

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_Y\DATA\VY110719\
 Data File : VY000583.D
 Acq On : 07 Nov 2019 16:12
 Operator : SY/MD
 Sample : K5723-14
 Misc : 4.51G/5ML/MSVOA_Y/SOIL
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 10-C

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	2.243	81	83	91	rVB2	9389	16460	1.20%	0.171%
2	4.724	476	490	503	rBV2	22109	69039	5.04%	0.717%
3	5.767	650	661	675	rVB3	29012	92320	6.74%	0.959%
4	7.730	970	983	989	rBV	181874	437706	31.98%	4.546%
5	7.803	989	995	1008	rVB2	315068	710080	51.88%	7.375%
6	8.157	1043	1053	1063	rBV	188547	412956	30.17%	4.289%
7	8.699	1133	1142	1153	rBV	524324	1015848	74.22%	10.551%
8	10.181	1377	1385	1393	rBV	797620	1368778	100.00%	14.217%
9	11.492	1592	1600	1611	rBV	734175	1201936	87.81%	12.484%
10	12.327	1729	1737	1746	rBV4	10494	20648	1.51%	0.214%
11	12.479	1754	1762	1774	rBV	586526	910606	66.53%	9.458%
12	13.302	1884	1897	1903	rBV2	71062	116758	8.53%	1.213%
13	13.424	1910	1917	1924	rBV	721176	1106844	80.86%	11.497%
14	13.528	1930	1934	1940	rVB4	10246	15950	1.17%	0.166%
15	14.204	2028	2045	2058	rBV4	79689	364111	26.60%	3.782%
16	14.613	2101	2112	2116	rVB	30057	48144	3.52%	0.500%
17	15.265	2211	2219	2225	rBV	313536	545133	39.83%	5.662%
18	15.332	2225	2230	2236	rVB	209301	355102	25.94%	3.688%
19	15.418	2237	2244	2254	rVB2	342011	620753	45.35%	6.448%
20	15.881	2315	2320	2325	rVB3	21218	39649	2.90%	0.412%
21	16.015	2336	2342	2345	rBV	18326	37689	2.75%	0.391%
22	16.088	2350	2354	2361	rVB5	9626	22326	1.63%	0.232%
23	16.289	2380	2387	2393	rBV	35543	64929	4.74%	0.674%
24	16.485	2413	2419	2425	rBV6	15719	33798	2.47%	0.351%

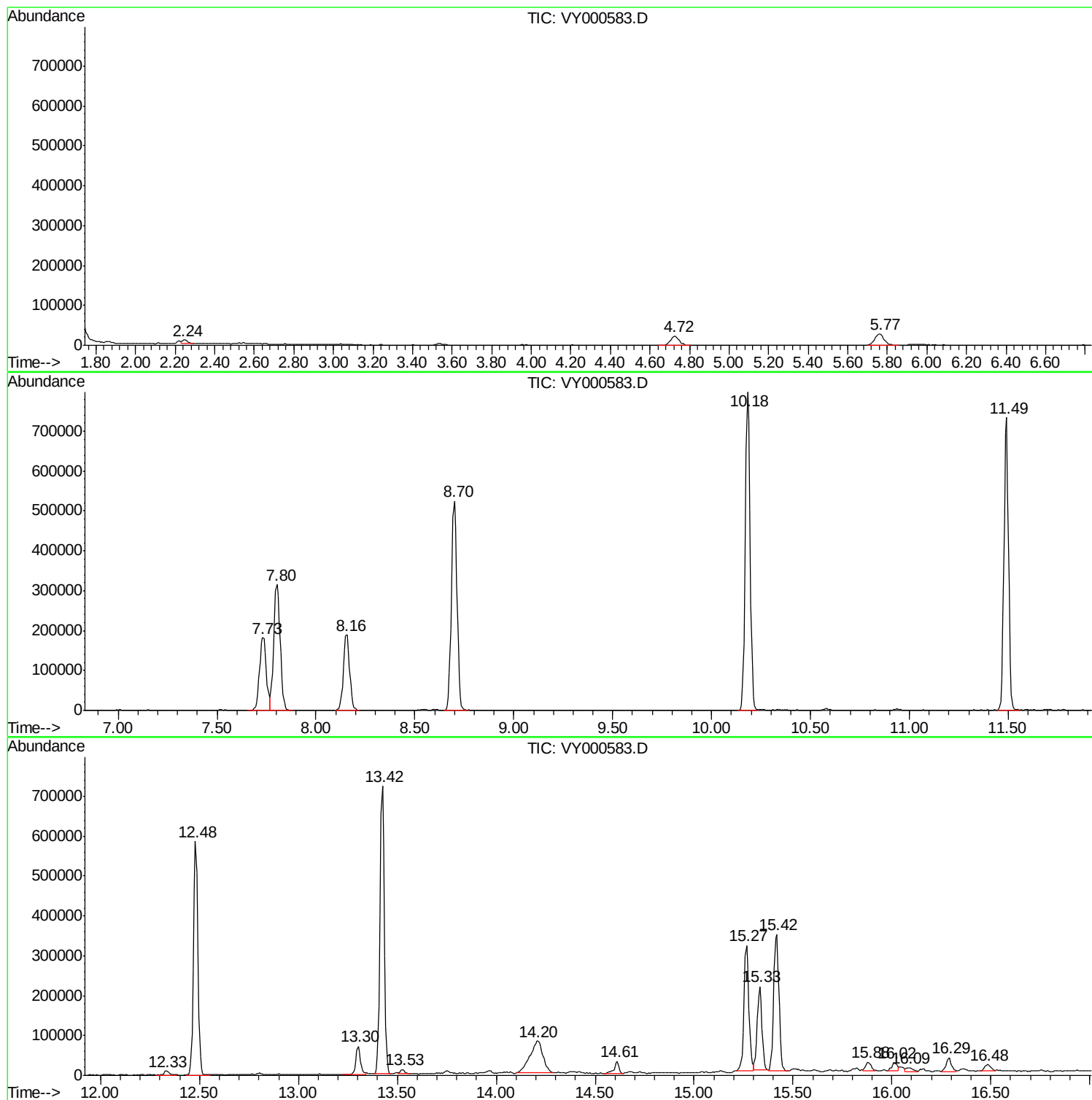
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Quant Method : Z:\V0ASRV\HPCHEM1\MSV0A_Y\METHODS\82Y103019S.M
Quant Title : SW846 8260

