

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_Y\DATA\VY110719\
 Data File : VY000582.D
 Acq On : 07 Nov 2019 15:49
 Operator : SY/MD
 Sample : K5723-13
 Misc : 6.11G/5ML/MSVOA_Y/SOIL
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 10-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	3.529	287	294	304	rBV3	6781	16480	1.20%	0.176%
2	4.724	478	490	498	rBV2	11993	36551	2.66%	0.391%
3	5.761	646	660	677	rBV3	37928	123044	8.96%	1.316%
4	7.730	971	983	988	rBV	186723	435073	31.69%	4.654%
5	7.797	988	994	1008	rVB	309807	714847	52.07%	7.647%
6	8.151	1043	1052	1064	rVB	197054	422865	30.80%	4.524%
7	8.693	1133	1141	1153	rBV	504631	1018472	74.19%	10.895%
8	10.181	1377	1385	1393	rBV	815673	1372881	100.00%	14.686%
9	11.485	1590	1599	1609	rBV	730140	1216555	88.61%	13.014%
10	12.333	1731	1738	1744	rBV3	33455	54187	3.95%	0.580%
11	12.479	1754	1762	1775	rVB	607332	939789	68.45%	10.053%
12	13.302	1892	1897	1901	rBV3	29711	51182	3.73%	0.548%
13	13.339	1901	1903	1910	rVB5	14254	17476	1.27%	0.187%
14	13.424	1910	1917	1924	rBV	743371	1126447	82.05%	12.050%
15	13.528	1930	1934	1941	rVB2	15096	24963	1.82%	0.267%
16	13.967	2001	2006	2012	rVB3	16563	27546	2.01%	0.295%
17	14.046	2012	2019	2027	rBV3	4647	15863	1.16%	0.170%
18	14.204	2027	2045	2060	rVV4	168529	730328	53.20%	7.813%
19	14.607	2107	2111	2116	rVB2	14450	20658	1.50%	0.221%
20	15.265	2202	2219	2225	rBV	186505	381785	27.81%	4.084%
21	15.332	2225	2230	2236	rVV2	116245	203490	14.82%	2.177%
22	15.411	2236	2243	2252	rVB2	177575	342252	24.93%	3.661%
23	15.881	2316	2320	2329	rVB5	11406	24380	1.78%	0.261%
24	16.009	2338	2341	2345	rBV2	7525	13882	1.01%	0.149%
25	16.295	2381	2388	2392	rVB8	7411	16923	1.23%	0.181%

