

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV012820\
 Data File : VV014417.D
 Acq On : 28 Jan 2020 13:39
 Operator : SY/MD
 Sample : L1253-08
 Misc : 25.0mL/MSVOA V/WATER
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 H0AC5

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.1
 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_V\METHOD\SOMVTR010220WMA.M
 Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.499	119	127	151	rBV	2556042	3564808	4.80%	2.561%
2	2.245	350	359	372	rVB	988588	1463979	1.97%	1.052%
3	3.968	876	895	929	rBV	13252700	32183647	43.30%	23.121%
4	4.405	1019	1031	1045	rBV	324278	751567	1.01%	0.540%
5	5.097	1229	1246	1274	rBV2	1394959	3117011	4.19%	2.239%
6	5.669	1401	1424	1442	rBV	1019583	2177371	2.93%	1.564%
7	5.961	1495	1515	1545	rBV	37600418	74331438	100.00%	53.400%
8	6.132	1551	1568	1586	rBV3	728593	1927417	2.59%	1.385%
9	6.254	1588	1606	1627	rVB2	1422044	3721549	5.01%	2.674%
10	6.460	1661	1670	1700	rVB	771176	1428254	1.92%	1.026%
11	7.154	1873	1886	1905	rBV	632699	1345892	1.81%	0.967%
12	7.376	1944	1955	1970	rBV	1565676	2632544	3.54%	1.891%
13	8.151	2182	2196	2216	rBV	1343157	2622849	3.53%	1.884%
14	8.900	2417	2429	2446	rBV	1407194	2347422	3.16%	1.686%
15	10.977	3067	3075	3091	rVB	676006	1051773	1.41%	0.756%
16	11.292	3161	3173	3191	rVB	1430586	2356794	3.17%	1.693%
17	11.669	3278	3290	3309	rVB	1312902	2173703	2.92%	1.562%

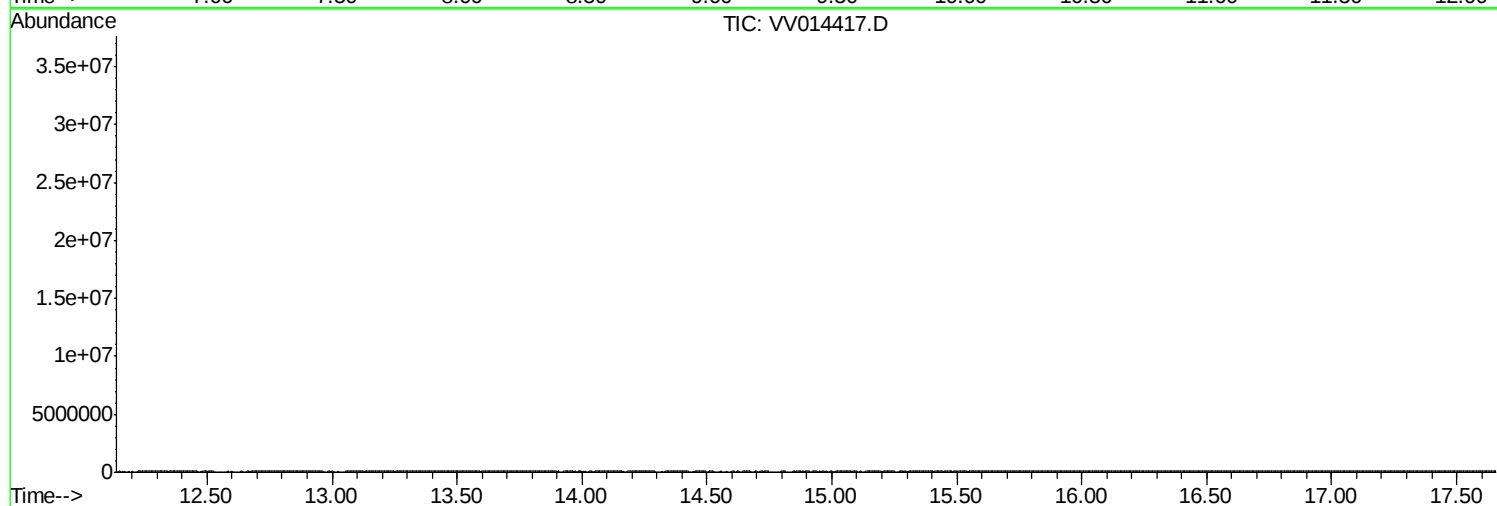
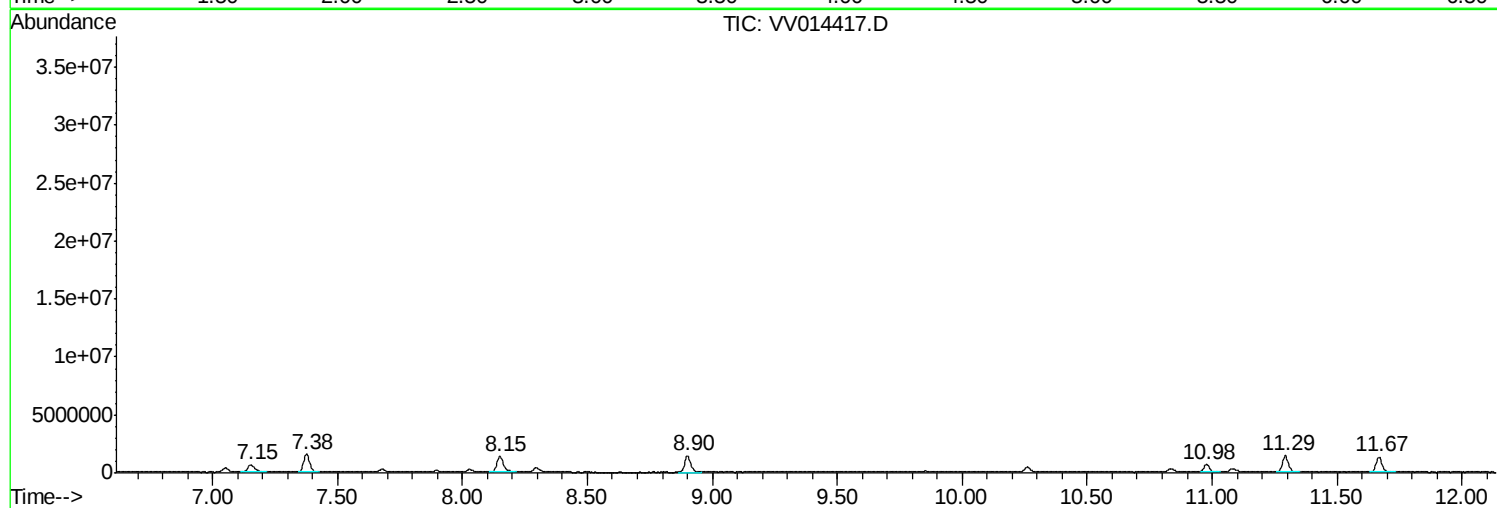
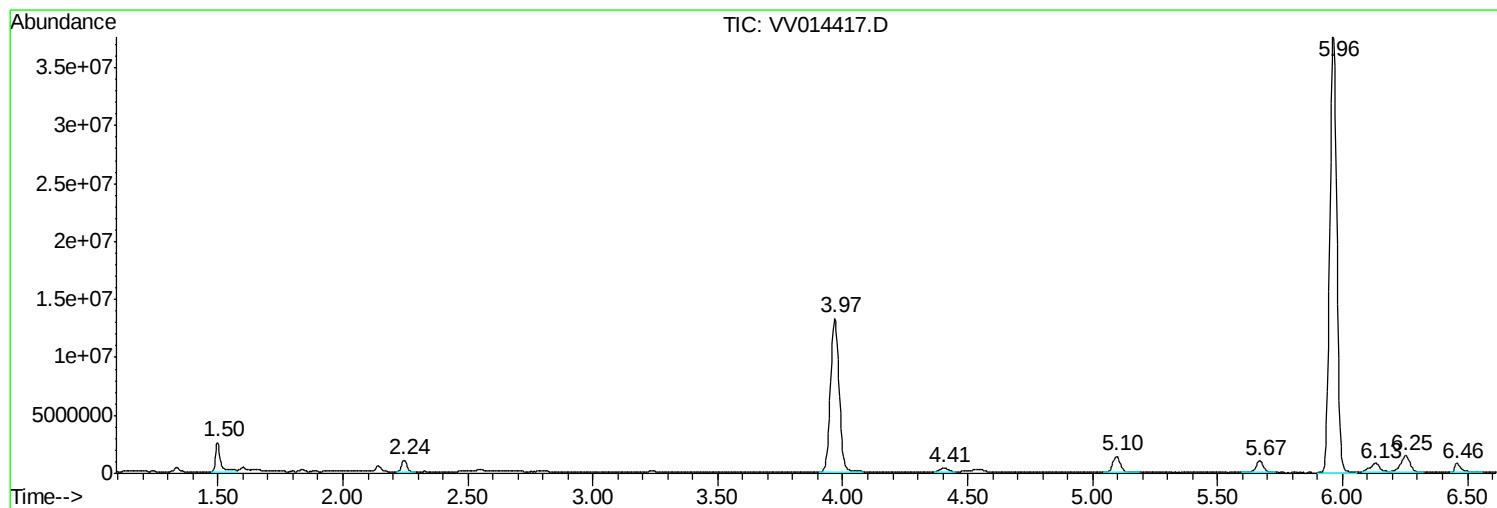
Sum of corrected areas: 139198018

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Quant Title : TRACE VOA SOM01.0