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



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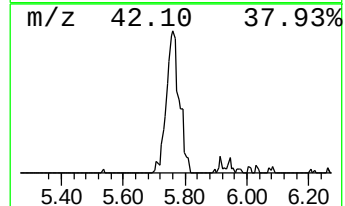
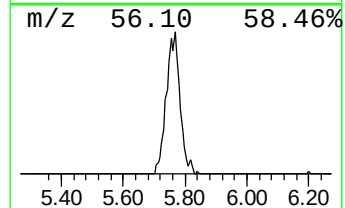
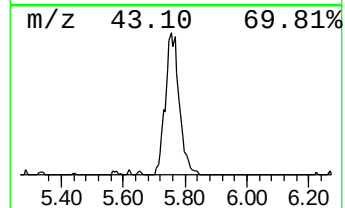
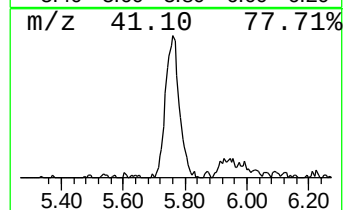
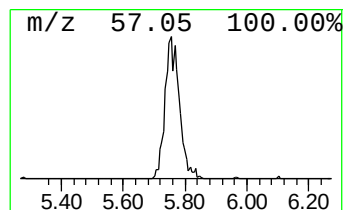
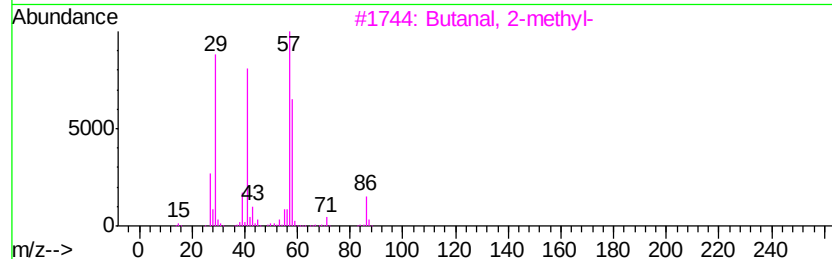
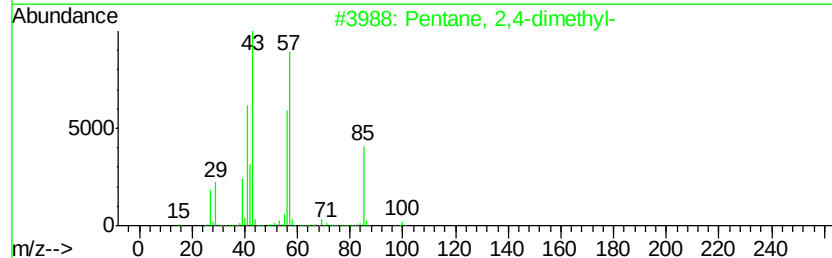
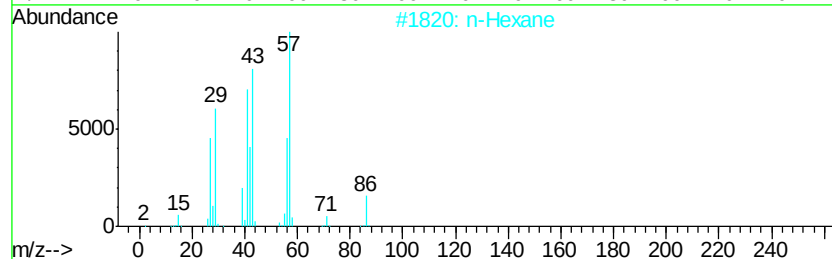
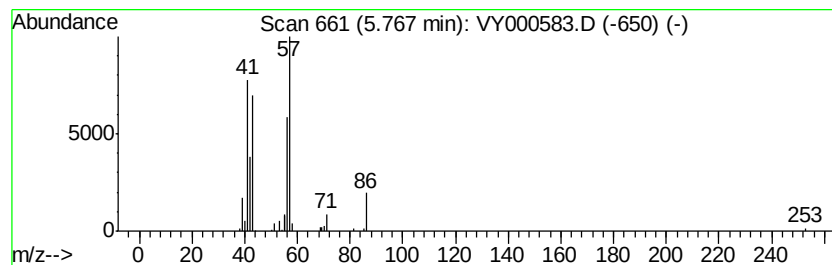
Quant Method : Z:\V0ASRV\HPCHEM1\MSV0A_Y\METHODS\82Y103019S.M
Quant Title : SW846 8260

