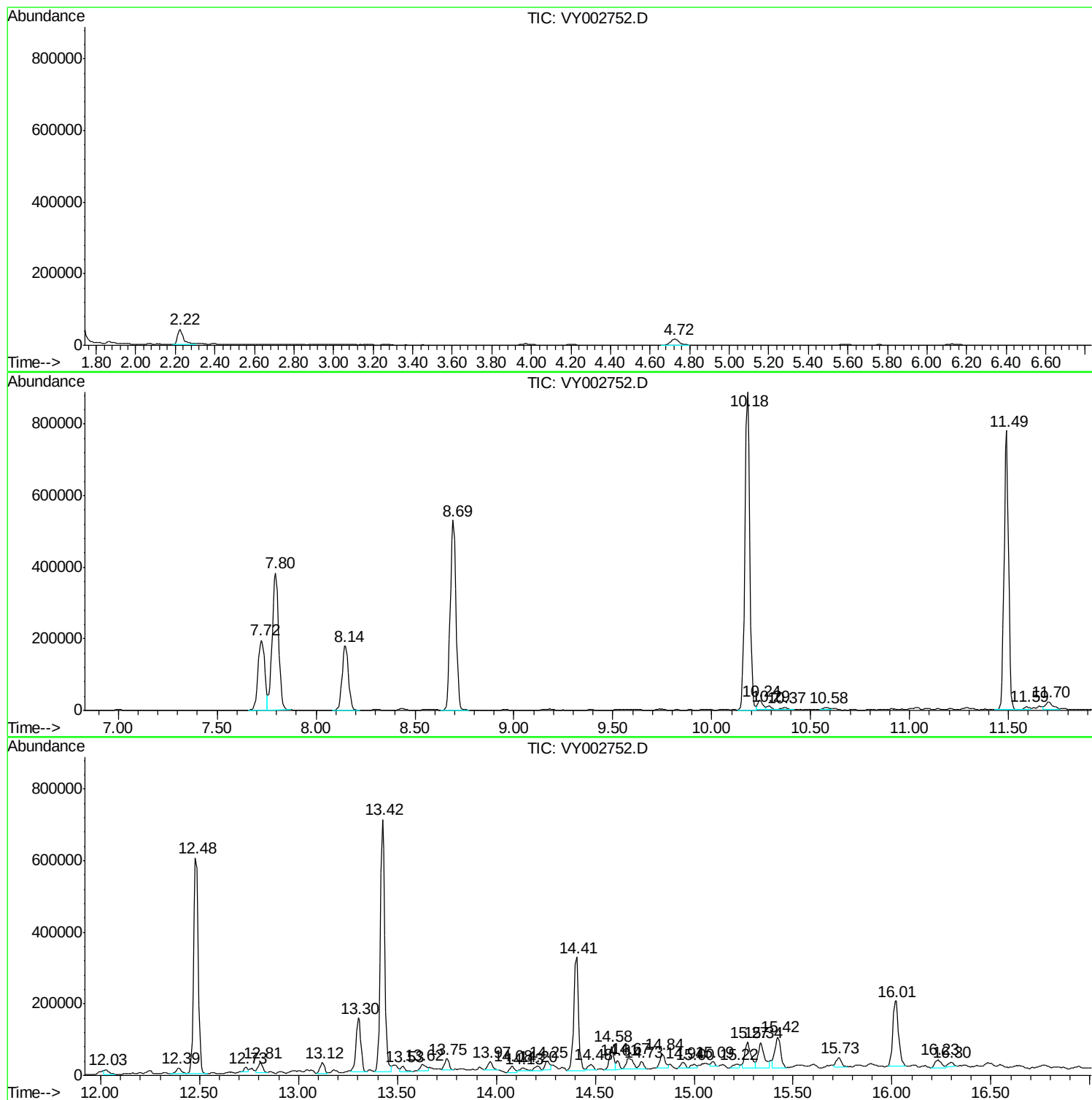
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_Y\METHODS\82Y051520S.M
Quant Title : SW846 8260