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



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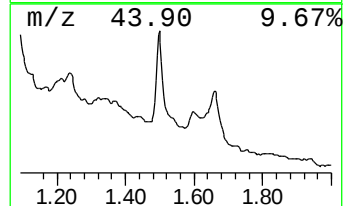
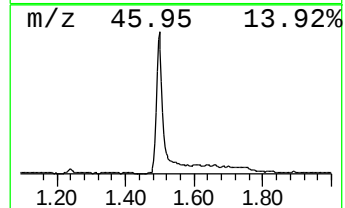
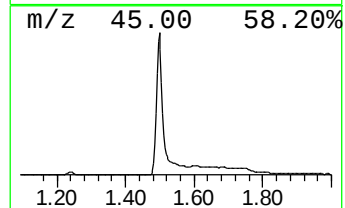
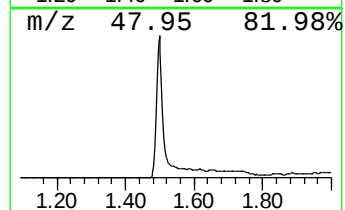
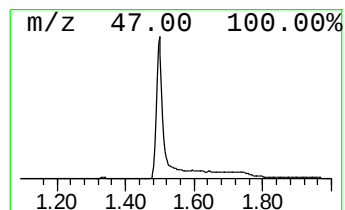
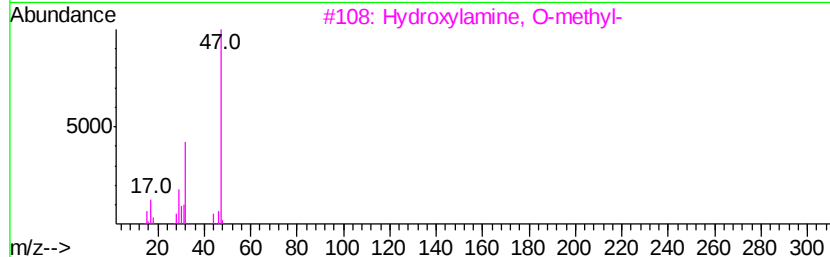
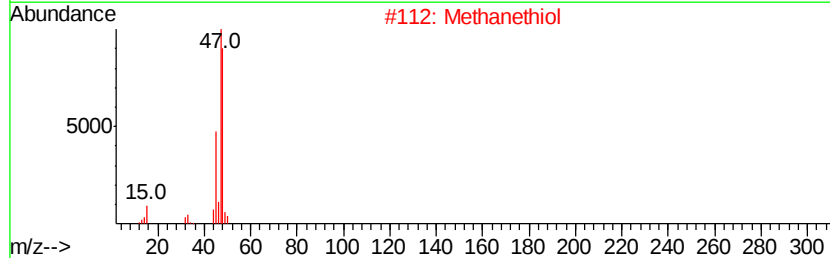
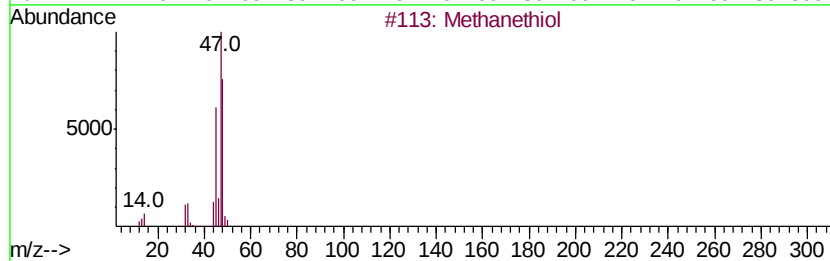
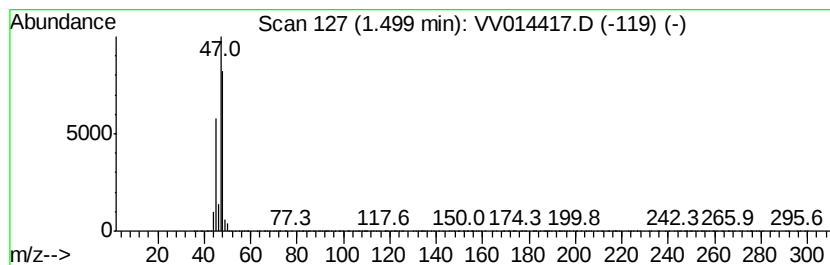
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Methanethiol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.50	8.19 ug/L	3564810	1,4-Difluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methanethiol	48	CH4S	000074-93-1	91
2		Methanethiol	48	CH4S	000074-93-1	90