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

Peak Number 1 n-Hexane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.77	6.50 ug/l	92320	Pentafluorobenzene	7.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexane	86	C6H14	000110-54-3	86
2		Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	39
3		Butanal, 2-methyl-	86	C5H10O	000096-17-3	38
4		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	36
5		Cyclobutane	56	C4H8	000287-23-0	35



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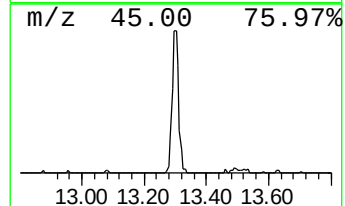
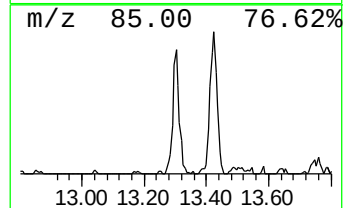
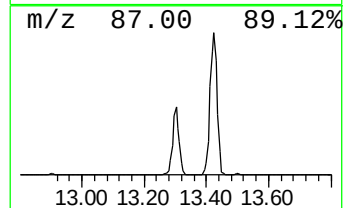
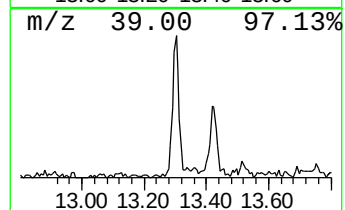
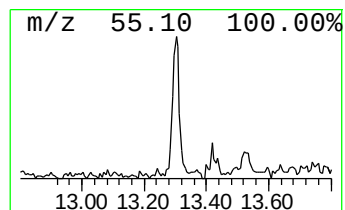
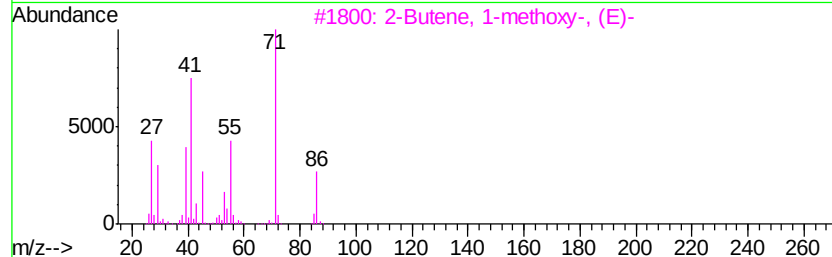
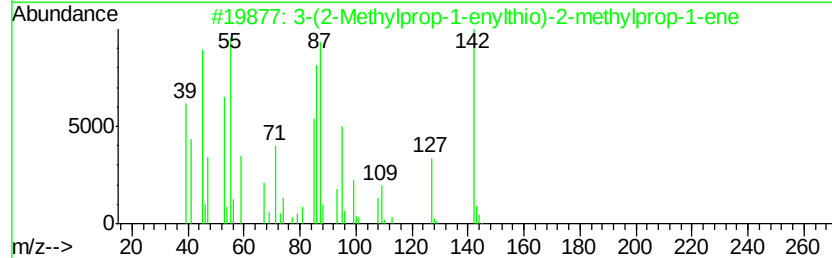
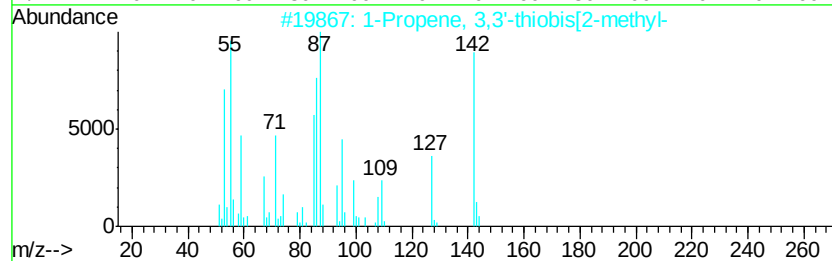
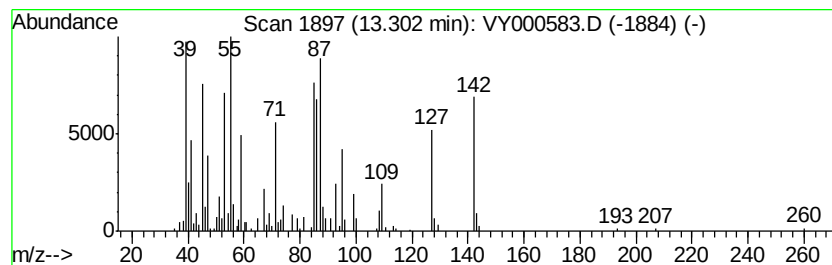
Instrument :
MSVOA_Y
ClientSampled :
10-C

