

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV040521\
 Data File : VV020915.D
 Acq On : 05 Apr 2021 15:20
 Operator : SY/MD
 Sample : M1879-14
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 EW1B5

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M

Title : VOC Analysis

Signal : TIC: VV020915.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.307	77	83	95	rVB	285832	288209	12.62%	1.344%
2	1.388	103	108	123	rBV	36397	54886	2.40%	0.256%
3	1.571	159	165	177	rVB	227979	263227	11.53%	1.228%
4	2.031	299	308	322	rBV	1021525	1417164	62.08%	6.611%
5	2.108	324	332	347	rVB	516879	737178	32.29%	3.439%
6	3.015	612	614	619	rVB4	951	535	0.02%	0.002%
7	3.108	641	643	646	rBV2	652	339	0.01%	0.002%
8	3.413	736	738	742	rBV3	745	589	0.03%	0.003%
9	3.519	768	771	773	rBV	310	198	0.01%	0.001%
10	3.548	776	780	781	rBV2	552	294	0.01%	0.001%
11	3.564	781	785	786	rBV2	282	229	0.01%	0.001%
12	3.603	794	797	801	rBV4	611	456	0.02%	0.002%
13	3.629	801	805	806	rBV	410	278	0.01%	0.001%
14	3.661	814	815	816	rBV	259	72	0.00%	0.000%
15	3.712	828	831	832	rBV2	513	346	0.02%	0.002%
16	3.728	832	836	838	rBV4	2231	1835	0.08%	0.009%
17	3.812	852	862	879	rBV2	45540	107937	4.73%	0.503%
18	3.902	879	890	909	rBV	123259	407543	17.85%	1.901%
19	4.352	1015	1030	1052	rBV2	395894	975633	42.74%	4.551%
20	4.908	1201	1203	1204	rBV	277	68	0.00%	0.000%
21	5.047	1230	1246	1275	rBV2	888323	2282932	100.00%	10.649%
22	5.619	1412	1424	1453	rBV	690690	1386950	60.75%	6.470%
23	6.072	1553	1565	1588	rBV	492128	979764	42.92%	4.570%
24	6.776	1782	1784	1788	rBV3	640	486	0.02%	0.002%
25	6.854	1807	1808	1810	rBV	700	257	0.01%	0.001%
26	6.895	1818	1821	1822	rBV2	459	320	0.01%	0.001%
27	6.931	1829	1832	1833	rBV2	572	279	0.01%	0.001%
28	6.989	1839	1850	1871	rBV	301644	544930	23.87%	2.542%
29	7.320	1941	1953	1970	rBV	1086413	1866090	81.74%	8.705%
30	7.622	2037	2047	2068	rBV2	206361	376179	16.48%	1.755%
31	8.030	2169	2174	2178	rBV5	1925	2268	0.10%	0.011%
32	8.091	2183	2193	2233	rVV	542354	1050210	46.00%	4.899%
33	8.657	2365	2369	2371	rBV3	924	743	0.03%	0.003%
34	8.722	2380	2389	2402	rVB4	17931	33772	1.48%	0.158%
35	8.857	2413	2431	2455	rBV	1067866	1713539	75.06%	7.993%
36	9.268	2554	2559	2561	rBV5	1201	1019	0.04%	0.005%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Min Area: 0 % of largest Peak

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Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M