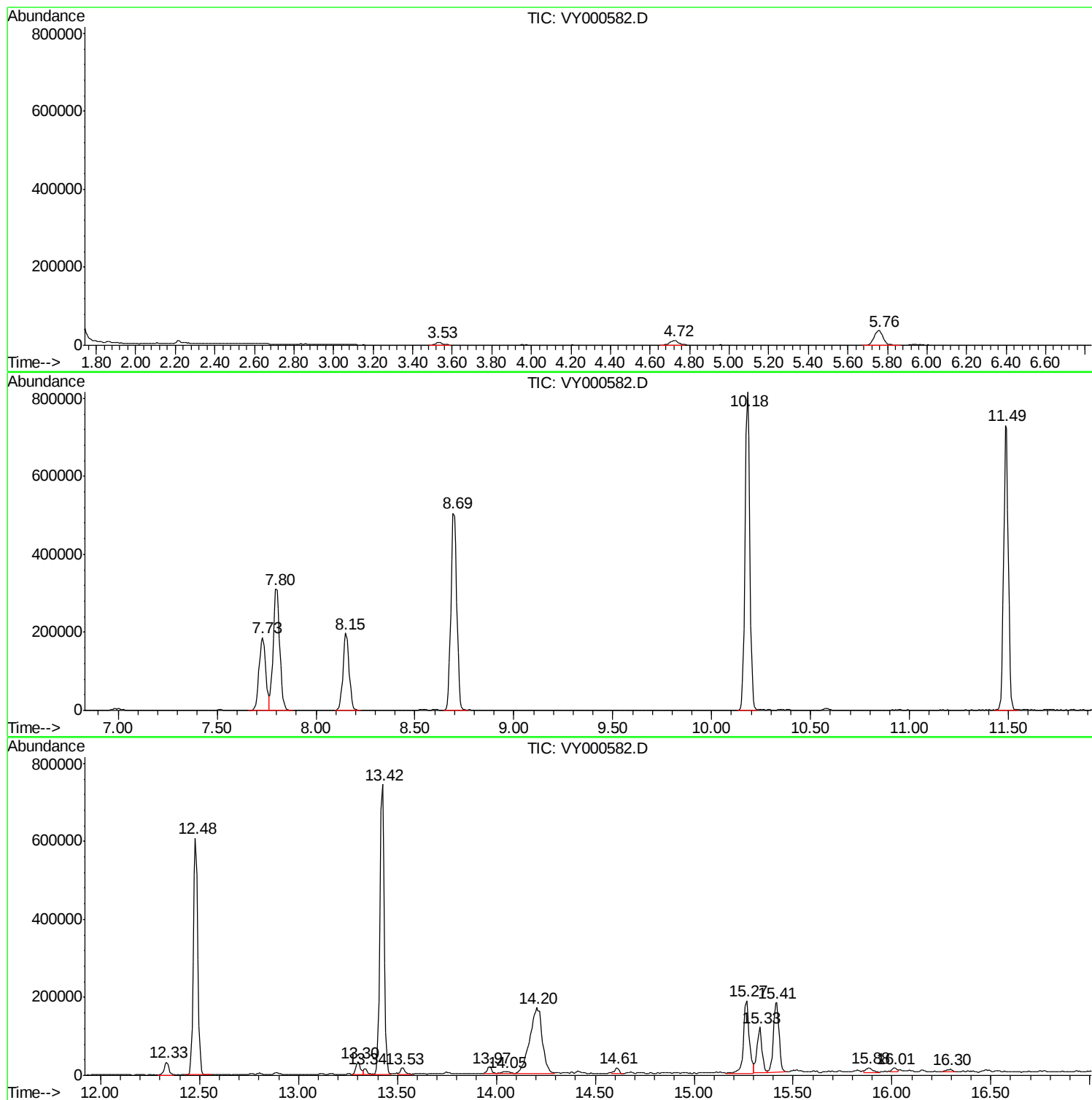
Sum of corrected areas: 9347919

Data Path : Z:\V0ASRV\HPCHEM1\MSV0A_Y\DATA\VY110719\
Data File : VY000582.D
Acq On : 07 Nov 2019 15:49
Operator : SY/MD
Sample : K5723-13
Misc : 6.11G/5ML/MSV0A_Y/SOIL
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSV0A_Y
ClientSampleId :
10-B

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



Data Path : Z:\V0ASRV\HPCHEM1\MSV0A_Y\DATA\VY110719\
Data File : VY000582.D
Acq On : 07 Nov 2019 15:49
Operator : SY/MD
Sample : K5723-13
Misc : 6.11G/5ML/MSV0A_Y/SOIL
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSV0A_Y
ClientSampleId :
10-B

