

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV033120\
 Data File : VV015311.D
 Acq On : 31 Mar 2020 14:11
 Operator : SY/MD
 Sample : L1975-12
 Misc : 5.0mL/MSVOA V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 ETTH5

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % 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\SOMVLM033020WMA.M
 Title : VOC Analysis

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	63	71	88	rVB2	742548	824927	15.21%	3.120%
2	1.399	90	96	111	rVV	59973	91998	1.70%	0.348%
3	1.579	146	152	174	rVB	271732	335386	6.19%	1.268%
4	2.045	288	297	310	rBV	912874	1286497	23.73%	4.866%
5	2.122	312	321	335	rVB	568440	837205	15.44%	3.166%
6	3.315	689	692	697	rVV7	1623	1425	0.03%	0.005%
7	3.370	704	709	713	rBV7	1825	1717	0.03%	0.006%
8	3.412	720	722	727	rVB5	1780	1502	0.03%	0.006%
9	3.482	739	744	748	rBV8	1606	1373	0.03%	0.005%
10	3.527	754	758	761	rBV5	3070	2233	0.04%	0.008%
11	3.579	772	774	779	rVB5	1512	1319	0.02%	0.005%
12	3.611	779	784	787	rBV7	2332	2031	0.04%	0.008%
13	3.743	816	825	839	rBV7	11055	28247	0.52%	0.107%
14	3.836	839	854	870	rBV3	46106	115660	2.13%	0.437%
15	3.929	871	883	903	rBV2	155560	524368	9.67%	1.983%
16	4.380	1008	1023	1044	rVV	343418	844982	15.58%	3.196%
17	4.553	1074	1077	1082	rVB7	1848	1811	0.03%	0.007%
18	4.627	1096	1100	1103	rBV5	1377	1116	0.02%	0.004%
19	4.781	1143	1148	1151	rBV7	1445	1434	0.03%	0.005%
20	4.826	1160	1162	1165	rBV4	1594	1181	0.02%	0.004%
21	5.074	1221	1239	1270	rBV2	843787	2114392	39.00%	7.997%
22	5.479	1363	1365	1368	rBV4	1917	1289	0.02%	0.005%
23	5.643	1403	1416	1444	rBV	684317	1450502	26.75%	5.486%
24	6.093	1544	1556	1579	rVB	481971	975462	17.99%	3.689%
25	6.212	1585	1593	1611	rVB3	33977	69633	1.28%	0.263%
26	6.534	1691	1693	1695	rBV2	1906	1153	0.02%	0.004%
27	6.746	1756	1759	1762	rVB5	2376	1391	0.03%	0.005%
28	6.775	1762	1768	1770	rBV7	2313	2132	0.04%	0.008%
29	6.868	1794	1797	1800	rBV5	2576	1876	0.03%	0.007%
30	7.006	1826	1840	1864	rBV	304169	553459	10.21%	2.093%
31	7.113	1868	1873	1875	rBV5	3364	3462	0.06%	0.013%
32	7.264	1915	1920	1923	rBV5	2714	2275	0.04%	0.009%
33	7.338	1931	1943	1966	rBV	1033792	1783822	32.90%	6.746%
34	7.643	2027	2038	2056	rVB	215777	363854	6.71%	1.376%

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Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM033020WMA.M
 Title : VOC Analysis