Title : VOC Analysis

37	9.358	2584	2587	2590	rBV3	986	858	0.04%	0.004%
38	9.423	2604	2607	2611	rBV5	1494	1339	0.06%	0.006%
39	9.490	2623	2628	2629	rBV	1081	773	0.03%	0.004%
40	9.519	2635	2637	2640	rBV3	493	289	0.01%	0.001%
41	9.612	2663	2666	2668	rBV4	1391	885	0.04%	0.004%
42	9.825	2723	2732	2737	rBV7	2470	4045	0.18%	0.019%
43	10.021	2780	2793	2817	rBV	1051631	1661343	72.77%	7.750%
44	10.220	2844	2855	2878	rVB	746877	1172272	51.35%	5.468%
45	10.744	3016	3018	3020	rBV2	877	401	0.02%	0.002%
46	11.021	3102	3104	3105	rBV2	592	241	0.01%	0.001%
47	11.255	3165	3177	3194	rBV	1165643	1796702	78.70%	8.381%
48	11.538	3258	3265	3280	rBV5	23423	41306	1.81%	0.193%
49	11.632	3282	3294	3315	rVB	1235400	1912365	83.77%	8.920%
50	12.085	3430	3435	3437	rBV4	2156	2040	0.09%	0.010%
51	12.249	3483	3486	3490	rBV5	1132	952	0.04%	0.004%
52	12.596	3592	3594	3596	rBV2	1043	564	0.02%	0.003%
53	12.747	3636	3641	3643	rBV4	1985	1945	0.09%	0.009%
54	12.837	3658	3669	3681	rBV2	220028	335746	14.71%	1.566%
55	12.953	3703	3705	3710	rVB3	1249	653	0.03%	0.003%
56	13.091	3740	3748	3752	rBV6	1782	2677	0.12%	0.012%
57	13.262	3797	3801	3806	rBV5	1446	1471	0.06%	0.007%
58	13.686	3931	3933	3937	rVB4	1531	775	0.03%	0.004%
59	13.779	3959	3962	3968	rBV4	837	921	0.04%	0.004%
60	14.075	4051	4054	4056	rBV3	903	745	0.03%	0.003%