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



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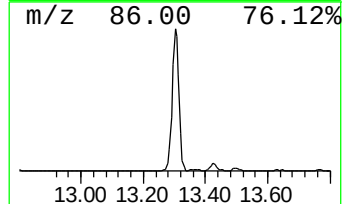
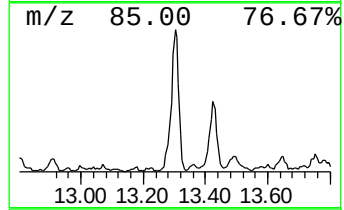
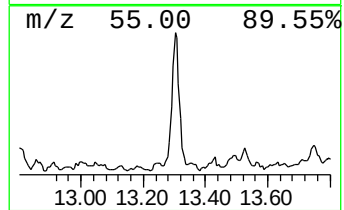
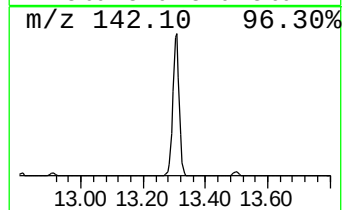
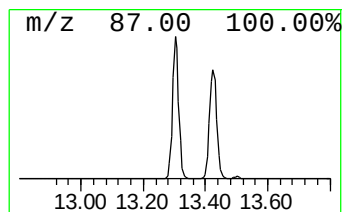
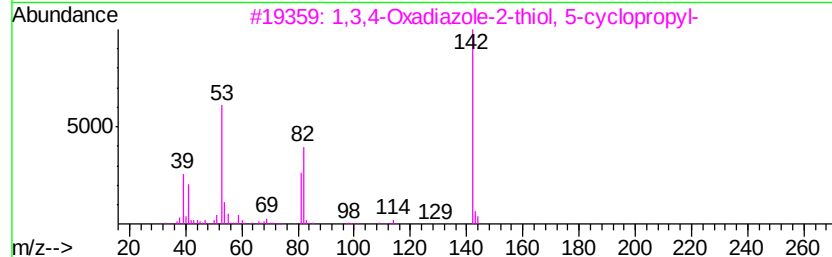
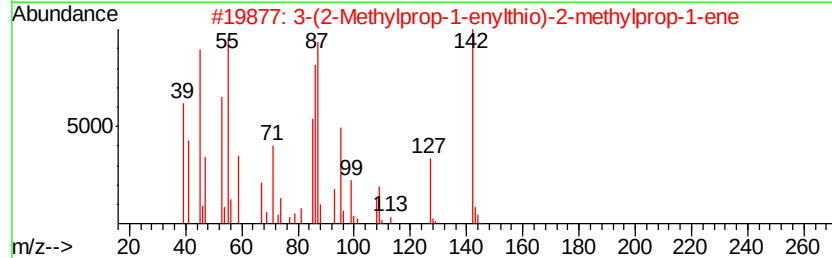
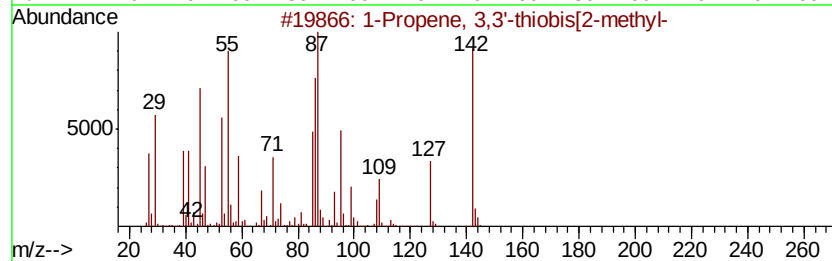
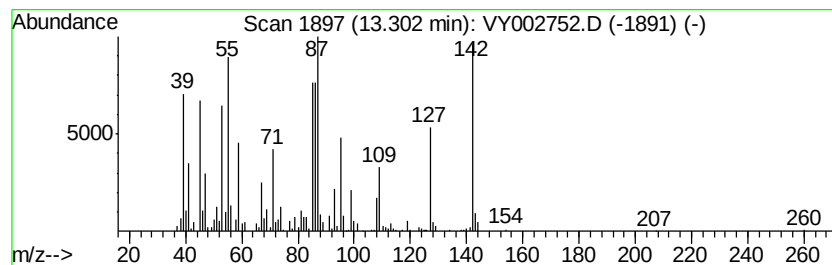
Instrument :
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ClientSampleId :
L-DRUM-COMP

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_Y\METHODS\82Y051520S.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 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.30	11.34 ug/l	248842	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	97
3	1,3,4-Oxadiazole-2-thiol, 5-cycl...	142 C5H6N2OS	064007-54-1	25
4	Methyl(methyl 4-O-methyl-.alpha....	236 C9H16O7	024916-47-0	14
5	Pyrazole-3-carboxylic acid, 5-am...	127 C4H5N3O2	124004-31-5	12