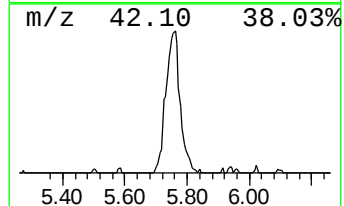
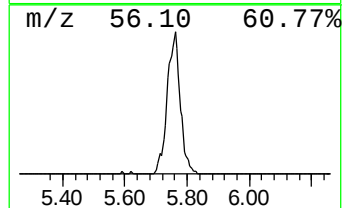
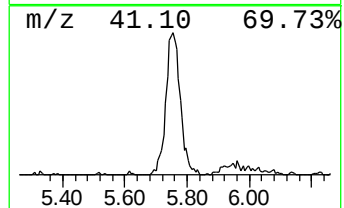
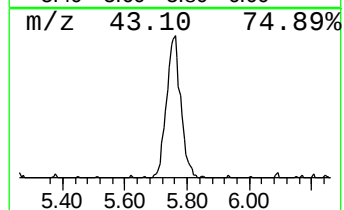
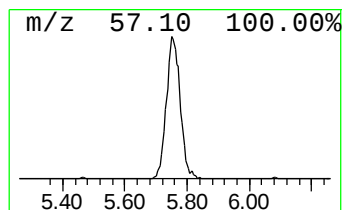
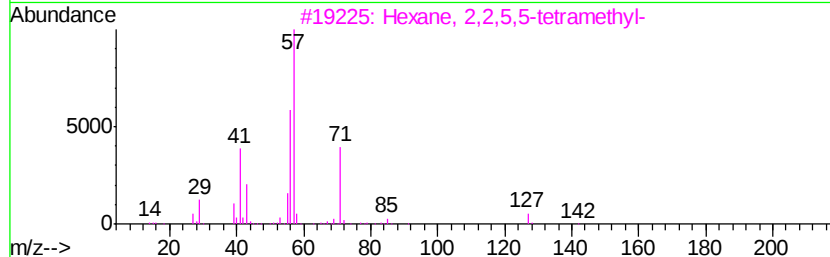
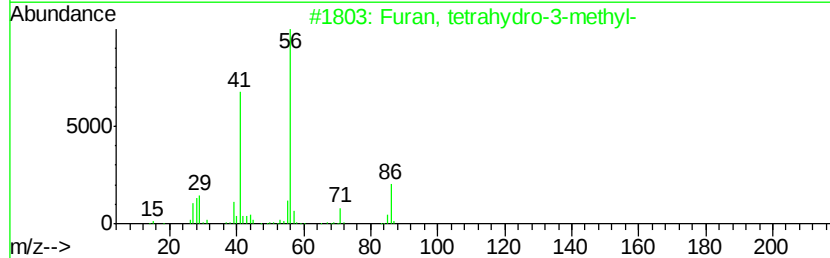
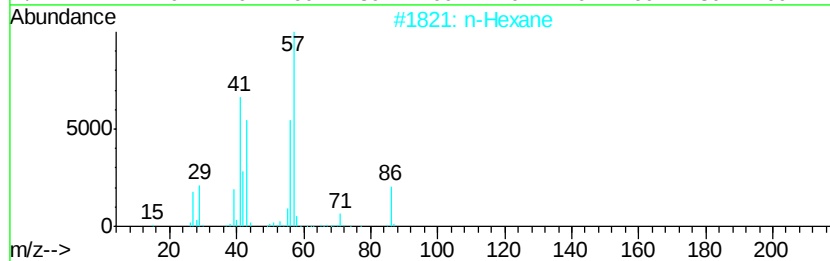
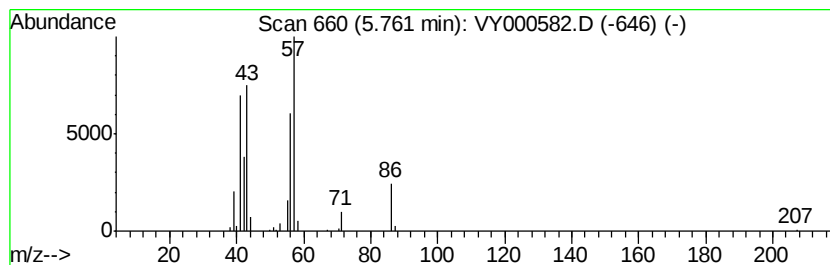
Quant Method : Z:\V0ASRV\HPCHEM1\MSV0A_Y\METHODS\82Y103019S.M
Quant Title : SW846 8260

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.
5.76	8.61 ug/l	123044	Pentafluorobenzene	7.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexane	86	C6H14	000110-54-3	91
2		Furan, tetrahydro-3-methyl-	86	C5H10O	013423-15-9	49
3		Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	47
4		Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	37
5		Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	36



Data Path : Z:\V0ASRV\HPCHEM1\MSV0A_Y\DATA\VY110719\
Data File : VY000582.D
Acq On : 07 Nov 2019 15:49
Operator : SY/MD
Sample : K5723-13
Misc : 6.11G/5ML/MSV0A_Y/SOIL
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSV0A_Y
ClientSampleId :
10-B