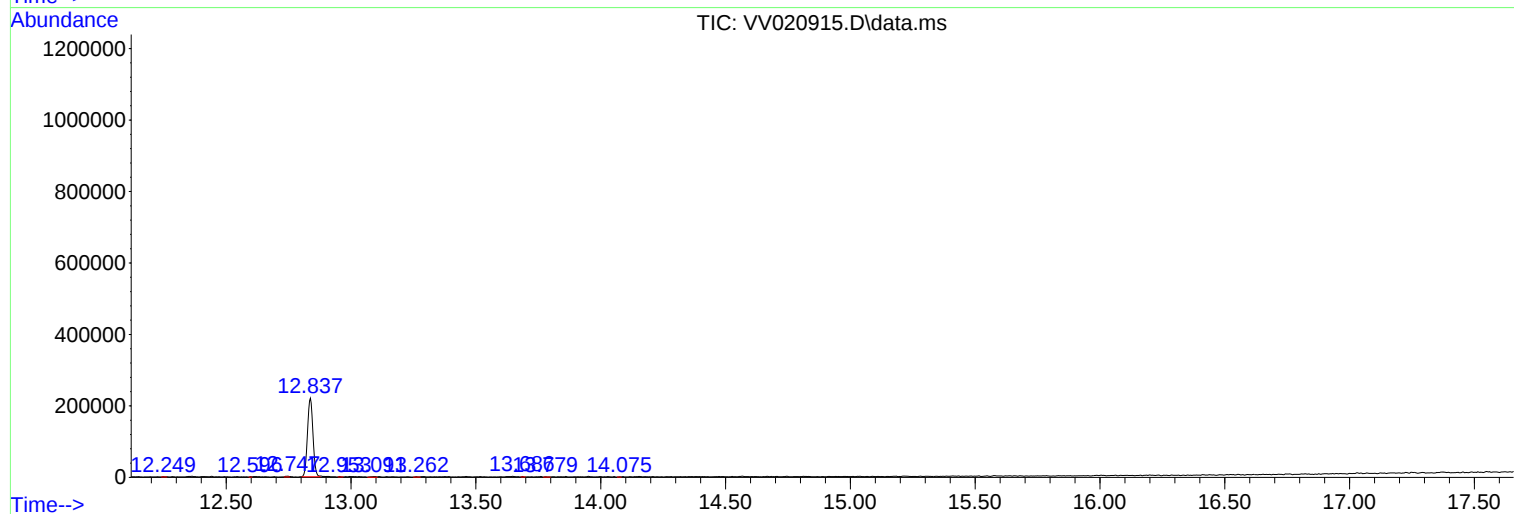
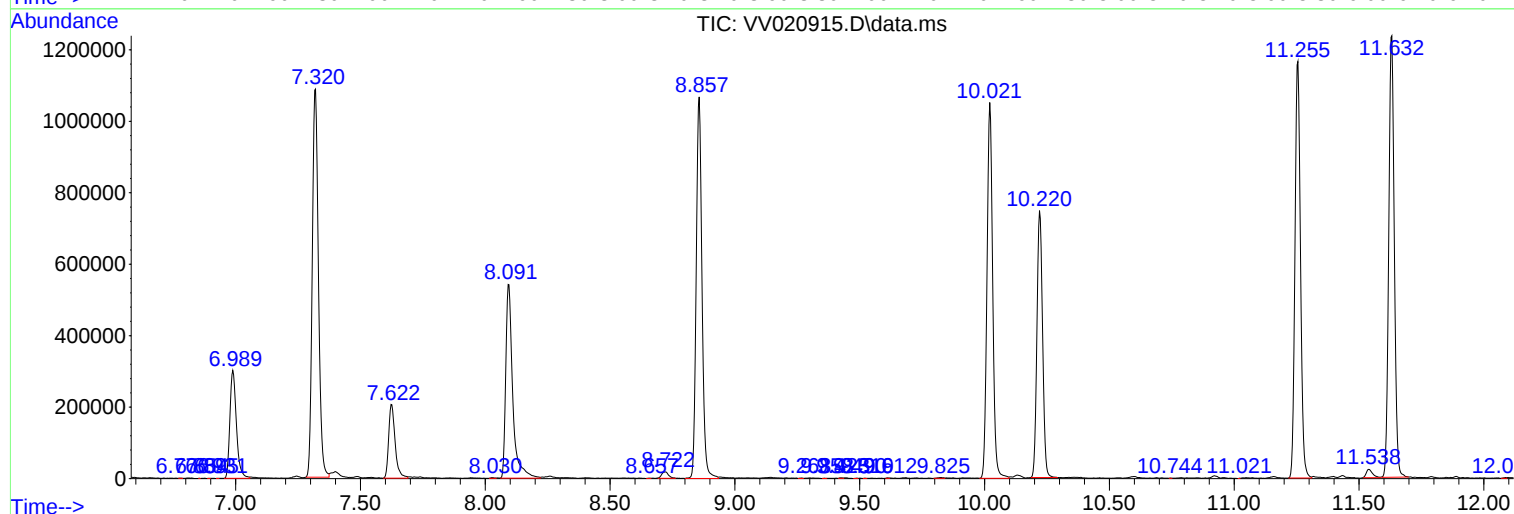
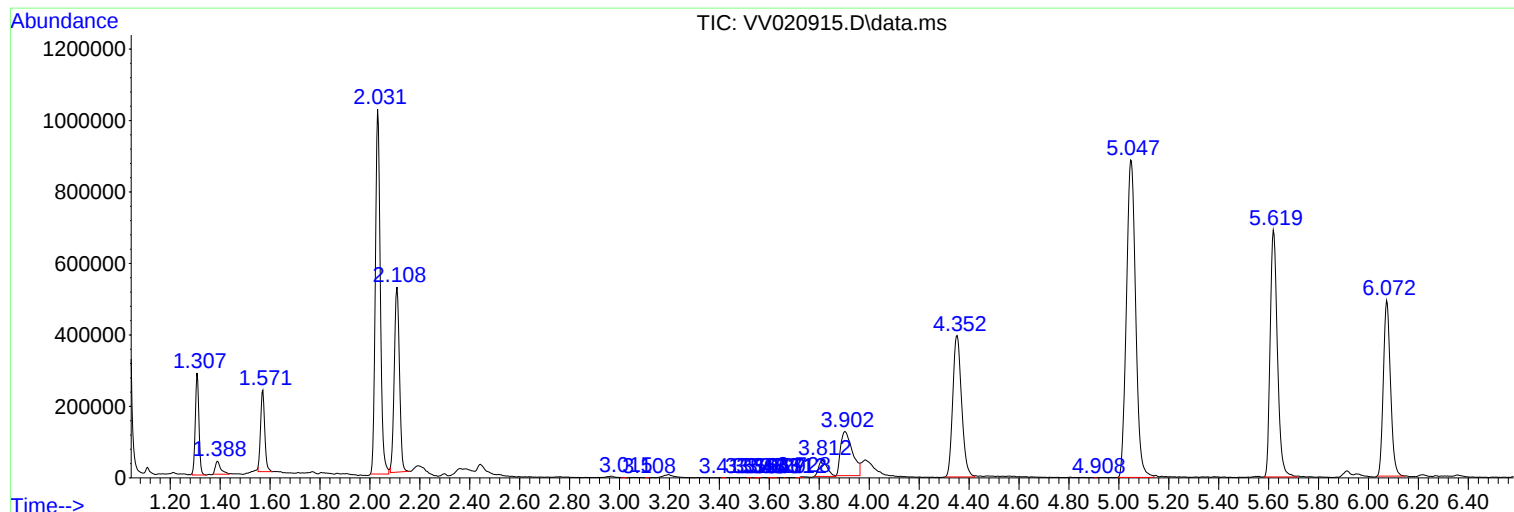
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Quant Title : VOC Analysis