3		Hvdroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
4		Hvdroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
5		Methane, nitroso-	45	CH3NO	000865-40-7	5



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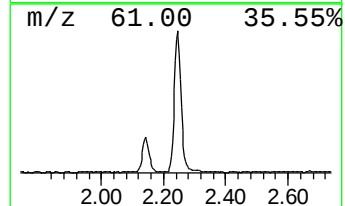
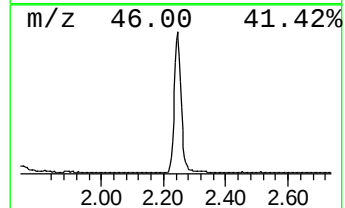
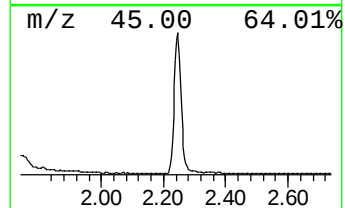
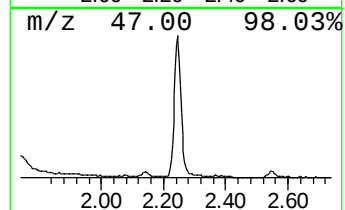
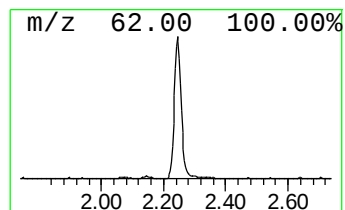
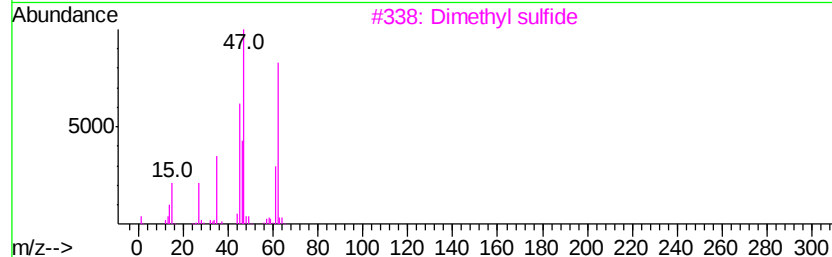
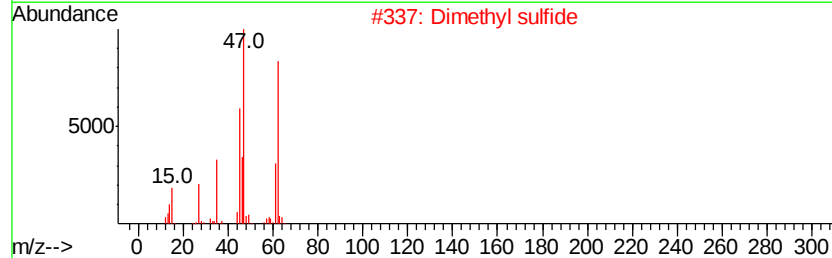
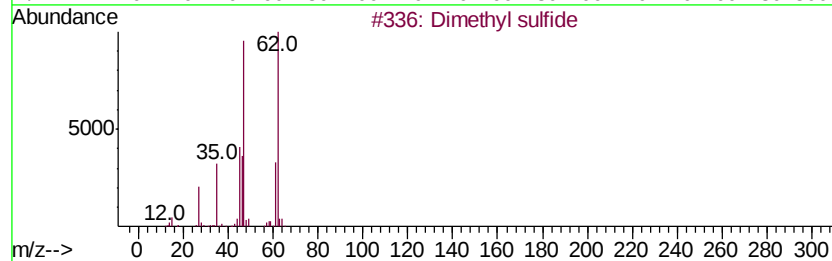
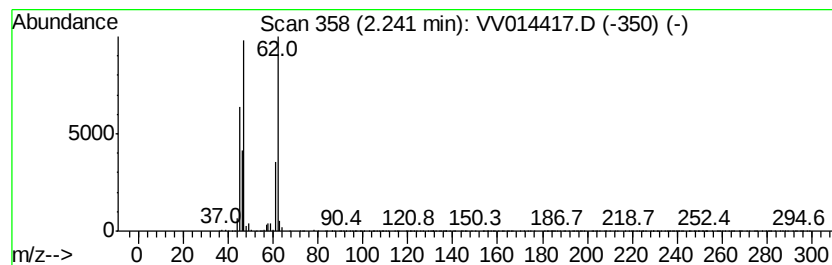
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 Dimethyl sulfide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.24	3.36 ug/L	1463980	1,4-Difluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dimethyl sulfide	62	C2H6S	000075-18-3	91