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Peak Number 2 1-Propene, 3,3'-thiobis[2-m... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.30	5.27 ug/l	116758	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	93
2	3-(2-Methylprop-1-enylthio)-2-me...	142 C8H14S	1000122-39-8	90
3	2-Butene, 1-methoxy-, (E)-	86 C5H10O	010034-14-7	47
4	2-Ethylprop-1-ene (1-3)sultine	132 C5H8O2S	084735-13-7	28
5	2-Butyn-1-ol, 4-methoxy-	100 C5H8O2	018857-03-9	27



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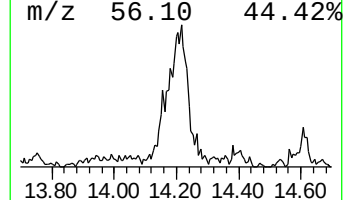
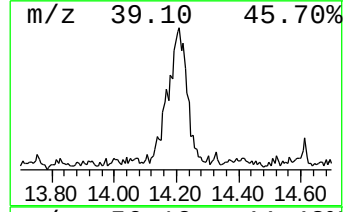
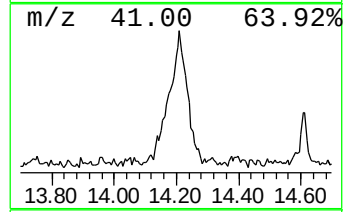
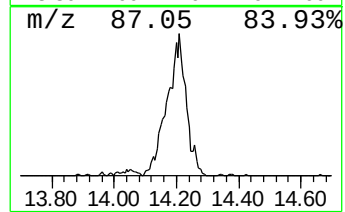
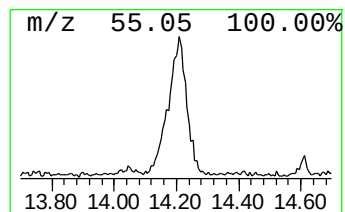
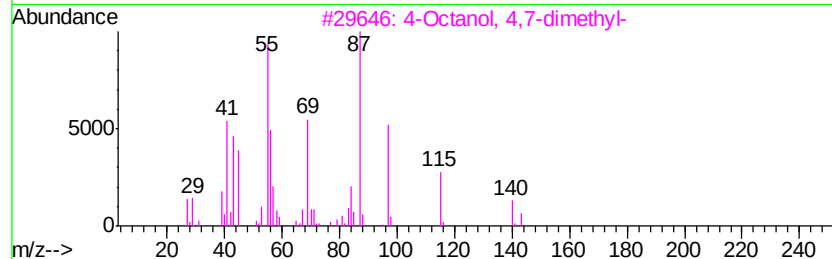
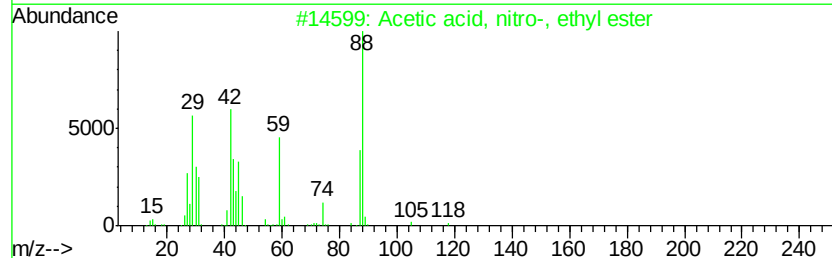
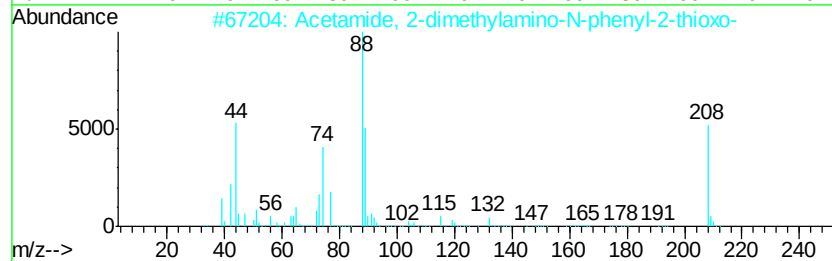
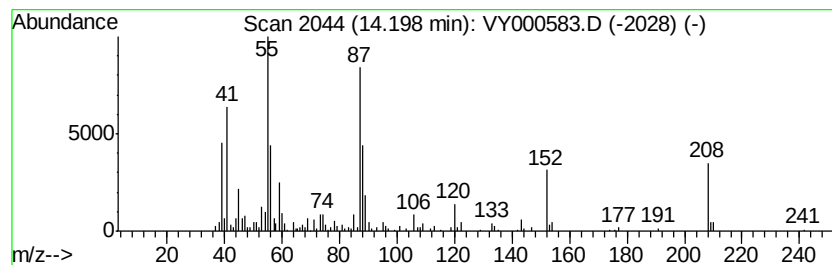
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Peak Number 3 unknown14.20 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.20	16.45 ug/l	364111	1,4-Dichlorobenzene-d4	13.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetamide, 2-dimethylamino-N-phe...	208	C10H12N2OS	1000303-49-5	27
2		Acetic acid, nitro-, ethyl ester	133	C4H7NO4	000626-35-7	14
3		4-Octanol, 4,7-dimethyl-	158	C10H22O	019781-13-6	12
4		2-Butyne, 1,4-dichloro-	122	C4H4Cl2	000821-10-3	10
5		2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	558	C25H50O13	1000351-91-9	10