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



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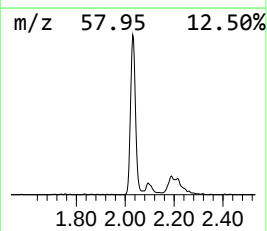
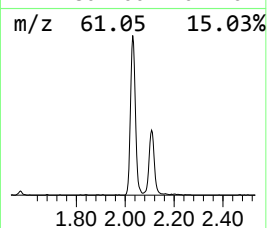
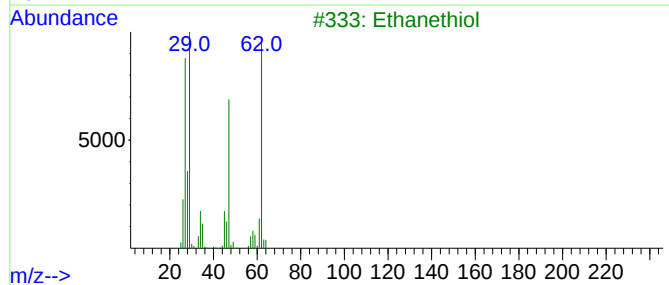
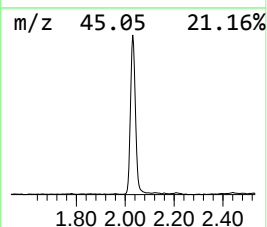
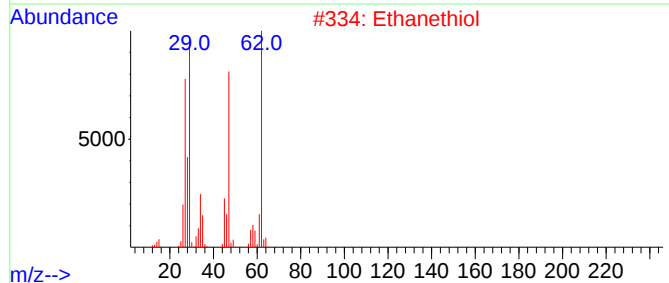
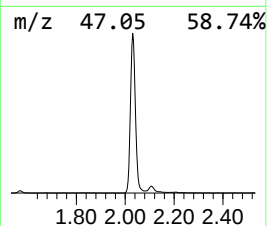
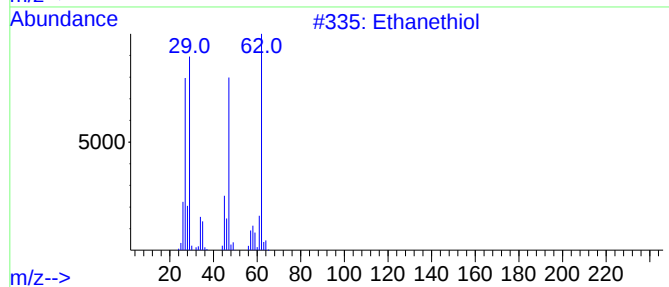
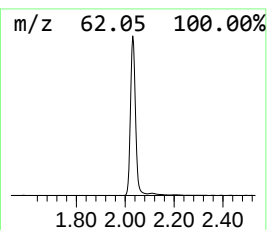
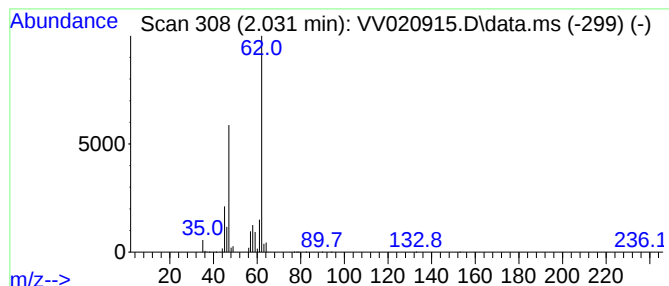
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Ethanethiol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.031	51.09 ug/L	1417160	1,4-Difluorobenzene	5.619