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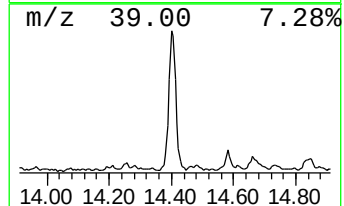
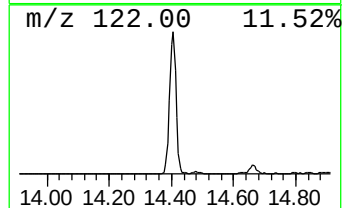
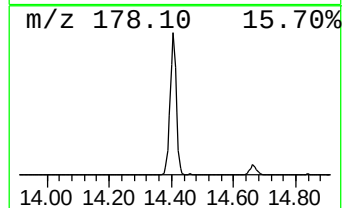
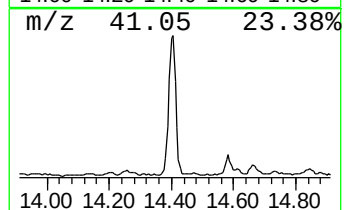
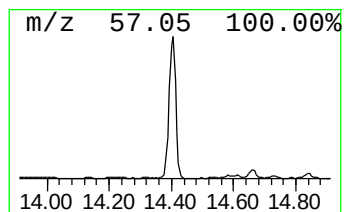
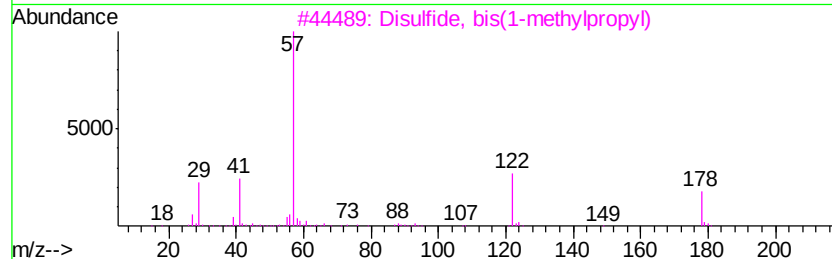
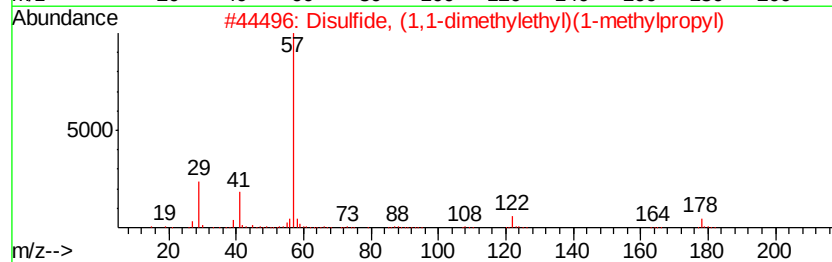
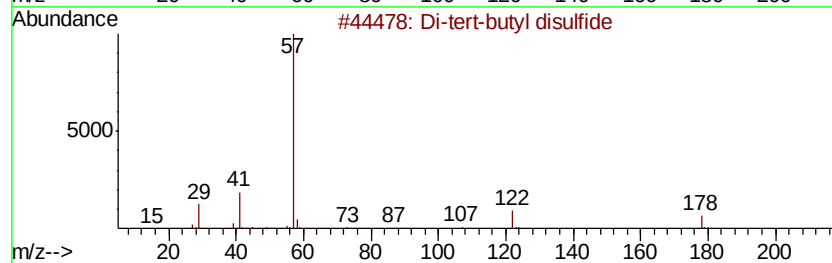
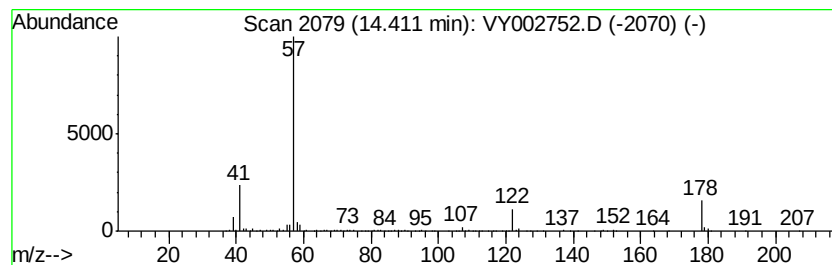
Instrument :
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Quant Title : SW846 8260

