

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX041720\
 Data File : VX015751.D
 Acq On : 17 Apr 2020 20:10
 Operator : JC/SP
 Sample : L2305-03
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 I-LG-C-1

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_X\METHOD\82X032720W.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	1.064	26	29	37	rBV	3815151	4578009	3.25%	1.336%
2	1.131	37	40	46	rVV	1869429	3481456	2.47%	1.016%
3	1.180	46	48	56	rVV	1218182	1920109	1.36%	0.560%
4	1.564	108	111	160	rVB2	51707974	131563073	93.41%	38.403%
5	2.253	218	224	245	rVB	2231851	4267421	3.03%	1.246%
6	2.417	245	251	256	rBV	3359083	5350008	3.80%	1.562%
7	2.557	266	274	309	rVB3	52327730	140850095	100.00%	41.114%
8	5.465	740	751	764	rBV	535555	1554469	1.10%	0.454%
9	5.636	768	779	793	rBV2	922336	2571023	1.83%	0.750%
10	6.038	835	845	851	rBV	583979	1572188	1.12%	0.459%
11	6.118	851	858	874	rVB	1648482	4280400	3.04%	1.249%
12	6.837	966	976	988	rBV	1429502	3473701	2.47%	1.014%
13	8.465	1235	1243	1251	rBV	5548310	9366288	6.65%	2.734%
14	8.697	1275	1281	1288	rBV	3047263	4802301	3.41%	1.402%
15	8.892	1303	1313	1322	rVB	1511193	2376670	1.69%	0.694%
16	10.099	1505	1511	1515	rBV	3343791	4422071	3.14%	1.291%
17	11.123	1673	1679	1685	rBV	3154595	3987630	2.83%	1.164%
18	11.702	1768	1774	1785	rVB	2241698	2986898	2.12%	0.872%
19	12.062	1827	1833	1839	rVB	3879400	4907757	3.48%	1.433%
20	13.818	2116	2121	2128	rVB	3472919	4270851	3.03%	1.247%