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



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Instrument :
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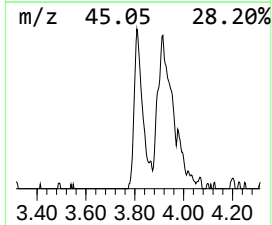
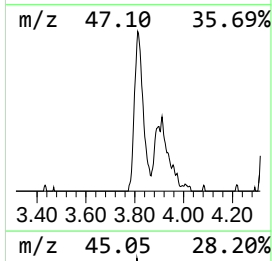
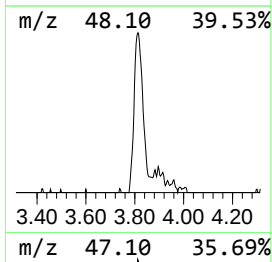
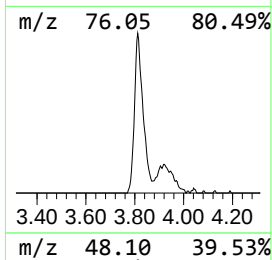
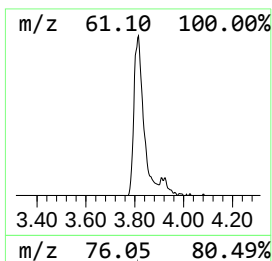
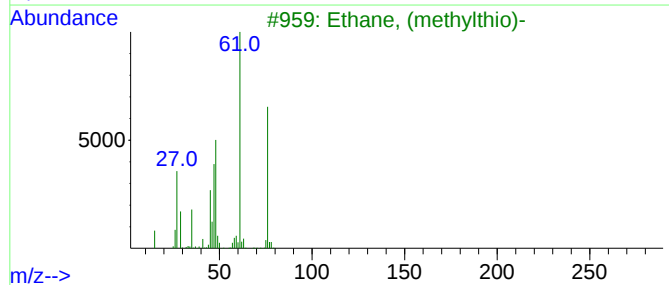
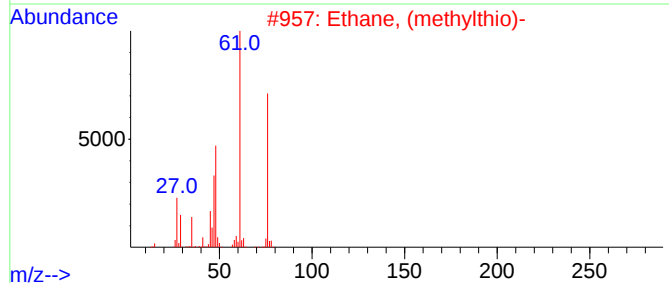
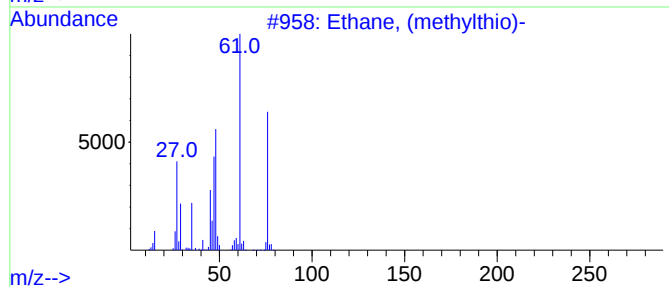
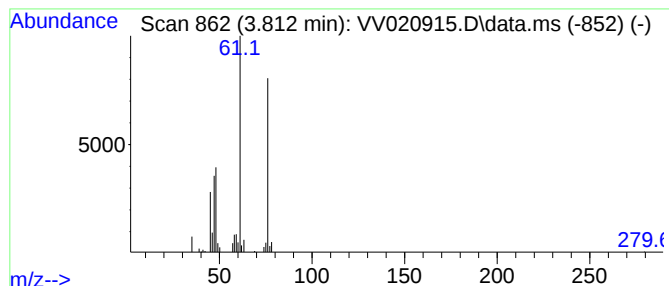
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Ethane, (methylthio)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.812	3.89 ug/L	107937	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, (methylthio)-	76	C3H8S	000624-89-5	91
2			Ethane, (methylthio)-	76	C3H8S	000624-89-5	91
3			Ethane, (methylthio)-	76	C3H8S	000624-89-5	91
4			p-Dithiane-2,5-diol	152	C4H8O2S2	040018-26-6	59
5			2-Aminoethylethyl sulfide	105	C4H11NS	036489-03-9	50