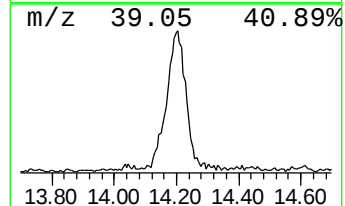
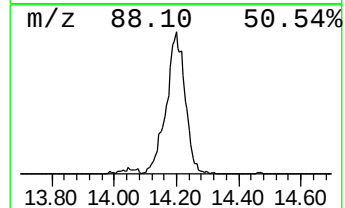
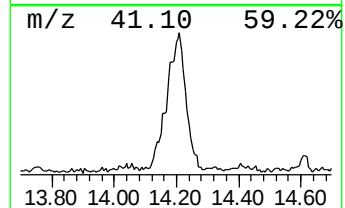
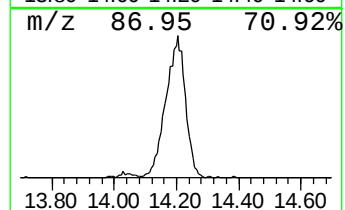
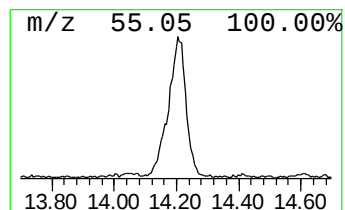
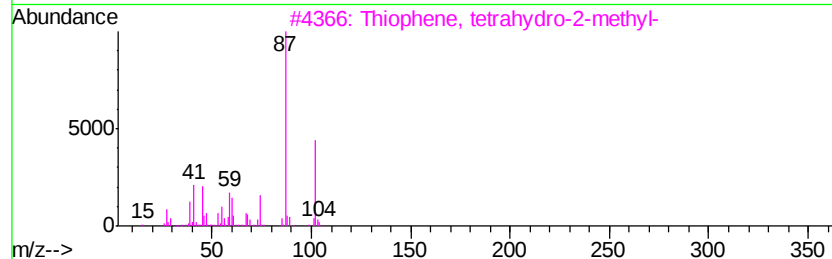
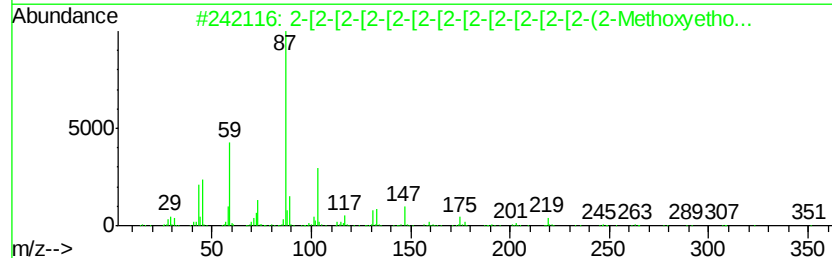
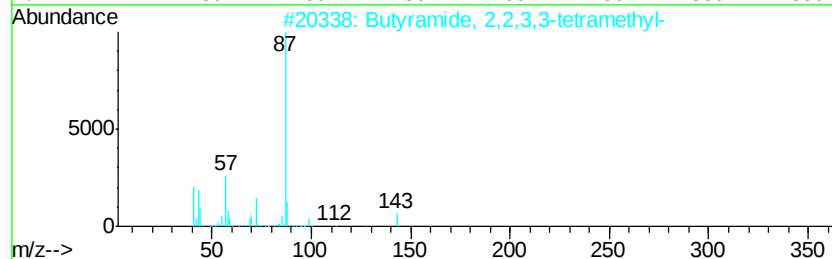
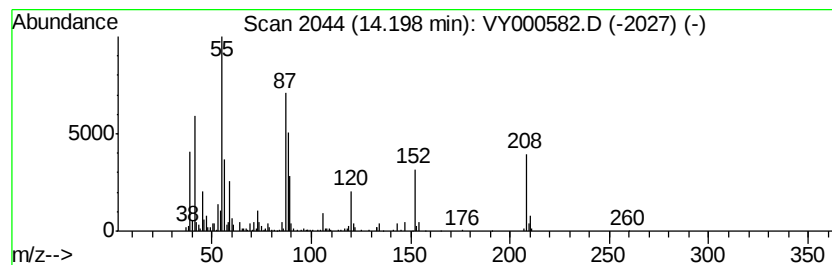
Quant Method : Z:\V0ASRV\HPCHEM1\MSV0A_Y\METHODS\82Y103019S.M
Quant Title : SW846 8260