2		Dimethyl sulfide	62	C2H6S	000075-18-3	91
3		Dimethyl sulfide	62	C2H6S	000075-18-3	91
4		Dimethyl sulfide	62	C2H6S	000075-18-3	91
5		Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	78



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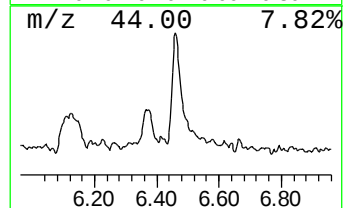
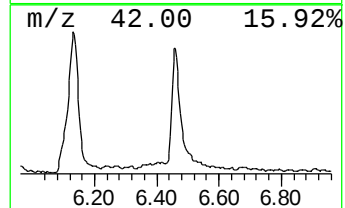
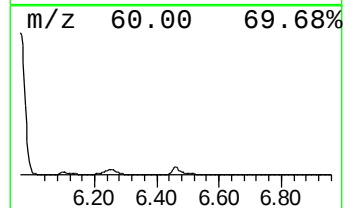
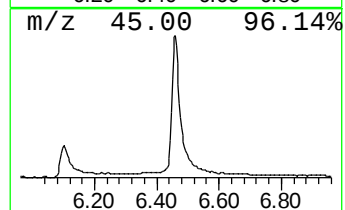
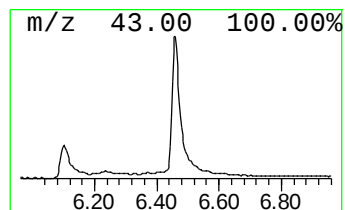
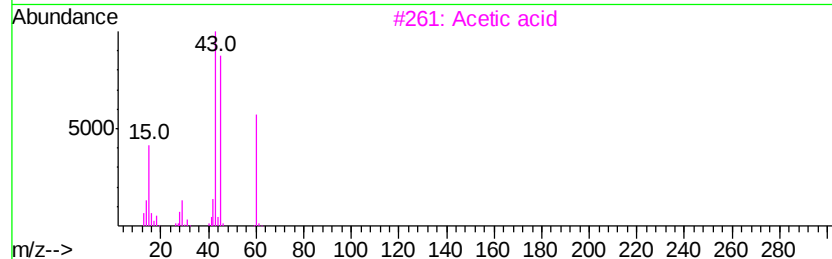
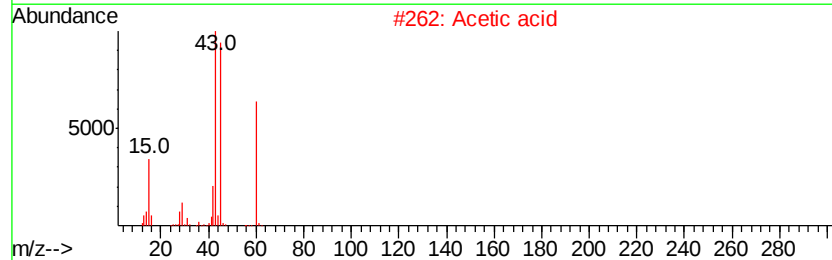
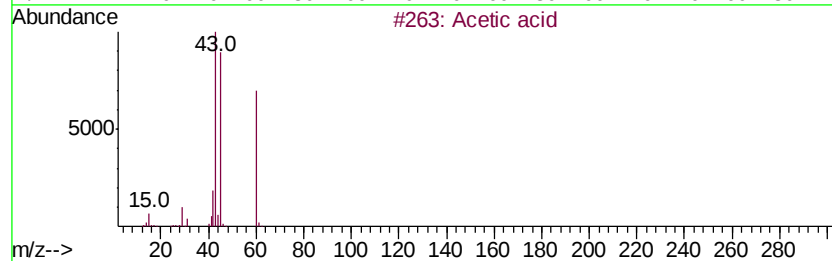
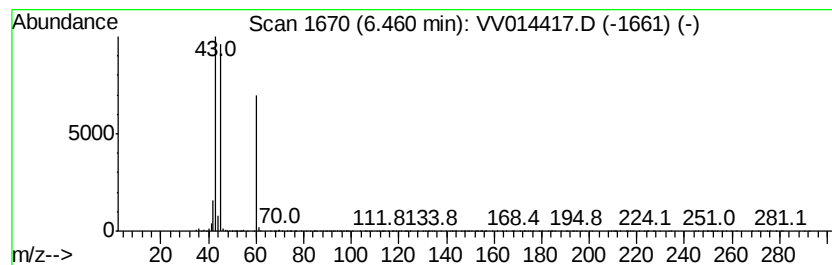
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 Acetic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	3.28 ug/L	1428250	1,4-Difluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid	60	C2H4O2	000064-19-7	91
