

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV092818\
 Data File : VV007986.D
 Acq On : 29 Sep 2018 06:23
 Operator : SY/MD
 Sample : J5062-14DL 10X
 Misc : 25.0 mL/MSVOA V/WATER
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 GAC14DL

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\SOMVTR092718WMA.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	1.319	52	71	80	rBV2	65607	172364	61.14%	5.915%
2	1.479	116	121	137	rVB	51800	64214	22.78%	2.204%
3	1.582	149	153	167	rVB	32991	41711	14.80%	1.431%
4	2.055	293	300	313	rVV	22311	34372	12.19%	1.179%
5	2.132	316	324	335	rVB	61941	87799	31.14%	3.013%
6	3.859	850	861	875	rVB3	2925	5972	2.12%	0.205%
7	3.990	883	902	923	rBV2	21285	89664	31.81%	3.077%
8	4.158	948	954	976	rVB3	5423	14347	5.09%	0.492%
9	4.408	1013	1032	1060	rVB2	51125	138907	49.27%	4.767%
10	5.097	1230	1246	1266	rBV2	114320	257017	91.17%	8.820%
11	5.669	1407	1424	1441	rBV	105448	206718	73.33%	7.094%
12	5.846	1469	1479	1485	rBV6	1687	3024	1.07%	0.104%
13	6.122	1552	1565	1587	rVB	63996	126393	44.83%	4.337%
14	6.666	1723	1734	1745	rBV8	3152	6287	2.23%	0.216%
15	7.032	1837	1848	1863	rBV	28462	49021	17.39%	1.682%
16	7.135	1867	1880	1902	rVB	39681	72095	25.57%	2.474%
17	7.363	1936	1951	1966	rBV	130429	223539	79.29%	7.671%
18	7.434	1966	1973	1981	rVB3	1785	2834	1.01%	0.097%
19	7.669	2030	2046	2060	rBV	17573	29221	10.37%	1.003%
20	7.987	2135	2145	2156	rBV3	5943	9906	3.51%	0.340%
21	8.145	2179	2194	2233	rBV	148048	281909	100.00%	9.674%
22	8.756	2374	2384	2401	rVB	39501	65378	23.19%	2.243%
23	8.900	2416	2429	2446	rBV	160193	261688	92.83%	8.980%
24	9.534	2621	2626	2640	rBV6	1435	2932	1.04%	0.101%
25	9.977	2759	2764	2774	rVB6	2449	3530	1.25%	0.121%
26	10.064	2781	2791	2801	rBV2	25669	39747	14.10%	1.364%
27	10.267	2842	2854	2866	rBV2	49243	77262	27.41%	2.651%
28	10.427	2894	2904	2913	rBV	8333	13299	4.72%	0.456%
29	10.839	3023	3032	3046	rBV2	6857	11027	3.91%	0.378%
30	11.299	3158	3175	3203	rBV	163074	270186	95.84%	9.272%
31	11.585	3254	3264	3275	rBV2	4594	8106	2.88%	0.278%
32	11.675	3278	3292	3309	rVB	136549	213415	75.70%	7.323%
33	11.929	3360	3371	3382	rBV2	9122	14203	5.04%	0.487%
34	12.296	3476	3485	3495	rBV7	1913	3776	1.34%	0.130%

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ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
GAC14DL

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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Title : TRACE VOA SOM01.0

35	12.884	3660	3668	3676	rbV3	5894	7951	2.82%	0.273%
36	14.090	4034	4043	4053	rbV2	2833	4341	1.54%	0.149%