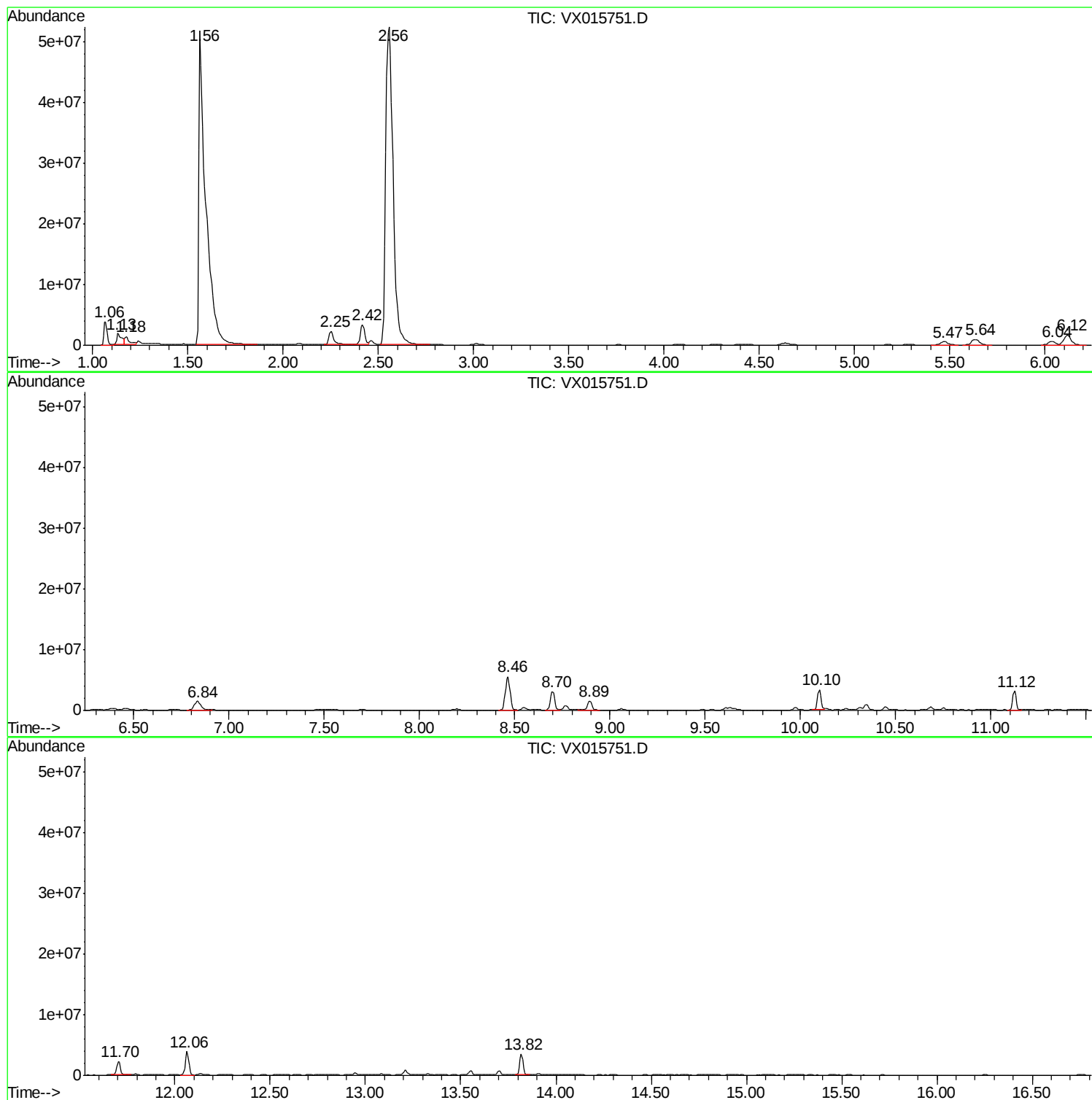
Sum of corrected areas: 342582418

Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX041720\
Data File : VX015751.D
Acq On : 17 Apr 2020 20:10
Operator : JC/SP
Sample : L2305-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
I-LG-C-1

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX041720\
Data File : VX015751.D
Acq On : 17 Apr 2020 20:10
Operator : JC/SP
Sample : L2305-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
I-LG-C-1