2		Acetic acid	60	C2H4O2	000064-19-7	90
3		Acetic acid	60	C2H4O2	000064-19-7	90
4		Acetic acid	60	C2H4O2	000064-19-7	90
5		Ammonium acetate	77	C2H7NO2	000631-61-8	83



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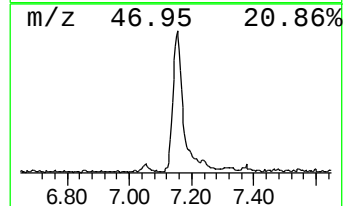
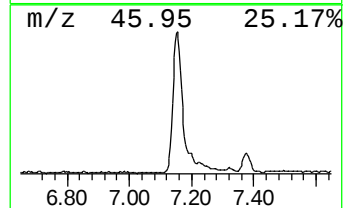
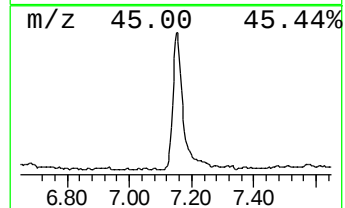
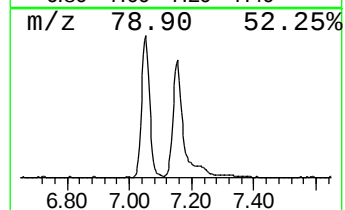
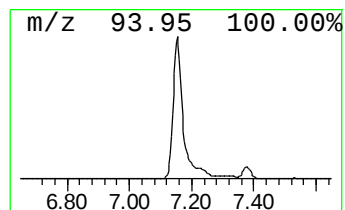
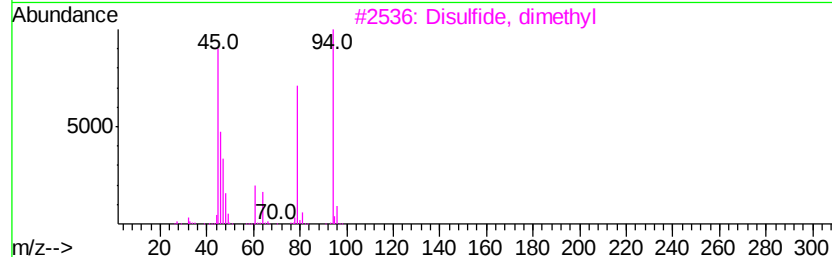
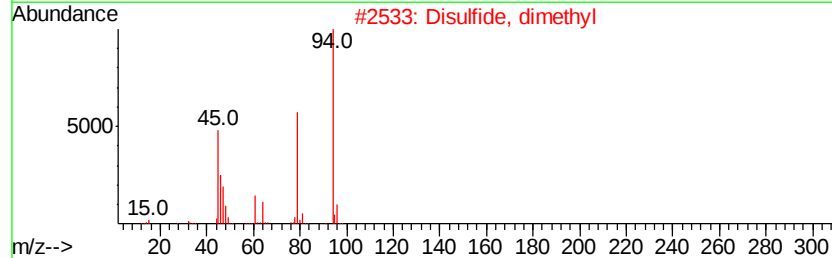
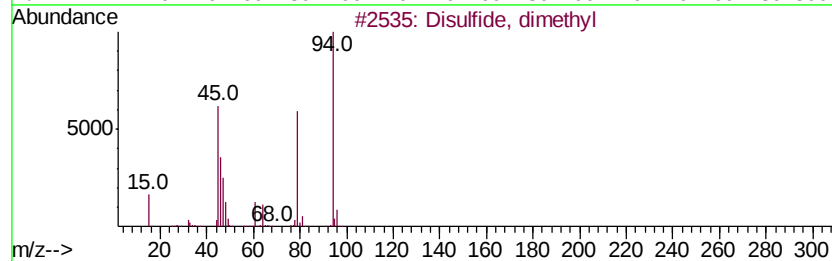
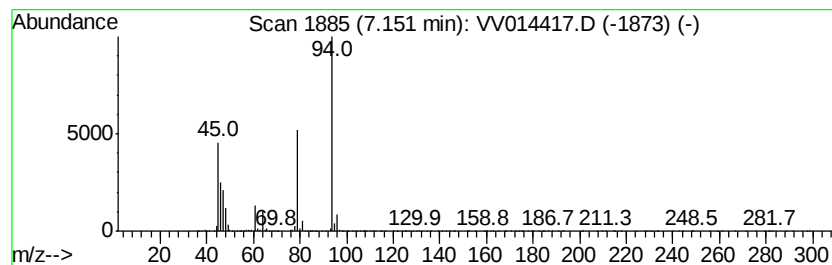
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Disulfide, dimethyl Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.15	3.09 ug/L	1345890	1,4-Difluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Disulfide, dimethyl	94	C2H6S2	000624-92-0	97