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

Peak Number 2 Di-tert-butyl disulfide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.41	23.91 ug/l	524905	1,4-Dichlorobenzene-d4	13.42
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Di-tert-butyl disulfide	178 C8H18S2	000110-06-5 86
2		Disulfide, (1,1-dimethylethyl)(1...	178 C8H18S2	072437-46-8 59
3		Disulfide, bis(1-methylpropyl)	178 C8H18S2	005943-30-6 53
4		Disulfide, bis(2-methylpropyl)	178 C8H18S2	001518-72-5 52
5		Disulfide, dibutyl	178 C8H18S2	000629-45-8 50



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Misc : 8.36G/5ML/MSVOA Y/SOIL
ALS Vial : 7 Sample Multiplier: 1

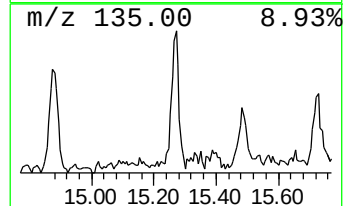
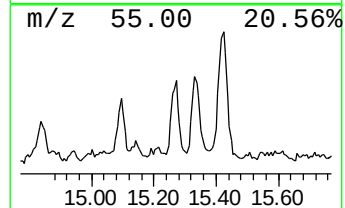
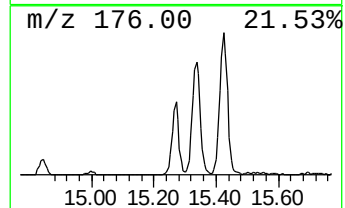
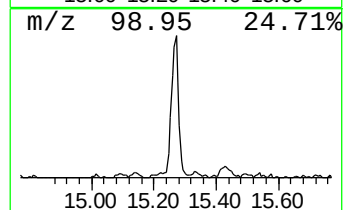
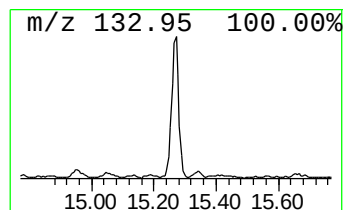
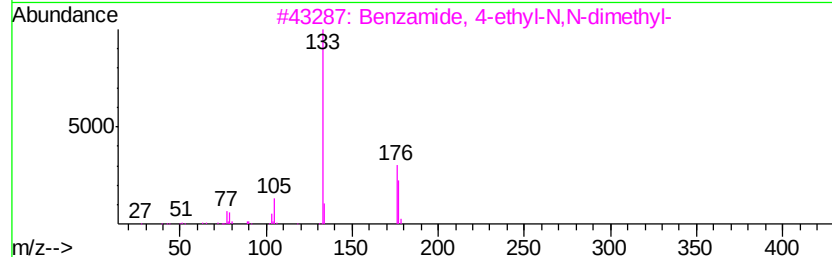
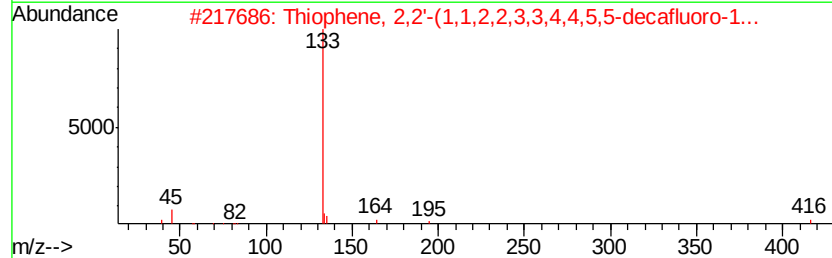
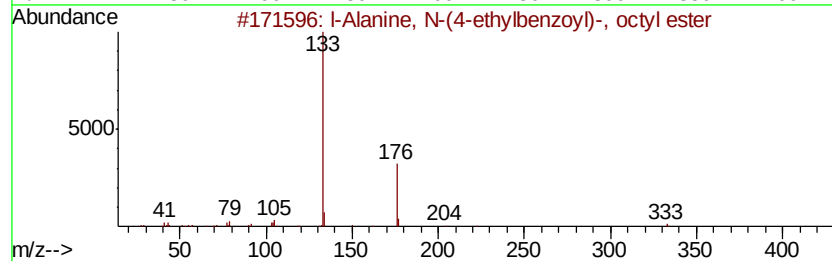
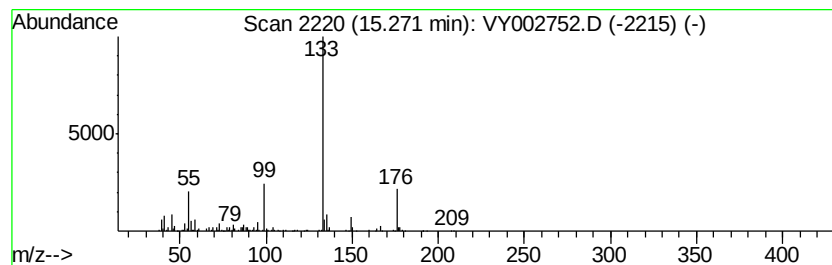
Instrument :
MSVOA_Y
ClientSampleId :
L-DRUM-COMP