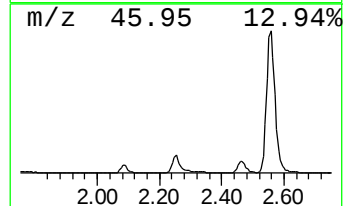
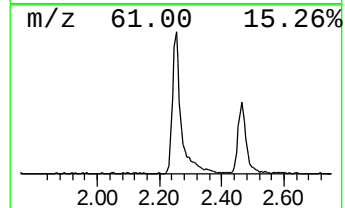
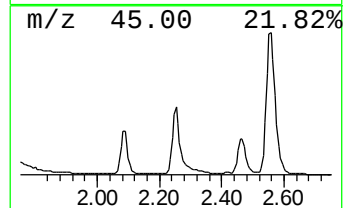
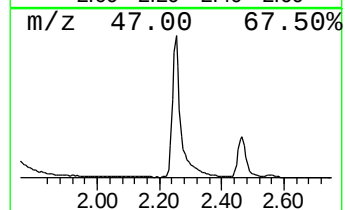
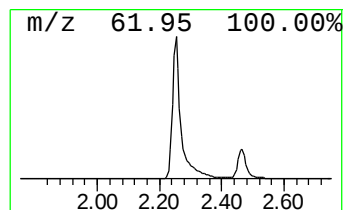
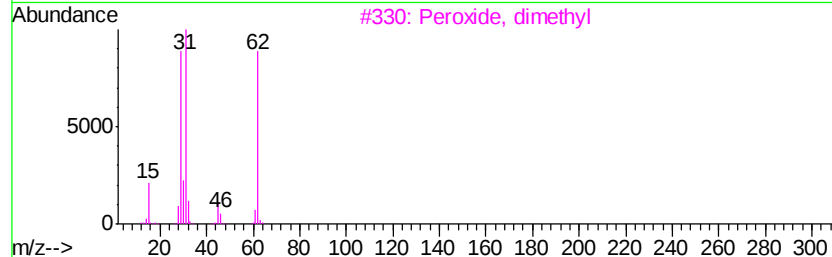
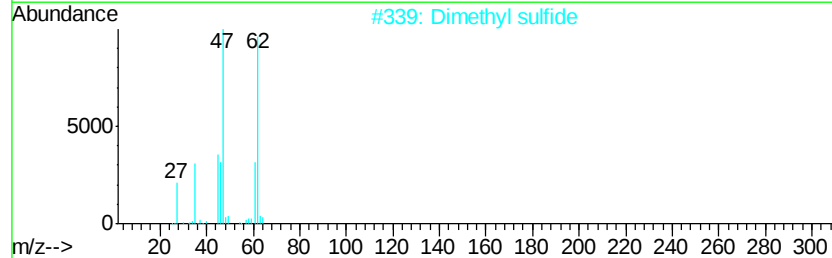
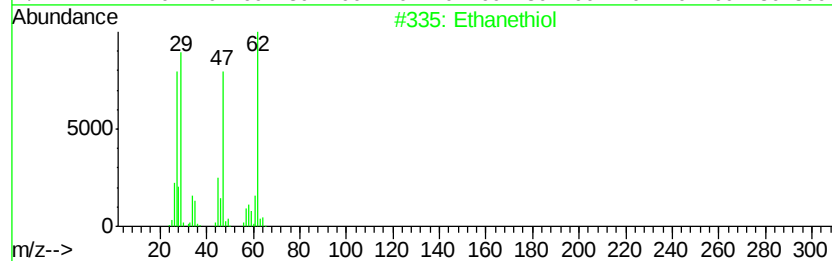
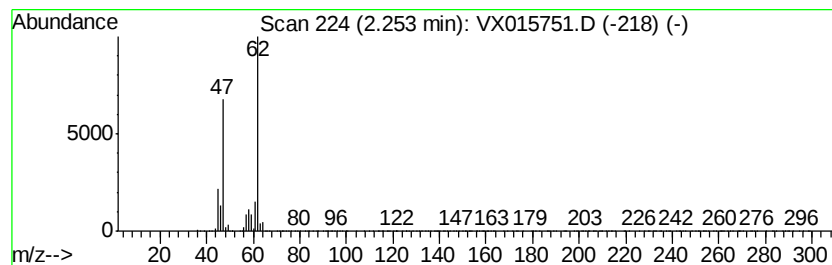
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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

Peak Number 5 Ethanethiol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	82.99 ug/l	4267420	Pentafluorobenzene	5.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanethiol	62	C2H6S	000075-08-1	91	
2	Dimethyl sulfide	62	C2H6S	000075-18-3	64	
3	Peroxide, dimethyl	62	C2H6O2	000690-02-8	64	
4	Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	25	
5	Ethene, chloro-	62	C2H3Cl	000075-01-4	9	



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX041720\
Data File : VX015751.D
Acq On : 17 Apr 2020 20:10
Operator : JC/SP
Sample : L2305-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
I-LG-C-1