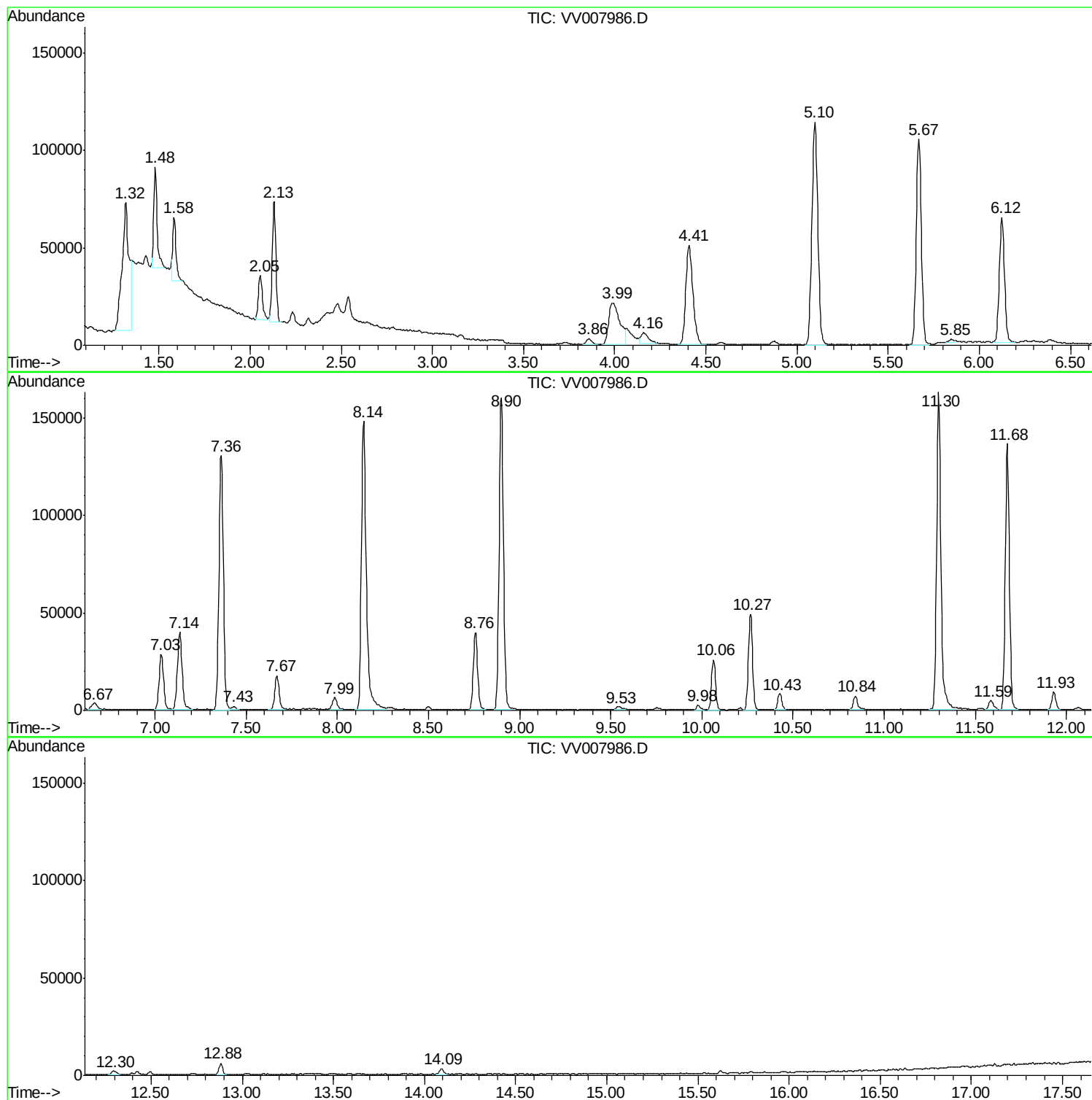
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Quant Title : TRACE VOA SOM01.0