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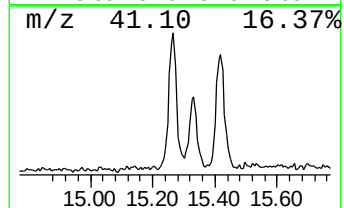
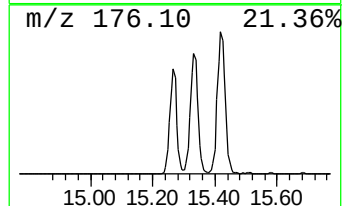
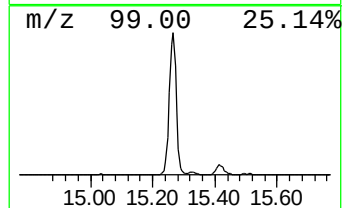
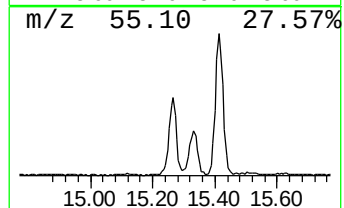
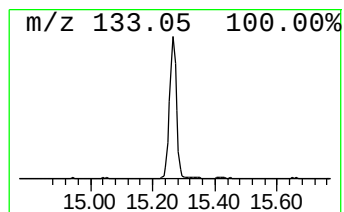
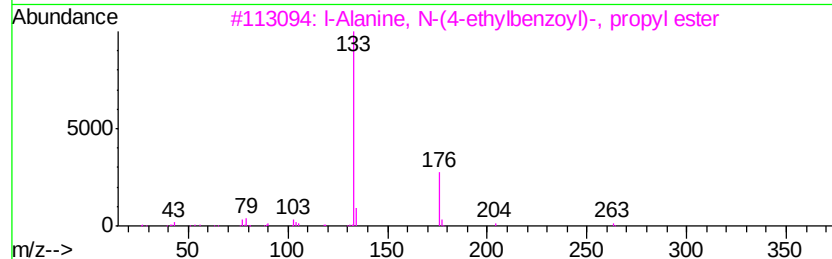
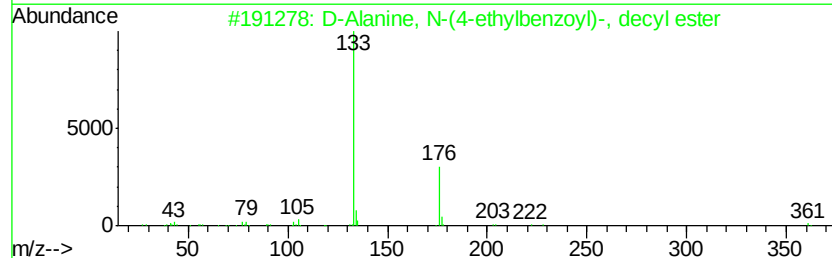
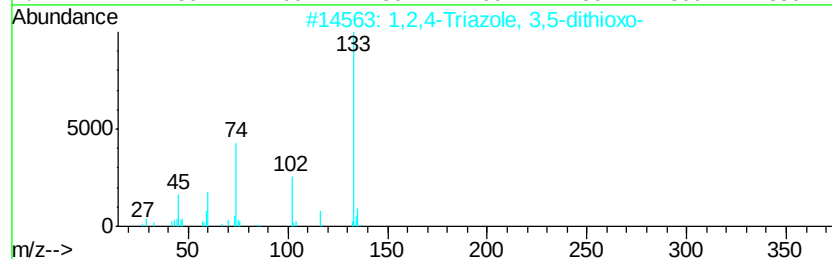
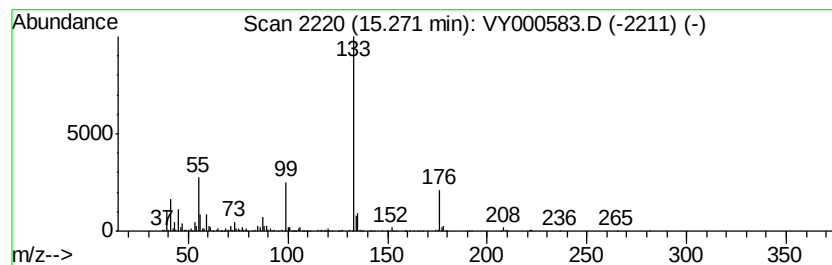
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Peak Number 4 unknown15.27 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	24.63 ug/l	545133	1,4-Dichlorobenzene-d4	13.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2,4-Triazole, 3,5-dithioxo-	133	C2H3N3S2	005650-03-3	40
2		D-Alanine, N-(4-ethylbenzoyl)-, ...	361	C22H35N03	1000354-09-1	33
3		L-Alanine, N-(4-ethylbenzoyl)-, ...	263	C15H21N03	1000314-15-9	33
4		1,2-Benzenediol, 0,0'-di(4-ethyl...	374	C24H22O4	1000325-97-5	33
5		1,2-Benzenediol, 0-(4-ethylbenzo...	414	C23H17F3O4	1000330-50-5	33