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_Y\METHODS\82Y051520S.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown15.27 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.27	6.92 ug/l	151828	1,4-Dichlorobenzene-d4	13.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	l-Alanine, N-(4-ethylbenzoyl)-, ...	333	C20H31NO3	1000314-16-3	40
2	Thiophene, 2,2'-(1,1,2,2,3,3,4,4...	416	C13H6F10S2	024014-44-6	38
3	Benzamide, 4-ethyl-N,N-dimethyl-	177	C11H15NO	1000340-34-4	33
4	Acetylthiosemicarbazide	133	C3H7N3OS	002302-88-7	28
5	(2-Methyl-[1,3]dithian-2-yl)phen...	240	C12H16OS2	078349-00-5	28



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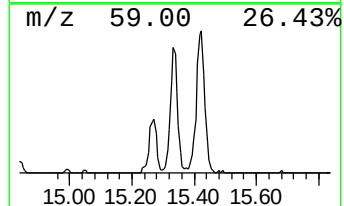
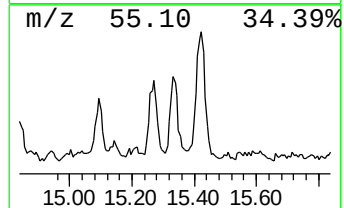
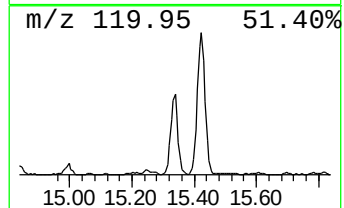
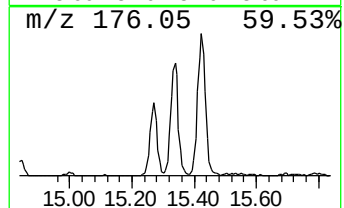
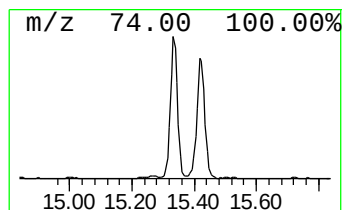
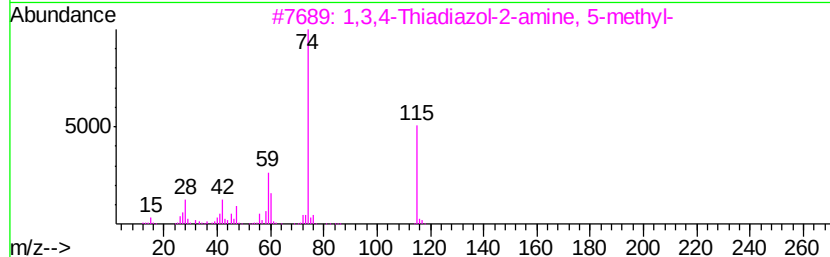
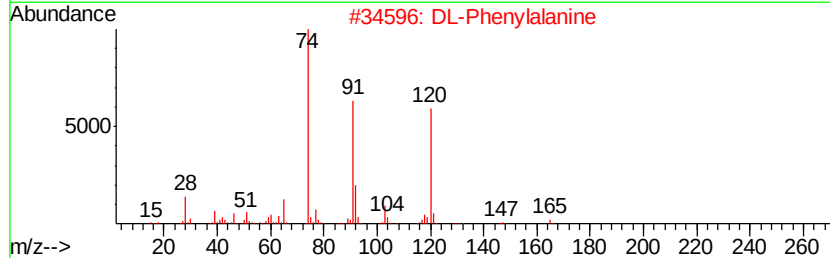
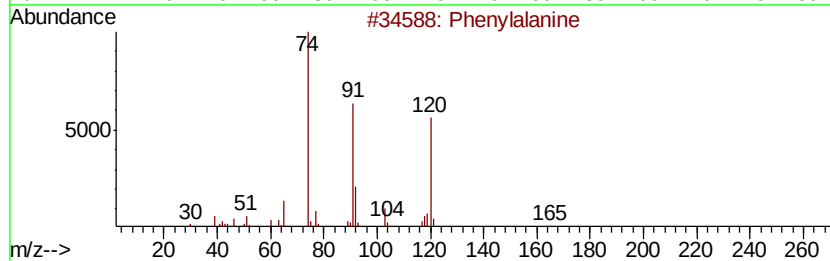
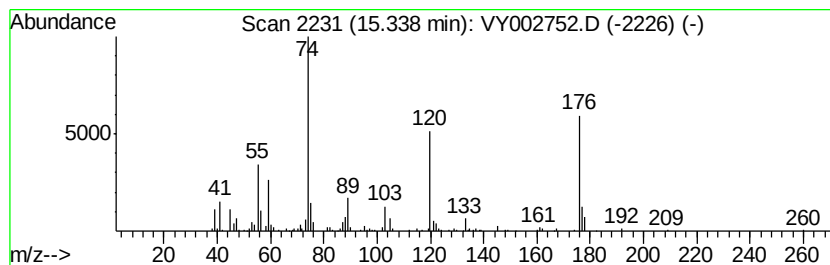
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Quant Title : SW846 8260