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



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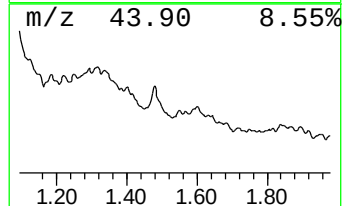
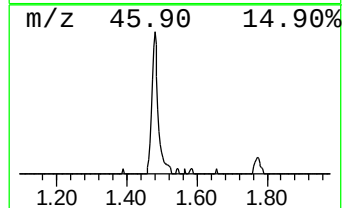
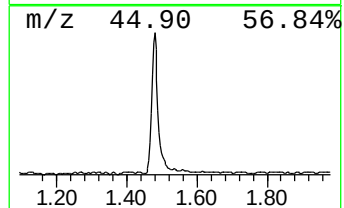
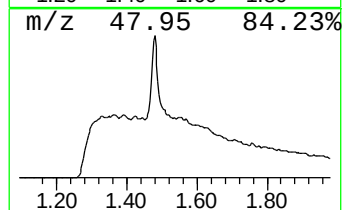
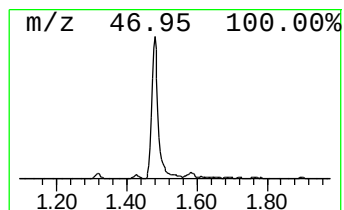
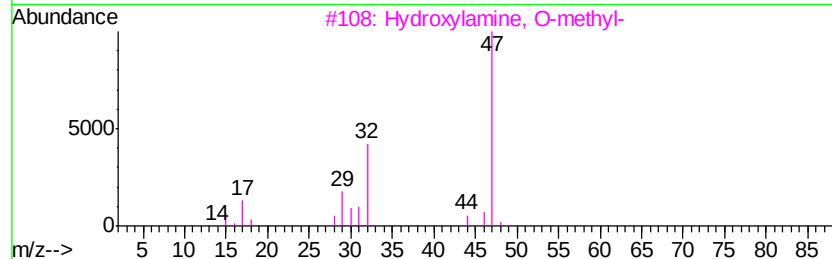
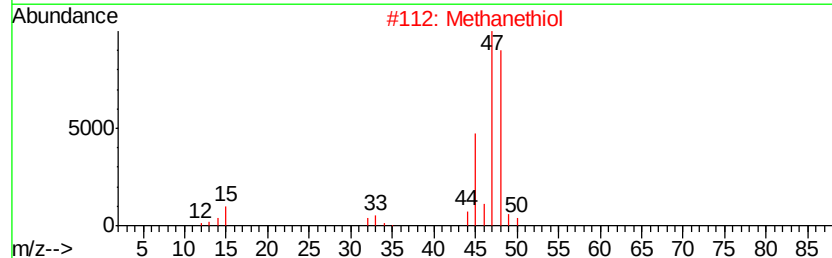
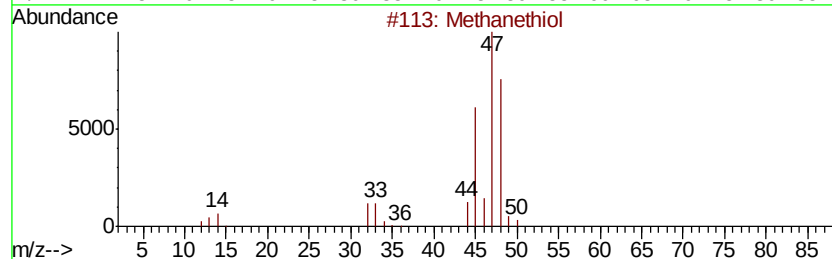
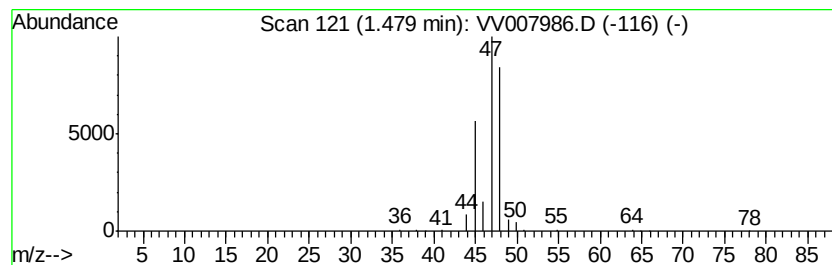
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Quant Title : TRACE VOA SOM01.0

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.
1.48	1.55 ug/L	64214	1,4-Difluorobenzene	5.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Methanethiol	48	CH4S	000074-93-1	90
2		Methanethiol	48	CH4S	000074-93-1	90
3		Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
4		Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	5
5		Ethane, fluoro-	48	C2H5F	000353-36-6	4