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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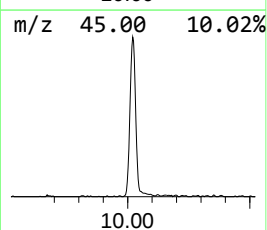
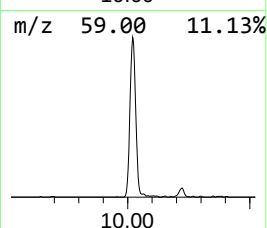
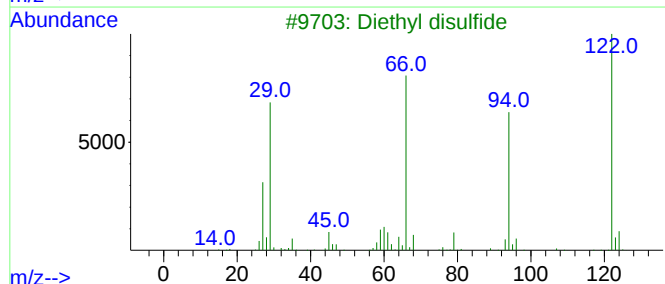
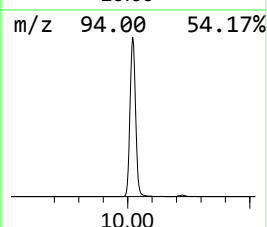
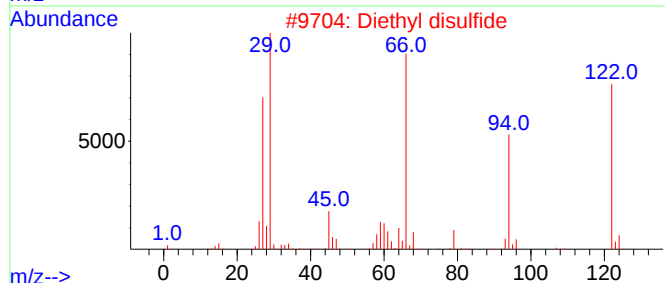
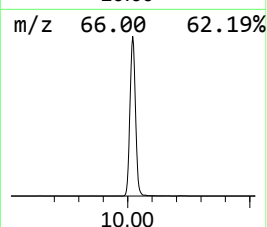
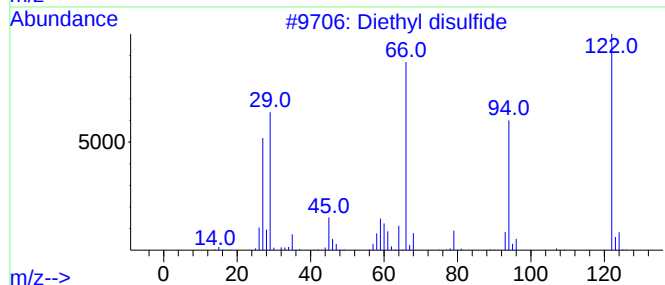
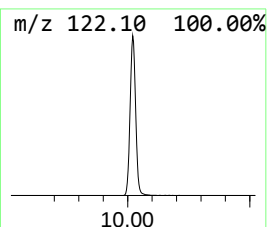
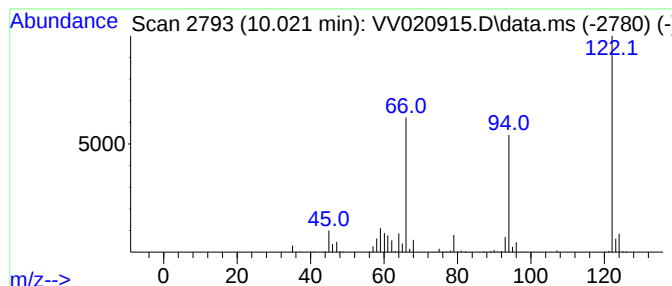
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Diethyl disulfide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.021	48.48 ug/L	1661340	Chlorobenzene-d5	8.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethyl disulfide	122	C4H10S2	000110-81-6	94
2			Diethyl disulfide	122	C4H10S2	000110-81-6	91
3			Diethyl disulfide	122	C4H10S2	000110-81-6	83
4			Diethyl sulfone	122	C4H10O2S	000597-35-3	38
5			5-exo-Methyl-5-norbornenol	124	C8H12O	003212-13-3	32