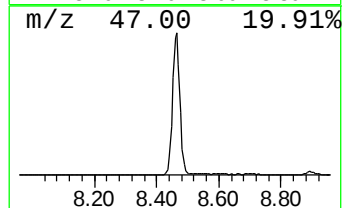
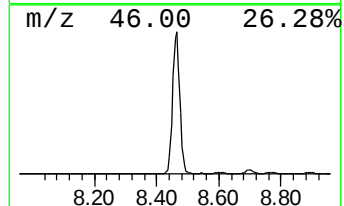
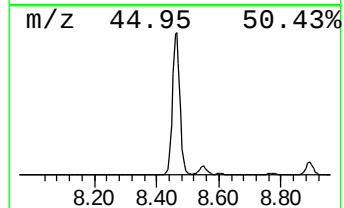
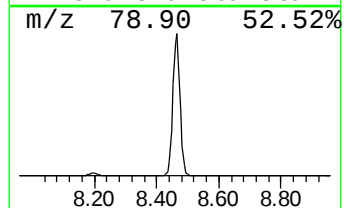
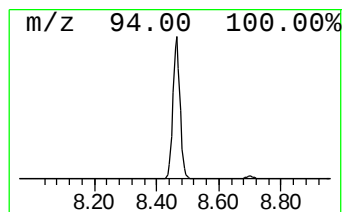
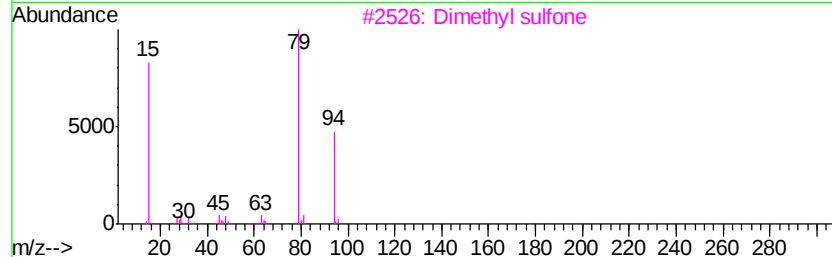
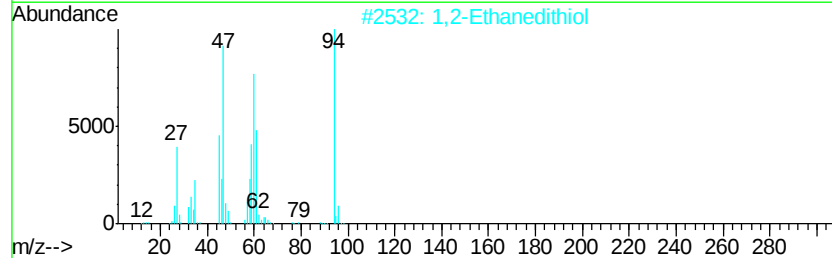
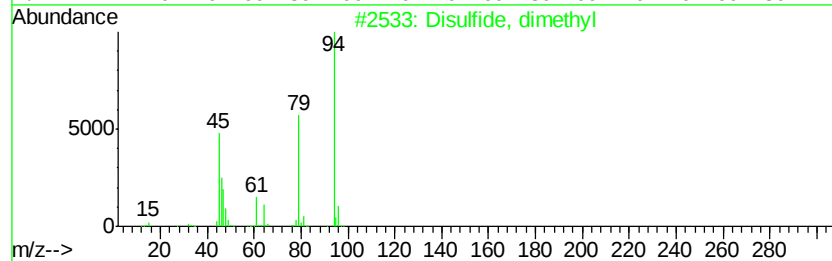
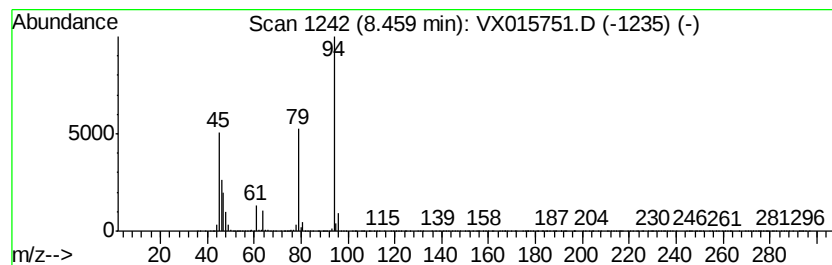
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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