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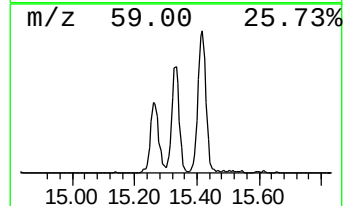
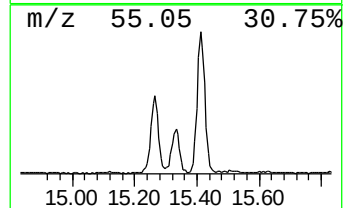
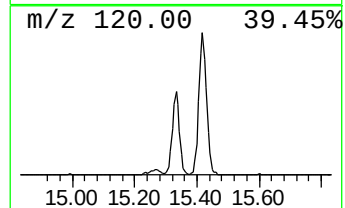
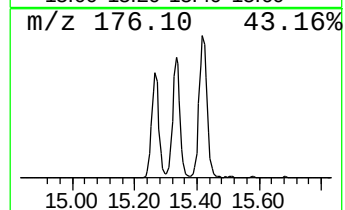
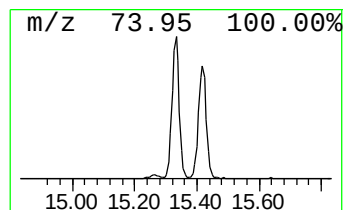
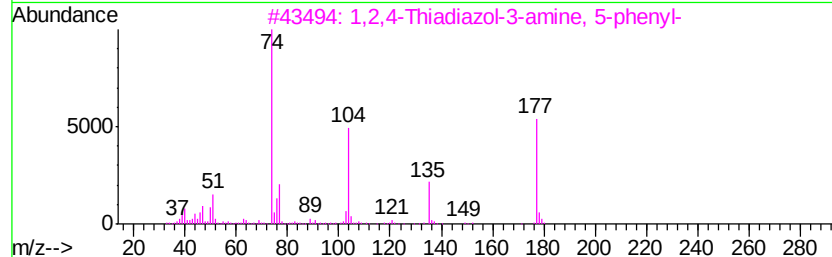
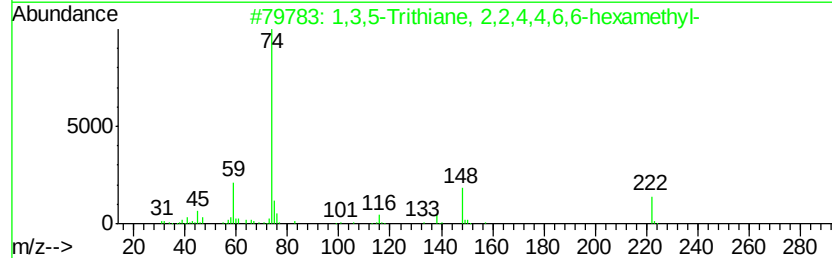
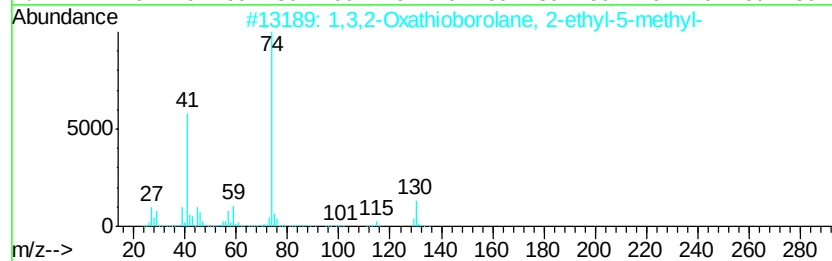
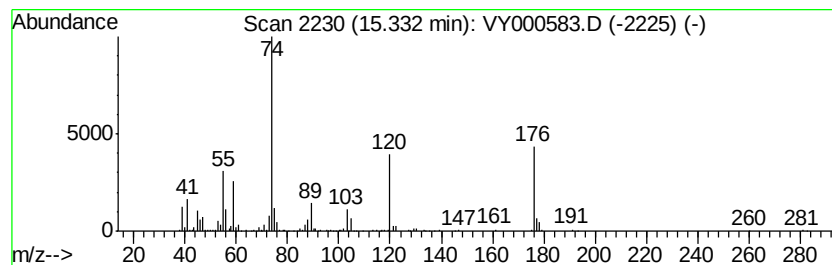
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 unknown15.33 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.33	16.04 ug/l	355102	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	35
2		1,3,5-Trithiane, 2,2,4,4,6,6-hex...	222	C9H18S3	000828-26-2	35
3		1,2,4-Thiadiazol-3-amine, 5-phenyl-	177	C8H7N3S	027182-54-3	17
4		1,3,4-Thiadiazol-2-amine, 5-methyl-	115	C3H5N3S	000108-33-8	17
5		tert-Butyldimethylsilylamine	131	C6H17NSi	1000366-62-1	12