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

Peak Number 4 unknown15.34 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.34	7.16 ug/l	157089	1,4-Dichlorobenzene-d4	13.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenylalanine	165	C9H11NO2	000063-91-2	38
2		DL-Phenylalanine	165	C9H11NO2	000150-30-1	38
3		1,3,4-Thiadiazol-2-amine, 5-methyl-	115	C3H5N3S	000108-33-8	32
4		Propanamide, N-[4-(2-chlorobenzo...	345	C17H16ClN3O3	314765-76-9	27
5		7-Methoxy-1-tetralone	176	C11H12O2	006836-19-7	27



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Instrument :
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ClientSampled :
L-DRUM-COMP

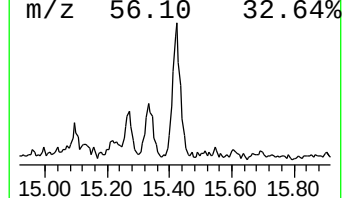
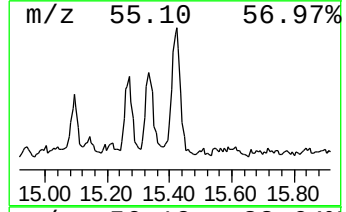
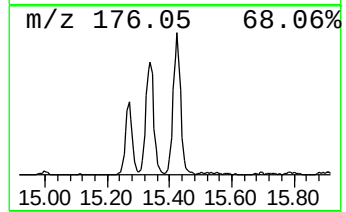
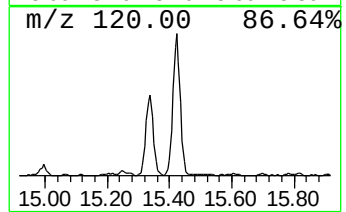
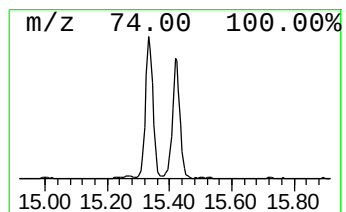
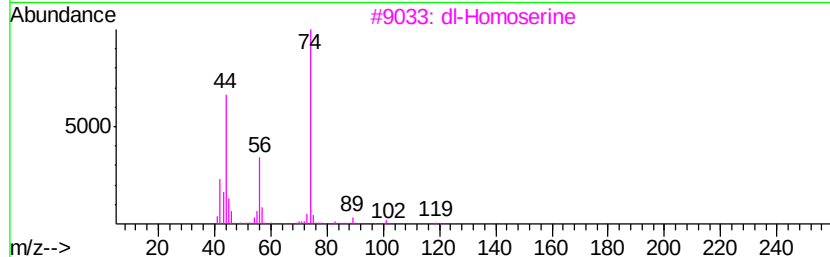
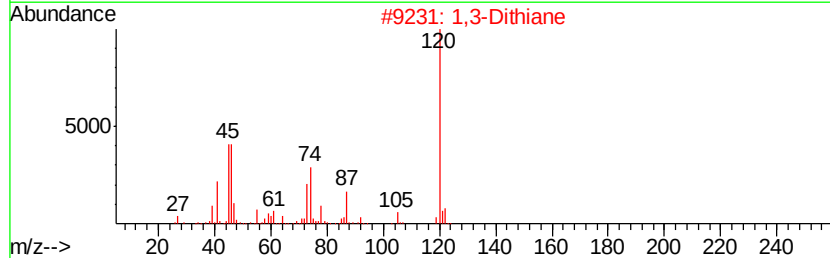
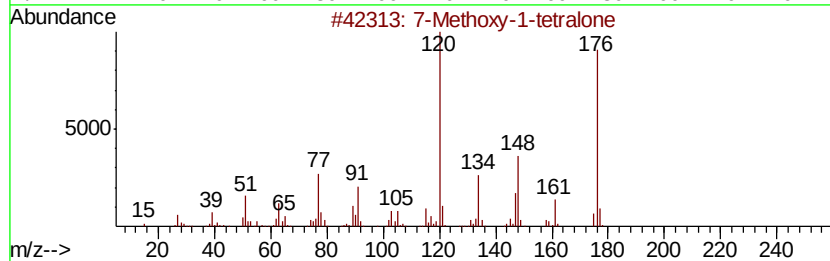
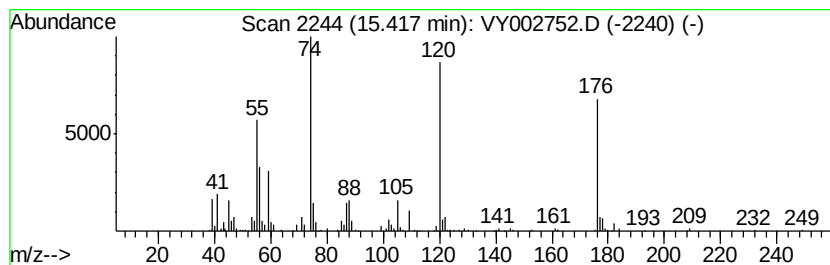
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Quant Title : SW846 8260