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

Peak Number 2 unknown14.20 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.20	32.42 ug/l	730328	1,4-Dichlorobenzene-d4	13.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butyramide, 2,2,3,3-tetramethyl-	143	C8H17NO	098486-62-5	10
2		2-[2-[2-[2-[2-[2-[2-[2-[2-...	646	C29H58O15	1000351-92-0	10
3		Thiophene, tetrahydro-2-methyl-	102	C5H10S	001795-09-1	10
4		2-Propenenitrile, 2-chloro-	87	C3H2ClN	000920-37-6	10
5		1,2,4-Trithiolane, 3,5-bis(1-met...	208	C8H16S3	054934-99-5	10



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_Y\DATA\VY110719\
Data File : VY000582.D
Acq On : 07 Nov 2019 15:49
Operator : SY/MD
Sample : K5723-13
Misc : 6.11G/5ML/MSVOA_Y/SOIL
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
10-B

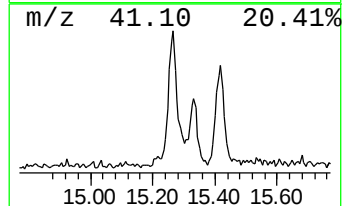
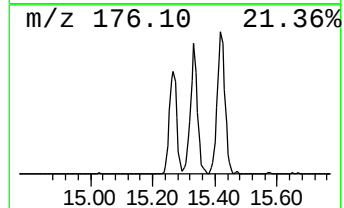
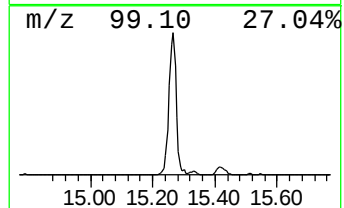
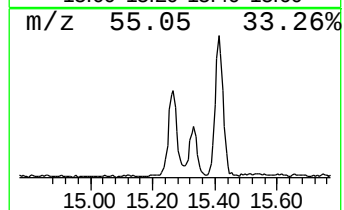
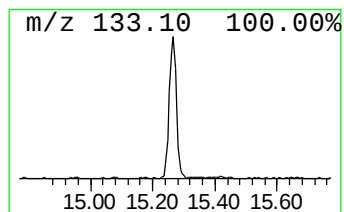
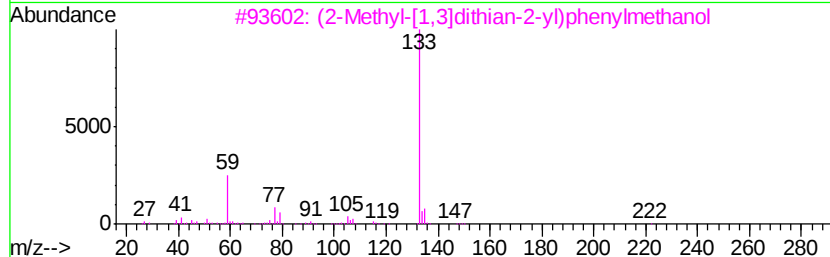
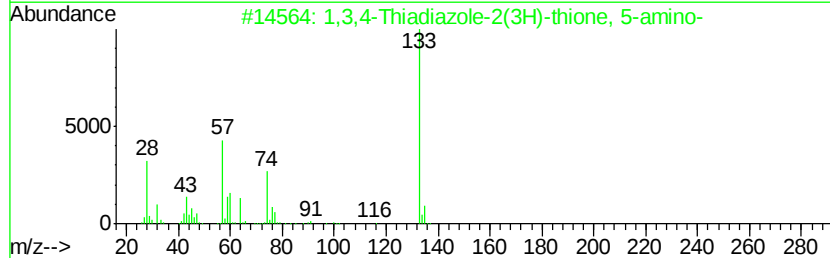
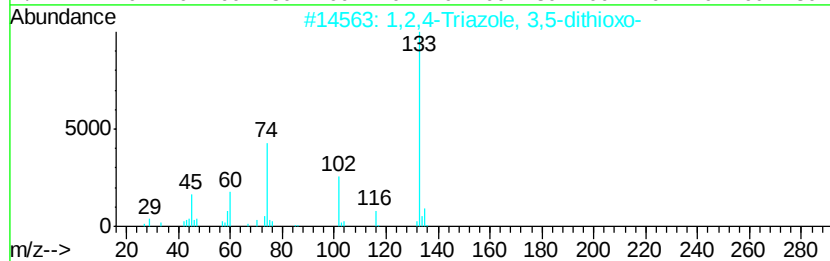
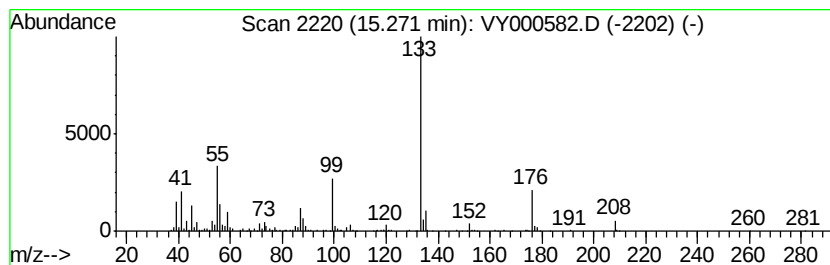
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_Y\METHODS\82Y103019S.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	16.95 ug/l	381785	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	52
2		1,3,4-Thiadiazole-2(3H)-thione, ...	133	C2H3N3S2	002349-67-9	52
3		(2-Methyl-[1,3]dithian-2-yl)phen...	240	C12H16OS2	078349-00-5	50
4		Rhodanine	133	C3H3NOS2	000141-84-4	50
5		Benzoic acid, 4-ethyl-, 4-cyanop...	251	C16H13NO2	056131-48-7	37