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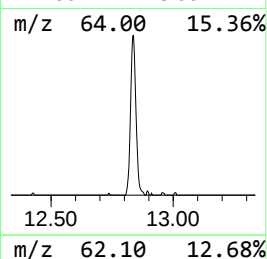
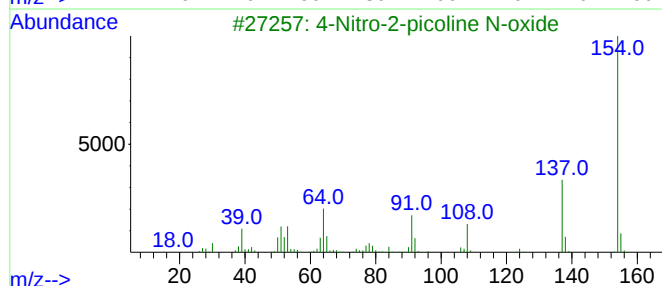
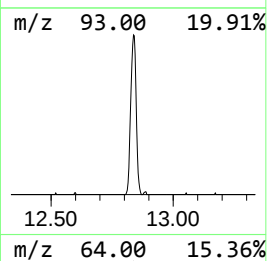
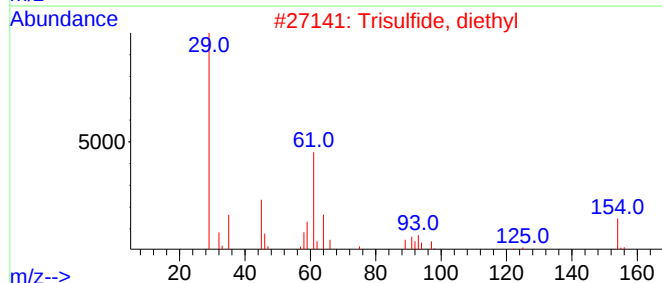
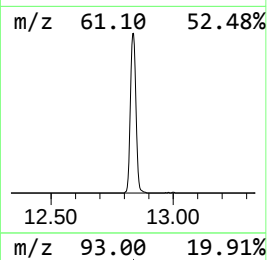
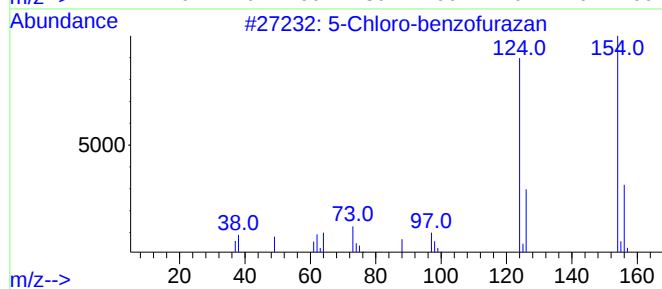
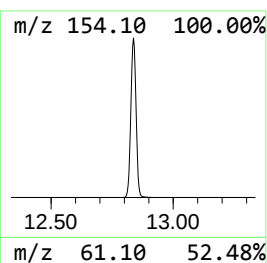
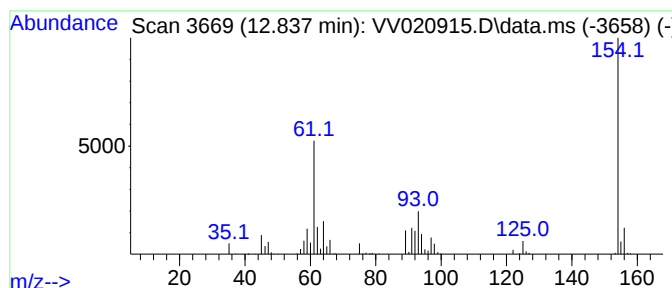
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.837	9.34 ug/L	335746	1,4-Dichlorobenzene-d4	11.255

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Chloro-benzofurazan	154	C6H3ClN2O	019155-86-3	46
2			Trisulfide, diethyl	154	C4H10S3	003600-24-6	43
3			4-Nitro-2-picoline N-oxide	154	C6H6N2O3	005470-66-6	16
4			2-(Dimethyl phosphino)-ethyl pho...	122	C4H12P2	054772-64-4	14
5			6-Chloropurine	154	C5H3ClN4	000087-42-3	12



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanethiol	2.031	51.1	ug/L	1417160	1	5.619	1386950	50.0
Ethane, (methyl...	3.812	3.9	ug/L	107937	1	5.619	1386950	50.0
Diethyl disulfide	10.021	48.5	ug/L	1661340	2	8.857	1713540	50.0
unknown-01	12.837	9.3	ug/L	335746	3	11.255	1796700	50.0