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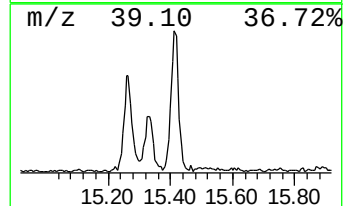
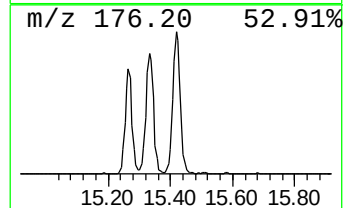
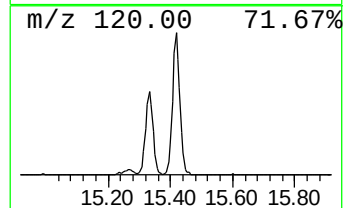
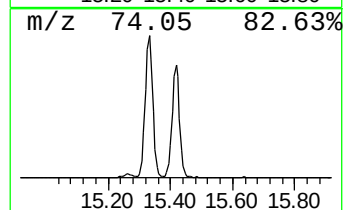
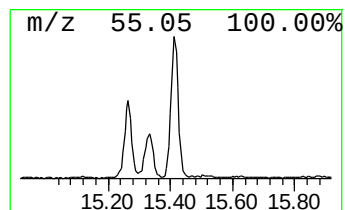
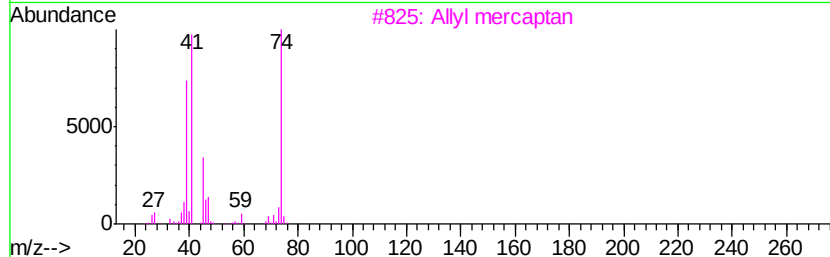
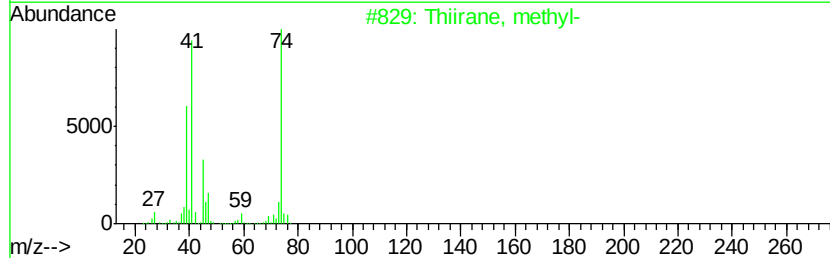
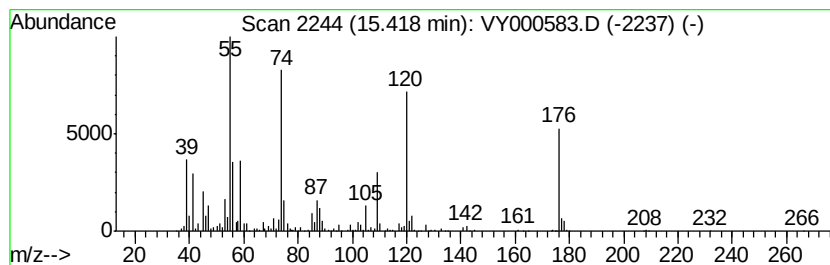
Quant Method : Z:\V0ASRV\HPCHEM1\MSV0A_Y\METHODS\82Y103019S.M
 Quant Title : SW846 8260

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

 Peak Number 6 unknown15.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.42	28.04 ug/l	620753	1,4-Dichlorobenzene-d4	13.42

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		D-Ribo-Hexose, 2,6-dideoxy-3-O-m...	162	C7H14O4	013089-76-4	38
2		Thiirane, methyl-	74	C3H6S	001072-43-1	25
3		Allyl mercaptan	74	C3H6S	000870-23-5	25
4		.alpha.-D-Glucopyranosiduronic a...	236	C9H16O7	031506-20-4	16
5		1,3-Dithiane	120	C4H8S2	000505-23-7	14



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_Y\DATA\VY110719\
Data File : VY000583.D
Acq On : 07 Nov 2019 16:12
Operator : SY/MD
Sample : K5723-14
Misc : 4.51G/5ML/MSVOA_Y/SOIL
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
10-C

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexane	5.77	6.5	ug/l	92320	1	7.80	710080	50.0
1-Propene, 3,3'-t...	13.30	5.3	ug/l	116758	4	13.42	1106840	50.0
unknown14.20	14.20	16.4	ug/l	364111	4	13.42	1106840	50.0
unknown15.27	15.27	24.6	ug/l	545133	4	13.42	1106840	50.0
unknown15.33	15.33	16.0	ug/l	355102	4	13.42	1106840	50.0
unknown15.42	15.42	28.0	ug/l	620753	4	13.42	1106840	50.0