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_Y\DATA\VY110719\
Data File : VY000582.D
Acq On : 07 Nov 2019 15:49
Operator : SY/MD
Sample : K5723-13
Misc : 6.11G/5ML/MSVOA_Y/SOIL
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
10-B

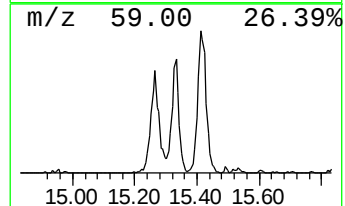
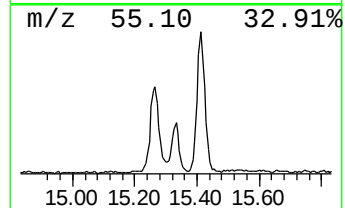
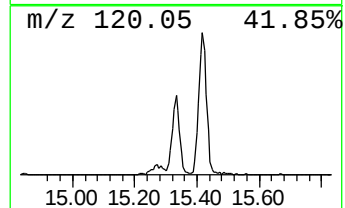
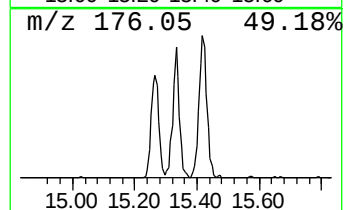
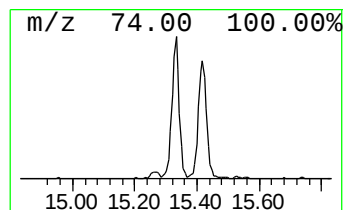
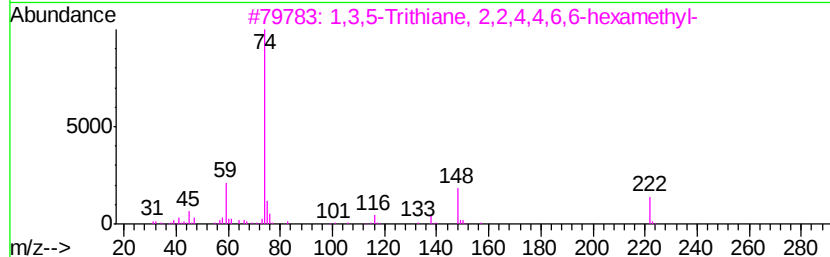
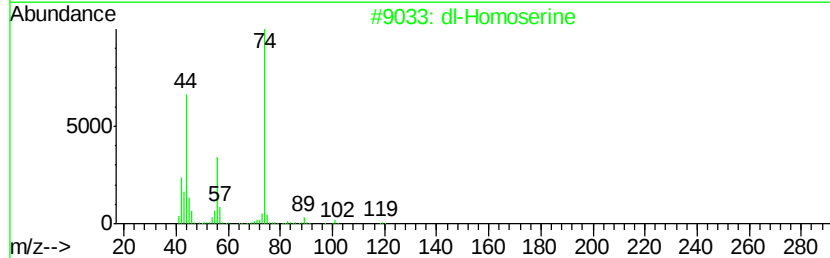
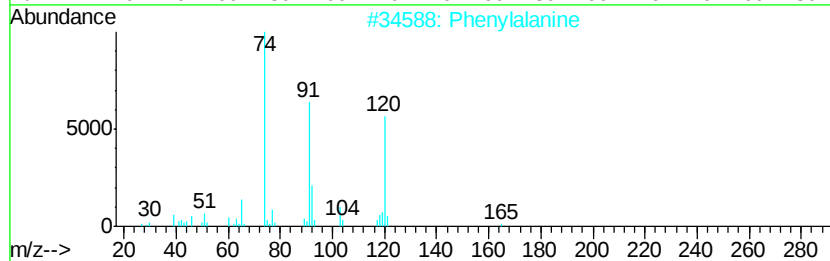
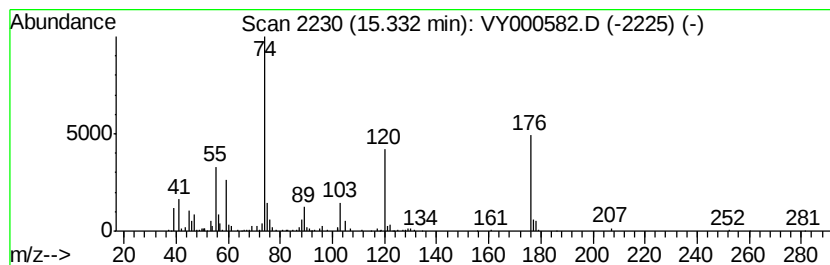
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_Y\METHODS\82Y103019S.M
Quant Title : SW846 8260