Peak Number 6 Disulfide, dimethyl Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.46	134.82 ug/l	9366290	1,4-Difluorobenzene	6.84

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Disulfide, dimethyl	94	C2H6S2	000624-92-0	97
2		1,2-Ethanedithiol	94	C2H6S2	000540-63-6	58
3		Dimethyl sulfone	94	C2H6O2S	000067-71-0	46
4		Methanesulfonyl chloride	114	CH3ClO2S	000124-63-0	7
5		Pyrazine, methyl-	94	C5H6N2	000109-08-0	5



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX041720\
Data File : VX015751.D
Acq On : 17 Apr 2020 20:10
Operator : JC/SP
Sample : L2305-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
I-LG-C-1

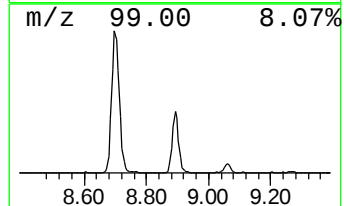
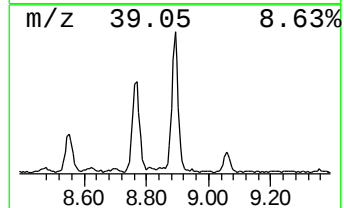
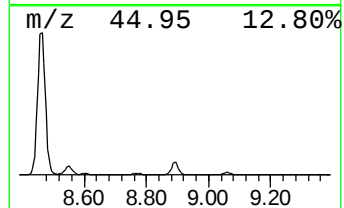
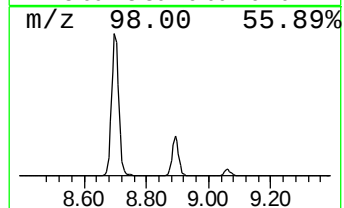
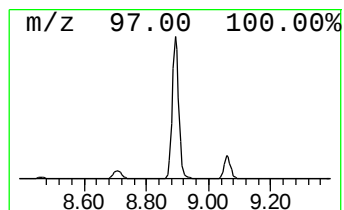
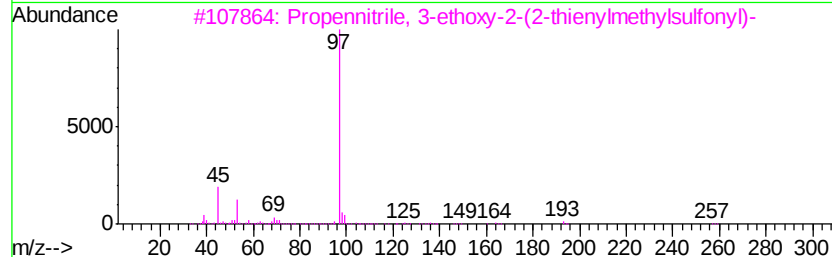
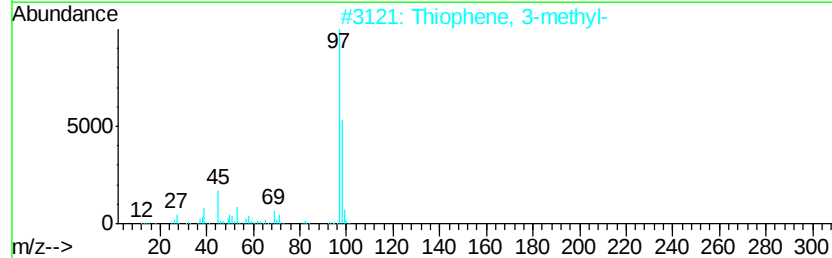
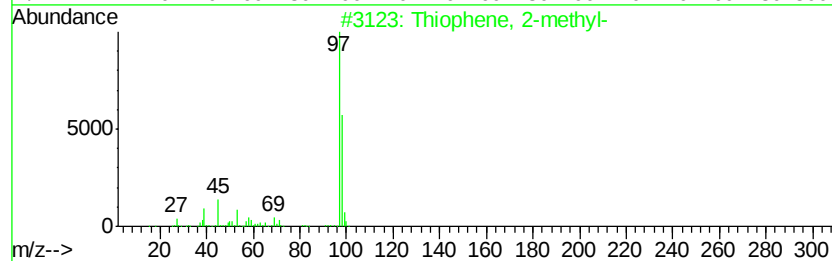
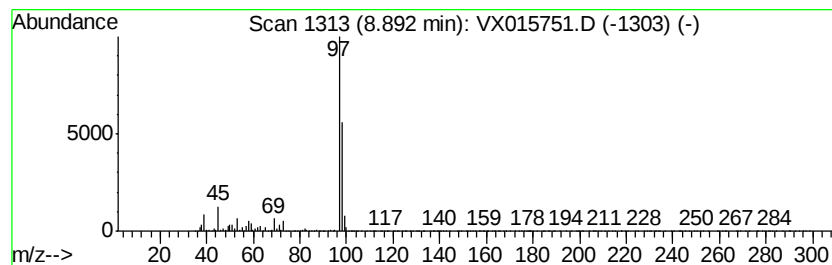
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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