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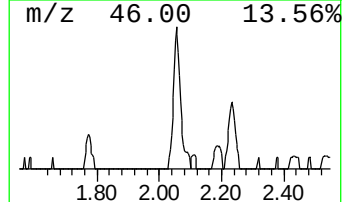
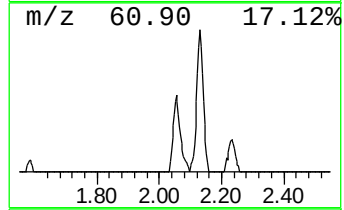
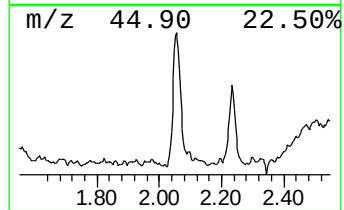
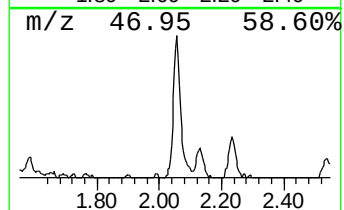
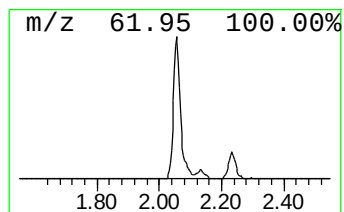
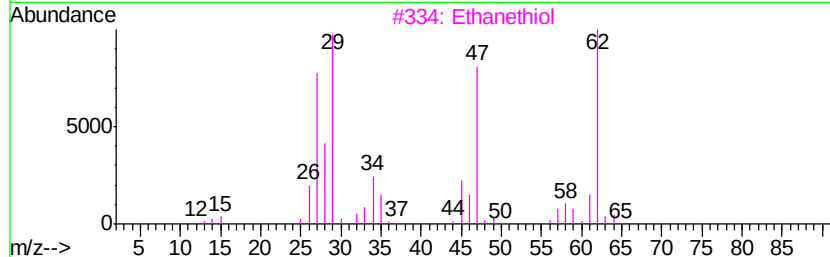
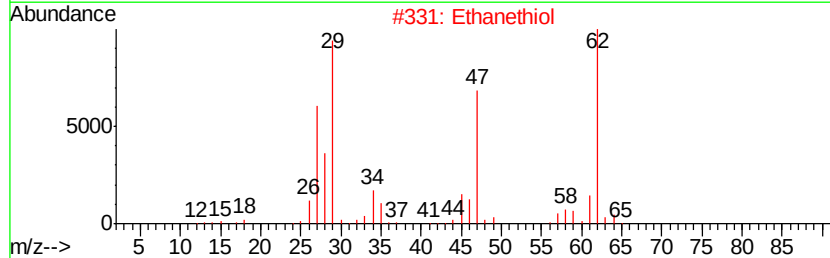
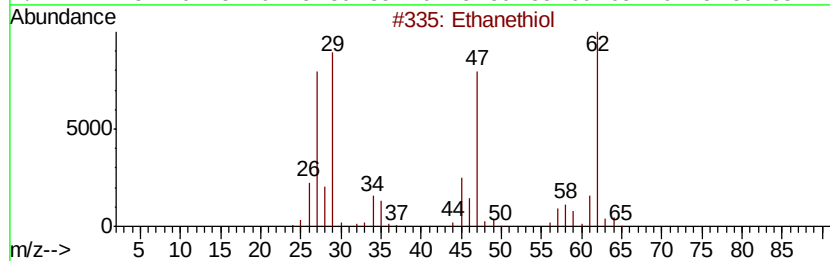
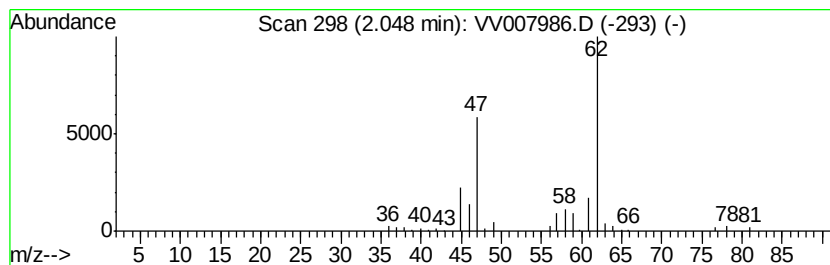
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR092718WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 Ethanethiol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.05	0.83 ug/L	34372	1,4-Difluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanethiol	62	C2H6S	000075-08-1	91
2		Ethanethiol	62	C2H6S	000075-08-1	91
3		Ethanethiol	62	C2H6S	000075-08-1	90
4		Ethanethiol	62	C2H6S	000075-08-1	90
5		Ethanethiol	62	C2H6S	000075-08-1	90