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

Peak Number 5 unknown15.42 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.42	7.83 ug/l	171956	1,4-Dichlorobenzene-d4	13.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	7-Methoxy-1-tetralone	176	C11H12O2	006836-19-7	32
2		1,3-Dithiane	120	C4H8S2	000505-23-7	22
3		dl-Homoserine	119	C4H9NO3	001927-25-9	14
4		Homoserine	119	C4H9NO3	000498-19-1	14
5		Xylopyranoside, methyl 4-azido-4...	203	C7H13N3O4	018390-81-3	12



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA Y\DATA\VY052220\
 Data File : VY002752.D
 Acq On : 22 May 2020 14:11
 Operator : SY/MD
 Sample : L2748-01
 Misc : 8.36G/5ML/MSVOA Y/SOIL
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 L-DRUM-COMP

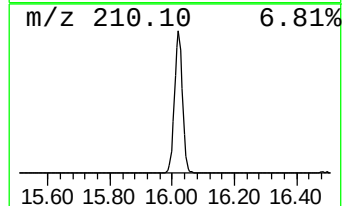
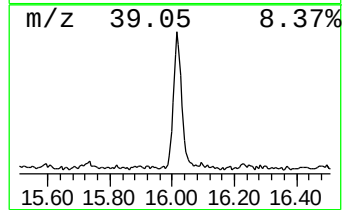
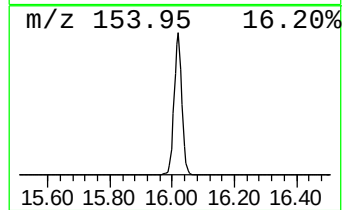
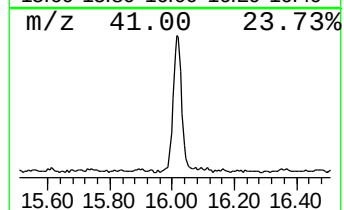
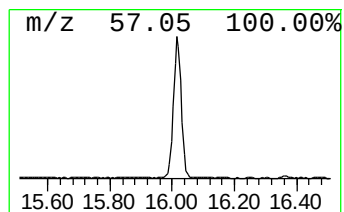
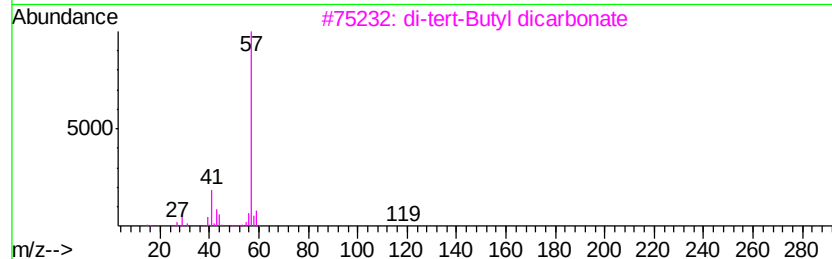
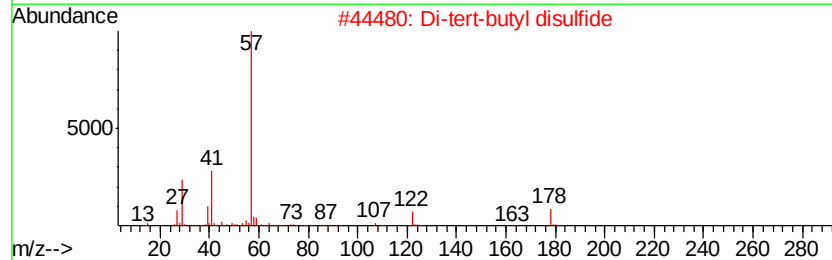
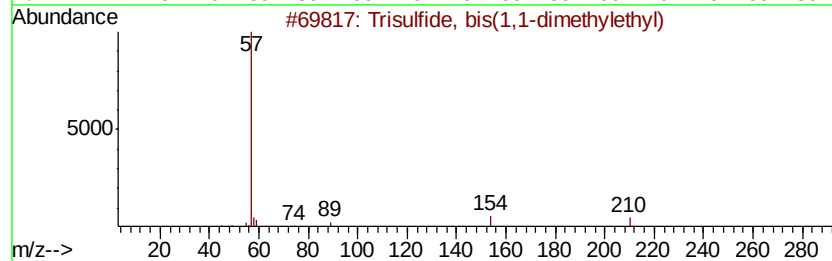
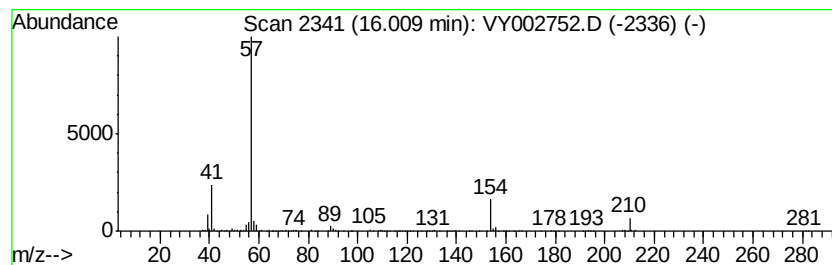
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_Y\METHODS\82Y051520S.M
 Quant Title : SW846 8260