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

Peak Number 4 unknown15.33 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.33	9.03 ug/l	203490	1,4-Dichlorobenzene-d4	13.42

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenylalanine	165	C9H11NO2	000063-91-2	28
2			dl-Homoserine	119	C4H9NO3	001927-25-9	27
3			1,3,5-Trithiane, 2,2,4,4,6,6-hex...	222	C9H18S3	000828-26-2	25
4			Urea, N-ethyl-N-nitroso-	117	C3H7N3O2	000759-73-9	17
5			1,3,2-Oxathioborolane, 2-ethyl-5...	130	C5H11BOS	1000163-05-5	16



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_Y\DATA\VY110719\
Data File : VY000582.D
Acq On : 07 Nov 2019 15:49
Operator : SY/MD
Sample : K5723-13
Misc : 6.11G/5ML/MSVOA_Y/SOIL
ALS Vial : 17 Sample Multiplier: 1

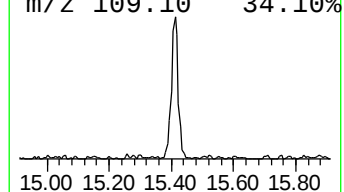
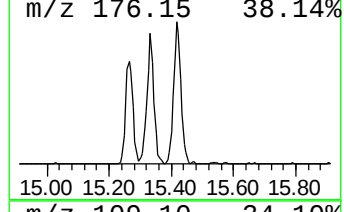
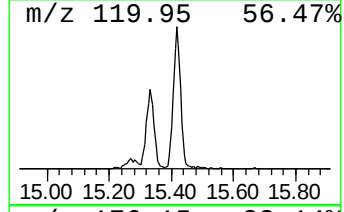
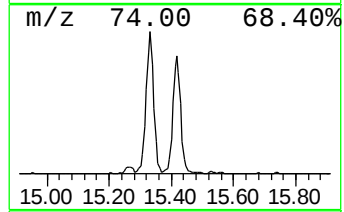
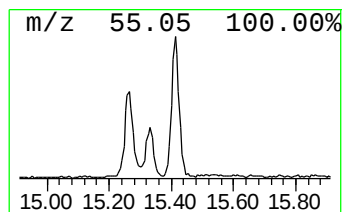
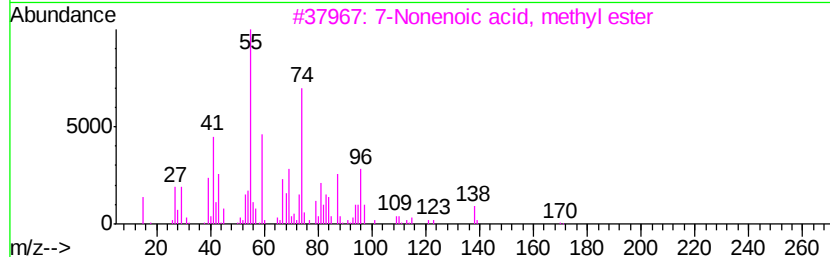
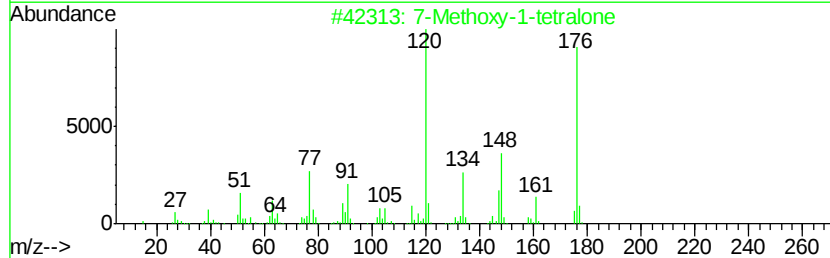
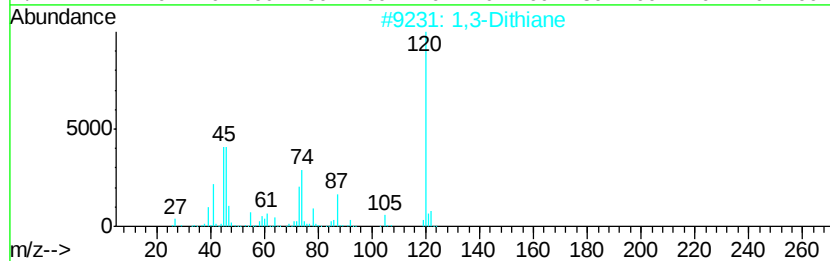
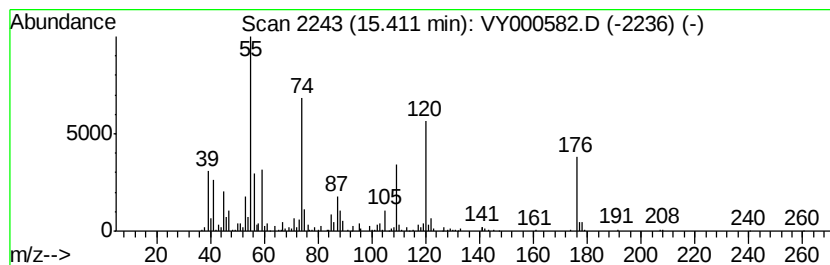
Instrument :
MSVOA_Y