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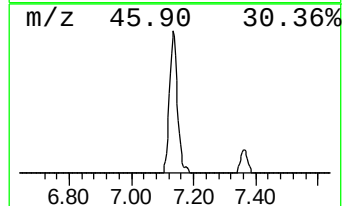
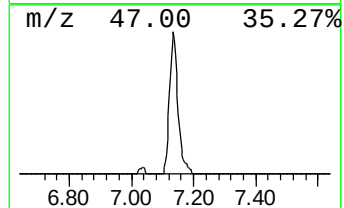
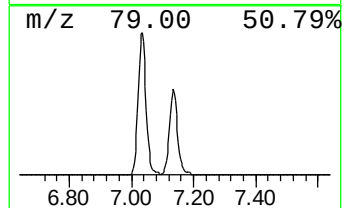
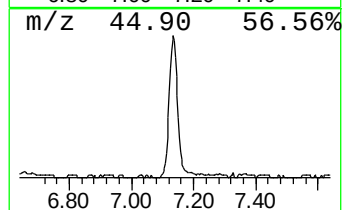
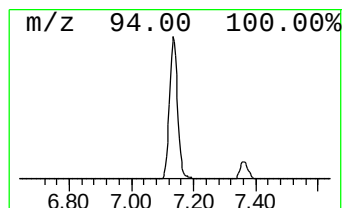
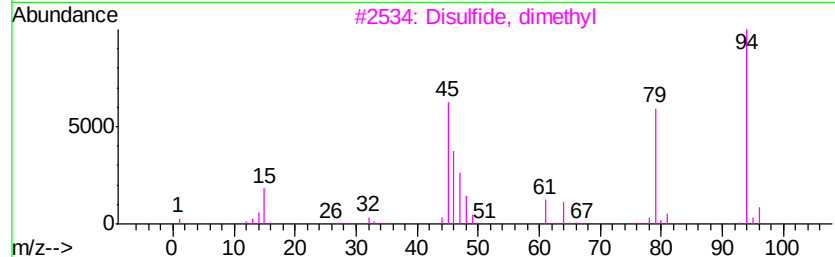
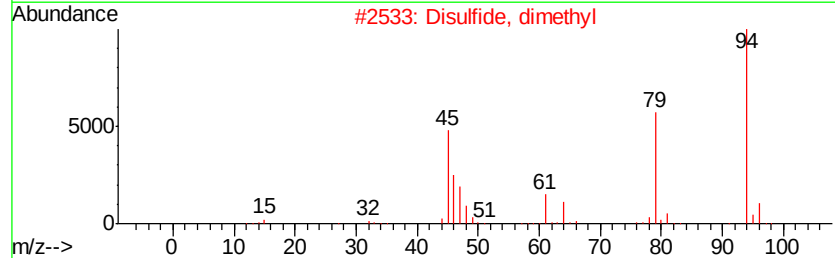
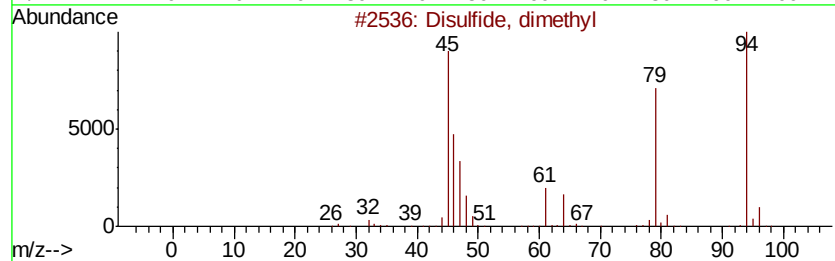
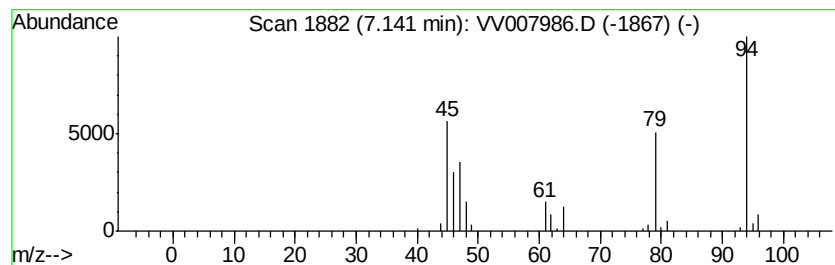
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 Disulfide, dimethyl Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.14	1.74 ug/L	72095	1,4-Difluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Disulfide, dimethyl	94	C2H6S2	000624-92-0	93
2		Disulfide, dimethyl	94	C2H6S2	000624-92-0	93
3		Disulfide, dimethyl	94	C2H6S2	000624-92-0	93
4		Disulfide, dimethyl	94	C2H6S2	000624-92-0	93
5		Disulfide, dimethyl	94	C2H6S2	000624-92-0	93