Peak Number 7 Thiophene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.89	26.87 ug/l	2376670	Chlorobenzene-d5	10.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Thiophene, 2-methyl-	98	C5H6S	000554-14-3	95
2		Thiophene, 3-methyl-	98	C5H6S	000616-44-4	93
3		Propennitrile, 3-ethoxy-2-(2-thi...	257	C10H11N03S2	1000267-97-5	50
4		3H-Pyrazol-3-one, 2,4-dihydro-5-...	98	C4H6N2O	000108-26-9	10
5		1H-Pyrazol-4-amine, 3-methyl-	97	C4H7N3	1000338-28-2	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX041720\
Data File : VX015751.D
Acq On : 17 Apr 2020 20:10
Operator : JC/SP
Sample : L2305-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

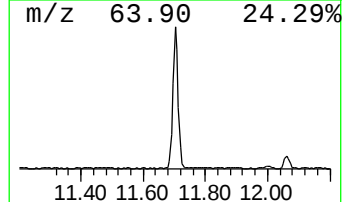
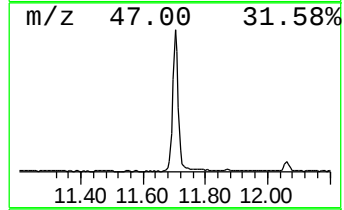
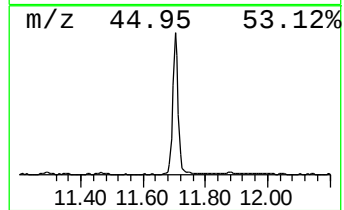
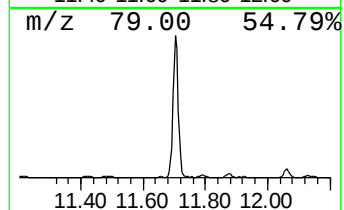
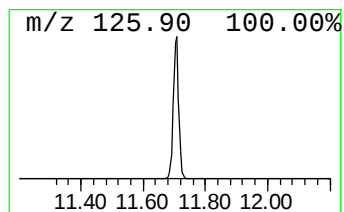
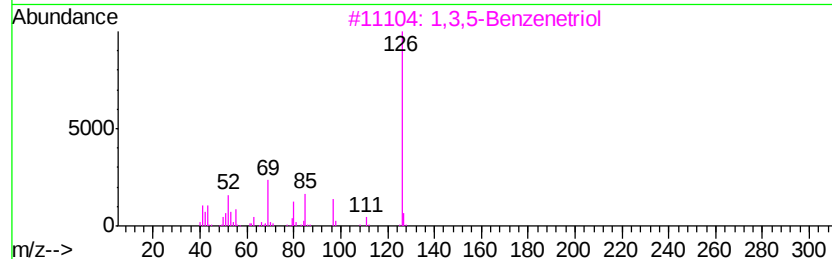
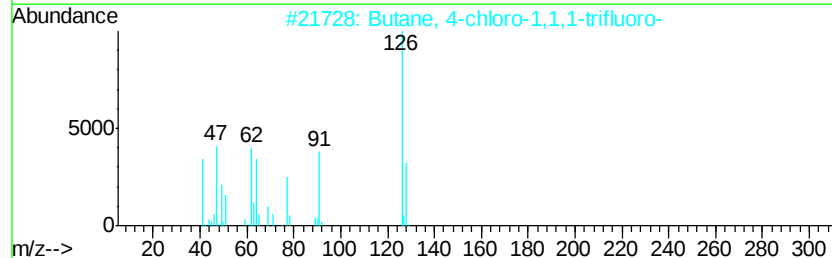
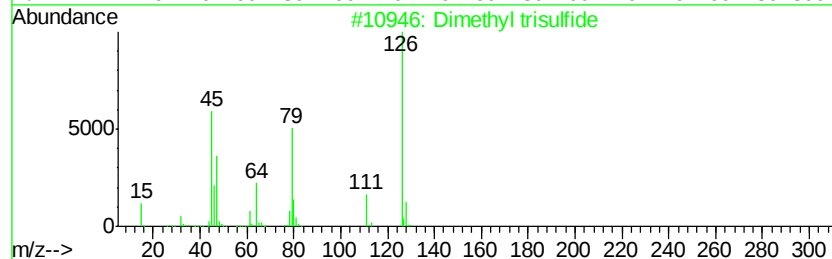
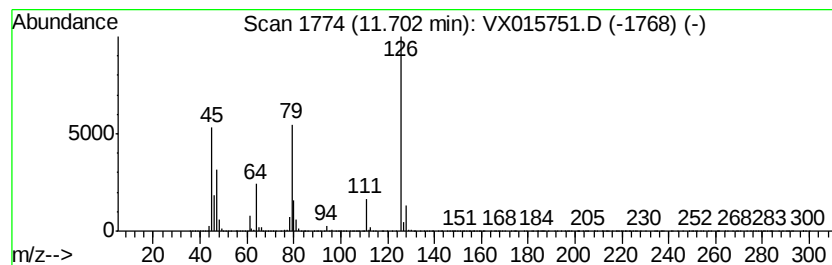
Instrument :
MSVOA_X
ClientSampleId :
I-LG-C-1

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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

Peak Number 8 Dimethyl trisulfide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	30.43 ug/l	2986900	1,4-Dichlorobenzene-d4	12.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Dimethyl trisulfide	126 C2H6S3	003658-80-8 96
2		Butane, 4-chloro-1,1,1-trifluoro-	146 C4H6ClF3	000406-85-9 23
3		1,3,5-Benzenetriol	126 C6H6O3	000108-73-6 12
4		Methyl 2-hydroxyethyl sulfoxide	108 C3H8O2S	021281-74-3 12
5		Dimethyldithiophosphinic acid	126 C2H7PS2	016367-68-3 10



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX041720\
Data File : VX015751.D
Acq On : 17 Apr 2020 20:10
Operator : JC/SP
Sample : L2305-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
I-LG-C-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.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
Ethanethiol	2.25	83.0	ug/l	4267420	1	5.64	2571020	50.0
Disulfide, dimethyl	8.46	134.8	ug/l	9366290	2	6.84	3473700	50.0
Thiophene, 2-methyl-	8.89	26.9	ug/l	2376670	3	10.10	4422070	50.0
Dimethyl trisulfide	11.70	30.4	ug/l	2986900	4	12.06	4907760	50.0