ClientSampleId :
10-B

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 5 unknown15.41 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.41	15.19 ug/l	342252	1,4-Dichlorobenzene-d4	13.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dithiane	120	C4H8S2	000505-23-7	14
2	7-Methoxy-1-tetralone	176	C11H12O2	006836-19-7	12
3	7-Nonenoic acid, methyl ester	170	C10H18O2	020731-22-0	12
4	1-(p-Tolyl)-2-imidazolidinone	176	C10H12N2O	090917-76-3	12
5	Thiirane, methyl-	74	C3H6S	001072-43-1	11



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_Y\DATA\VY110719\
Data File : VY000582.D
Acq On : 07 Nov 2019 15:49
Operator : SY/MD
Sample : K5723-13
Misc : 6.11G/5ML/MSVOA_Y/SOIL
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
10-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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexane	5.76	8.6	ug/l	123044	1	7.80	714847	50.0
unknown14.20	14.20	32.4	ug/l	730328	4	13.42	1126450	50.0
1,2,4-Triazole, 3...	15.27	16.9	ug/l	381785	4	13.42	1126450	50.0
unknown15.33	15.33	9.0	ug/l	203490	4	13.42	1126450	50.0
unknown15.41	15.41	15.2	ug/l	342252	4	13.42	1126450	50.0