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ALS Vial : 46 Sample Multiplier: 1

Instrument :
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ClientSampled :
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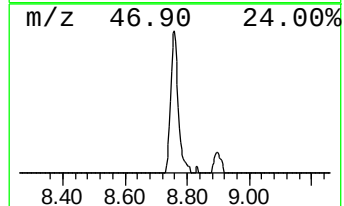
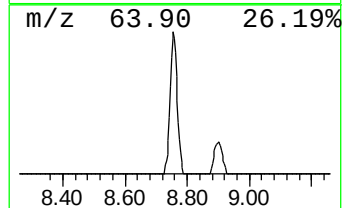
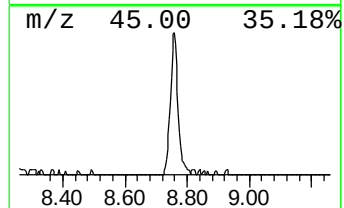
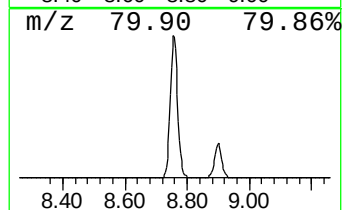
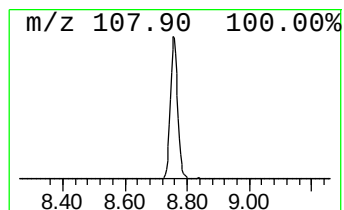
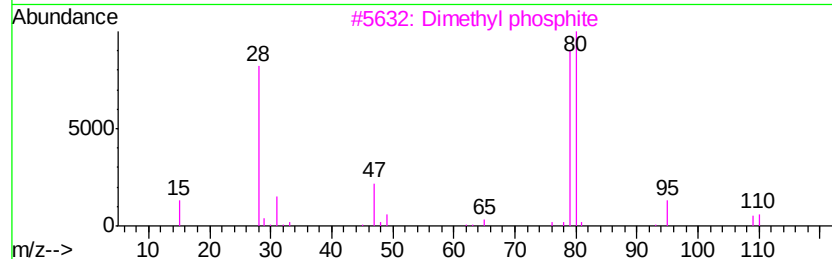
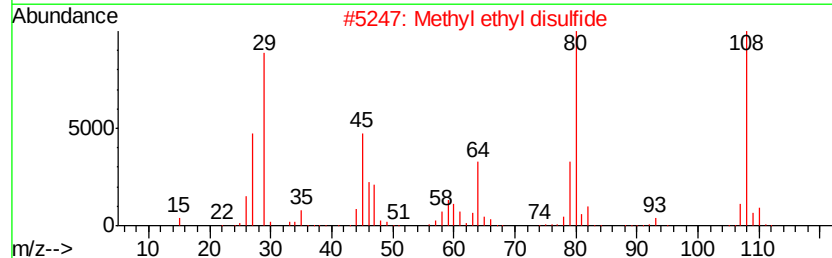
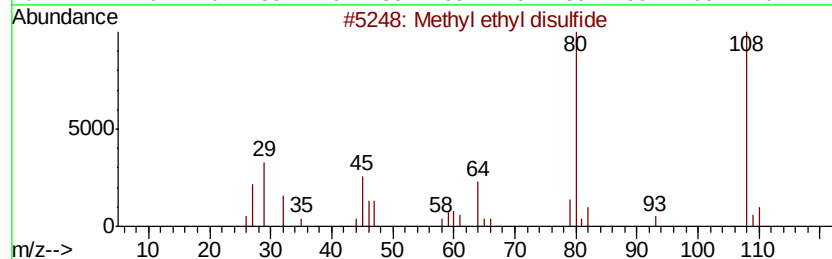
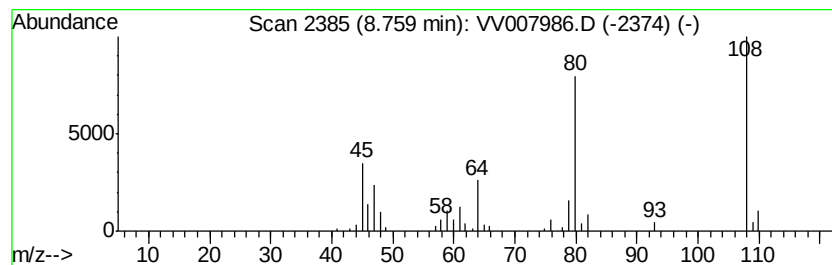
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 Methyl ethyl disulfide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.76	1.25 ug/L	65378	Chlorobenzene-d5	8.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methyl ethyl disulfide	108	C3H8S2	020333-39-5	83
2		Methyl ethyl disulfide	108	C3H8S2	020333-39-5	64
3		Dimethyl phosphite	110	C2H7O3P	000868-85-9	53
4		Methanesulfonic acid, methyl ester	110	C2H6O3S	000066-27-3	50
5		Nicotinyl alcohol	109	C6H7NO	000100-55-0	43