2		Disulfide, dimethyl	94	C2H6S2	000624-92-0	96
3		Disulfide, dimethyl	94	C2H6S2	000624-92-0	95
4		Disulfide, dimethyl	94	C2H6S2	000624-92-0	94
5		Disulfide, dimethyl	94	C2H6S2	000624-92-0	94



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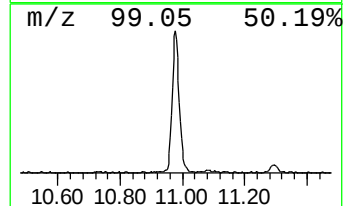
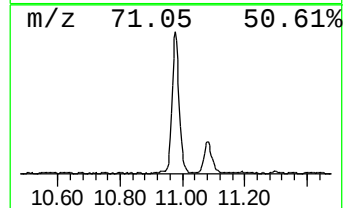
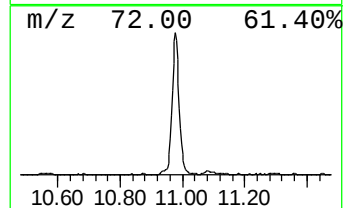
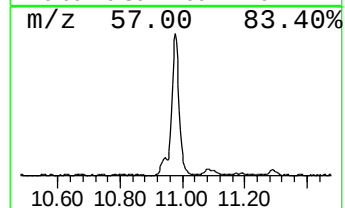
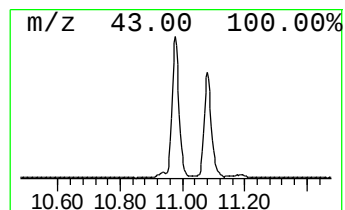
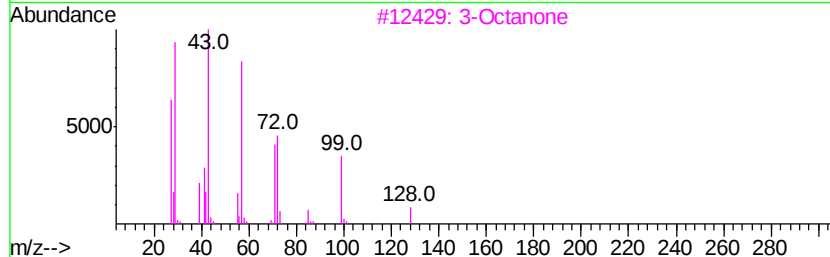
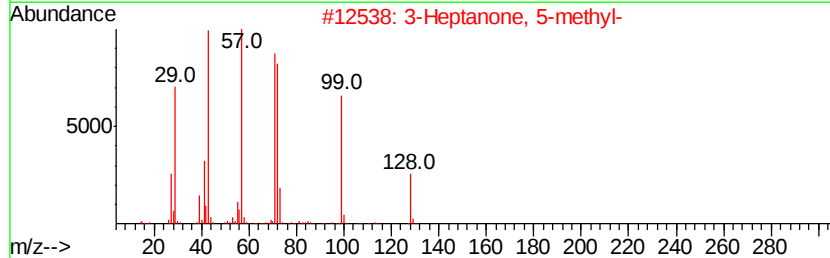
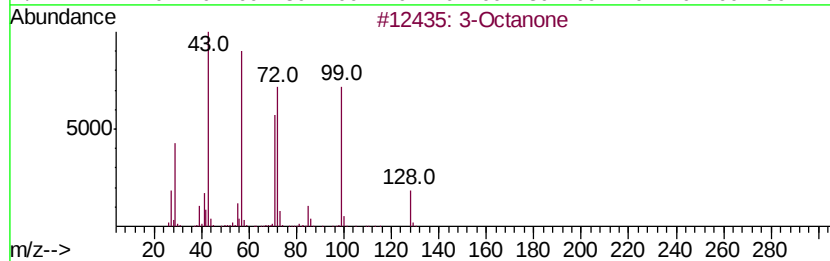
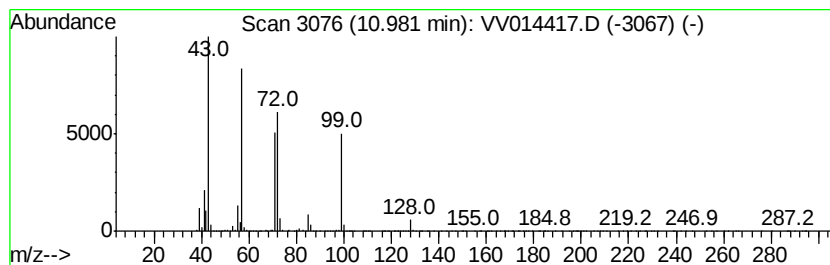
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 3-Octanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.98	2.23 ug/L	1051770	1,4-Dichlorobenzene-d4	11.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Octanone	128	C8H16O	000106-68-3	94
2		3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	72
3		3-Octanone	128	C8H16O	000106-68-3	64
4		3-Heptanone, 6-methyl-	128	C8H16O	000624-42-0	58
5		3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	53



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Quant Title : TRACE VOA SOM01.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Methanethiol	1.50	8.2	ug/L	3564810	1	5.67	2177370	5.0
Dimethyl sulfide	2.24	3.4	ug/L	1463980	1	5.67	2177370	5.0
Acetic acid	6.46	3.3	ug/L	1428250	1	5.67	2177370	5.0
Disulfide, dimethyl	7.15	3.1	ug/L	1345890	1	5.67	2177370	5.0
3-Octanone	10.98	2.2	ug/L	1051770	3	11.29	2356790	5.0