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

 Peak Number 6 Trisulfide, bis(1,1-dimethy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.01	16.98 ug/l	372795	1,4-Dichlorobenzene-d4	13.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	58
2		Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	32
3		di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	27
4		Disulfide, (1,1-dimethylethyl)(1...	178	C8H18S2	072437-46-8	23
5		Isobutyl ether	130	C8H18O	000628-55-7	17



Data Path : Z:\V0ASRV\HPCHEM1\MSV0A_Y\DATA\VY052220\
Data File : VY002752.D
Acq On : 22 May 2020 14:11
Operator : SY/MD
Sample : L2748-01
Misc : 8.36G/5ML/MSV0A_Y/SOIL
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSV0A_Y
ClientSampleId :
L-DRUM-COMP

Quant Method : Z:\V0ASRV\HPCHEM1\MSV0A_Y\METHODS\82Y051520S.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Propene, 3,3'-t...	13.30	11.3	ug/l	248842	4	13.42	1097540	50.0
Di-tert-butyl dis...	14.41	23.9	ug/l	524905	4	13.42	1097540	50.0
unknown15.27	15.27	6.9	ug/l	151828	4	13.42	1097540	50.0
unknown15.34	15.34	7.2	ug/l	157089	4	13.42	1097540	50.0
unknown15.42	15.42	7.8	ug/l	171956	4	13.42	1097540	50.0
Trisulfide, bis(1...	16.01	17.0	ug/l	372795	4	13.42	1097540	50.0