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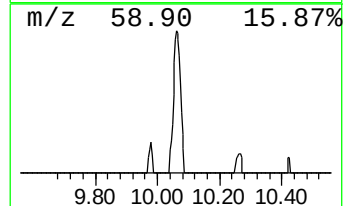
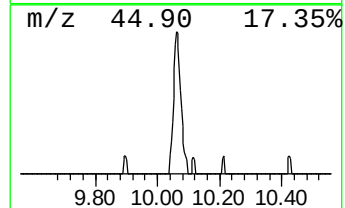
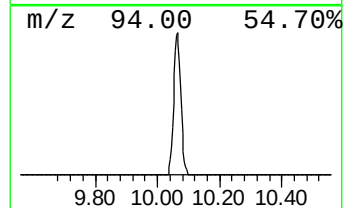
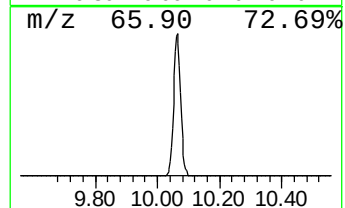
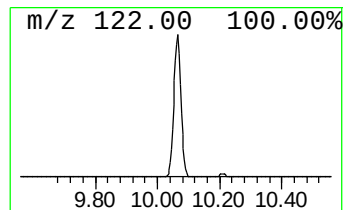
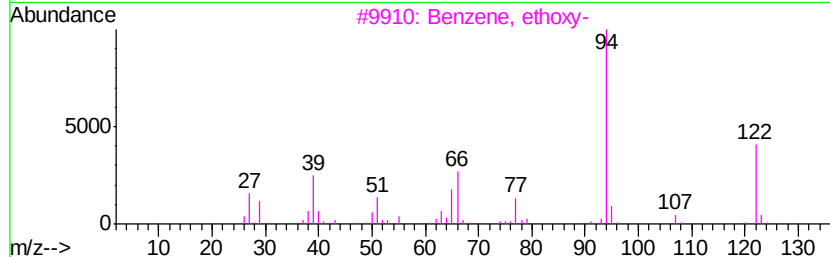
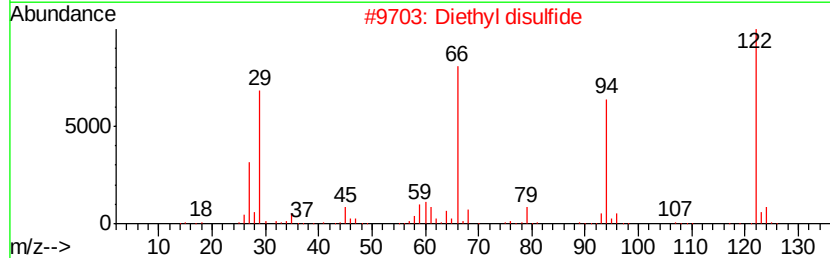
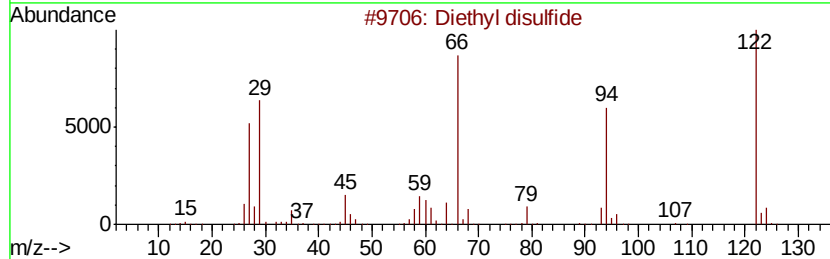
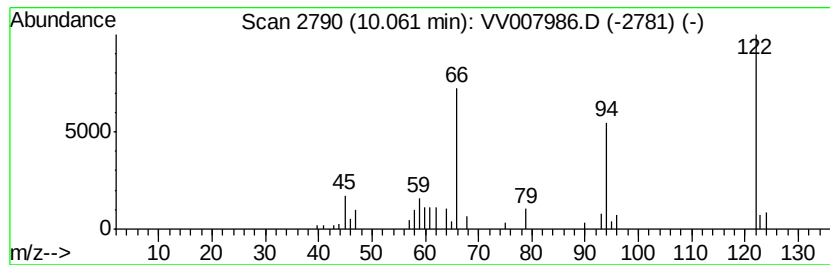
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR092718WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 Diethyl disulfide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.06	0.76 ug/L	39747	Chlorobenzene-d5	8.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Diethyl disulfide	122	C4H10S2	000110-81-6	94
2		Diethyl disulfide	122	C4H10S2	000110-81-6	87
3		Benzene, ethoxy-	122	C8H10O	000103-73-1	38
4		Diethyl sulfone	122	C4H10O2S	000597-35-3	38
5		Benzene, ethoxy-	122	C8H10O	000103-73-1	33



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ClientSampleId :
GAC14DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR092718WMA.M
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	1.48	1.6	ug/L	64214	1	5.67	206718	5.0
Ethanethiol	2.05	0.8	ug/L	34372	1	5.67	206718	5.0
Disulfide, dimethyl	7.14	1.7	ug/L	72095	1	5.67	206718	5.0
Methyl ethyl disu...	8.76	1.3	ug/L	65378	2	8.90	261688	5.0
Diethyl disulfide	10.06	0.8	ug/L	39747	2	8.90	261688	5.0