35	8.113	2172	2184	2216	rBV	774183	1414884	26.10%	5.351%
36	8.415	2270	2278	2282	rBV7	6783	11191	0.21%	0.042%
37	8.559	2318	2323	2325	rBV5	2760	2778	0.05%	0.011%
38	8.733	2366	2377	2399	rBV	145763	328722	6.06%	1.243%
39	8.875	2409	2421	2447	rVB	1084925	1738776	32.07%	6.576%
40	9.145	2502	2505	2507	rBV4	1667	1126	0.02%	0.004%
41	9.170	2508	2513	2514	rBV3	4565	4109	0.08%	0.016%
42	9.476	2606	2608	2613	rVB5	1893	1108	0.02%	0.004%
43	9.498	2613	2615	2622	rVB8	2031	1772	0.03%	0.007%
44	9.569	2635	2637	2643	rVB7	2129	1500	0.03%	0.006%
45	9.643	2657	2660	2663	rBV5	1819	1219	0.02%	0.005%
46	9.698	2668	2677	2685	rBV5	8654	17096	0.32%	0.065%
47	9.807	2709	2711	2714	rVB3	2144	1217	0.02%	0.005%
48	9.833	2714	2719	2725	rBV8	4009	4853	0.09%	0.018%
49	9.919	2743	2746	2749	rBV6	1661	1162	0.02%	0.004%
50	10.038	2769	2783	2816	rBV	3175114	5422029	100.00%	20.506%
51	10.238	2833	2845	2863	rBV	717653	1123954	20.73%	4.251%
52	10.347	2877	2879	2884	rBV6	2249	1831	0.03%	0.007%
53	10.521	2927	2933	2934	rBV6	2679	2106	0.04%	0.008%
54	10.598	2954	2957	2962	rBV6	3503	3850	0.07%	0.015%
55	10.993	3076	3080	3085	rBV8	2686	2298	0.04%	0.009%
56	11.032	3088	3092	3094	rBV4	1850	1411	0.03%	0.005%
57	11.148	3123	3128	3134	rVV9	2850	3641	0.07%	0.014%
58	11.177	3134	3137	3140	rBV5	1833	1467	0.03%	0.006%
59	11.273	3155	3167	3182	rBV	1114752	1697458	31.31%	6.420%
60	11.485	3231	3233	3240	rVB7	4116	4000	0.07%	0.015%
61	11.553	3248	3254	3270	rVB4	13282	23812	0.44%	0.090%
62	11.649	3270	3284	3308	rBV	1060143	1676030	30.91%	6.339%
63	11.804	3327	3332	3333	rBV5	3805	3172	0.06%	0.012%
64	11.836	3340	3342	3348	rBV7	1715	1216	0.02%	0.005%
65	11.903	3352	3363	3375	rBV4	22713	39905	0.74%	0.151%
66	12.257	3469	3473	3474	rBV3	2035	1472	0.03%	0.006%
67	12.302	3482	3487	3488	rBV5	1709	1327	0.02%	0.005%
68	12.405	3514	3519	3524	rBV9	1942	2311	0.04%	0.009%
69	12.450	3531	3533	3537	rVB4	2068	1479	0.03%	0.006%
70	12.476	3537	3541	3544	rBV6	2103	1298	0.02%	0.005%
71	12.505	3547	3550	3554	rVB5	1627	1383	0.03%	0.005%

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 Title : VOC Analysis

72	12.537	3556	3560	3565	rBV7	1870	1782	0.03%	0.007%
73	12.582	3570	3574	3575	rBV4	2480	1832	0.03%	0.007%
74	12.627	3584	3588	3594	rBV9	1762	1973	0.04%	0.007%
75	12.659	3594	3598	3602	rVB7	2335	1891	0.03%	0.007%
76	12.681	3602	3605	3607	rBV3	1567	1103	0.02%	0.004%
77	12.723	3615	3618	3621	rBV4	1701	1172	0.02%	0.004%
78	12.759	3627	3629	3633	rVV5	1368	1172	0.02%	0.004%
79	12.810	3641	3645	3648	rBV4	1839	1573	0.03%	0.006%
80	12.855	3648	3659	3672	rVV	403739	604991	11.16%	2.288%
81	13.090	3730	3732	3735	rVB4	2271	1236	0.02%	0.005%
82	13.167	3748	3756	3761	rBV4	4191	6376	0.12%	0.024%
83	13.315	3799	3802	3806	rVB5	1583	1109	0.02%	0.004%
84	13.337	3806	3809	3812	rBV5	1370	1147	0.02%	0.004%
85	13.450	3839	3844	3845	rBV4	2519	1818	0.03%	0.007%
86	13.514	3860	3864	3866	rBV5	1856	1431	0.03%	0.005%
87	13.948	3996	3999	4004	rVB7	1897	1370	0.03%	0.005%
88	14.103	4044	4047	4054	rVB8	3175	3117	0.06%	0.012%
89	14.135	4054	4057	4058	rBV3	2227	1299	0.02%	0.005%
90	14.521	4174	4177	4180	rBV4	2059	1384	0.03%	0.005%
91	14.553	4183	4187	4193	rBV8	2949	3925	0.07%	0.015%
92	14.601	4199	4202	4204	rBV4	2470	1622	0.03%	0.006%
93	14.643	4211	4215	4217	rBV4	1709	1094	0.02%	0.004%
94	14.836	4269	4275	4279	rBV9	3095	3384	0.06%	0.013%
95	14.910	4295	4298	4301	rBV5	2059	1448	0.03%	0.005%
96	15.125	4360	4365	4368	rBV6	2207	1882	0.03%	0.007%
97	15.482	4471	4476	4478	rBV6	3293	2965	0.05%	0.011%
98	15.614	4513	4517	4521	rBV6	2820	2377	0.04%	0.009%
99	15.951	4619	4622	4626	rBV5	2220	1841	0.03%	0.007%
100	16.019	4640	4643	4647	rBV6	2802	2639	0.05%	0.010%

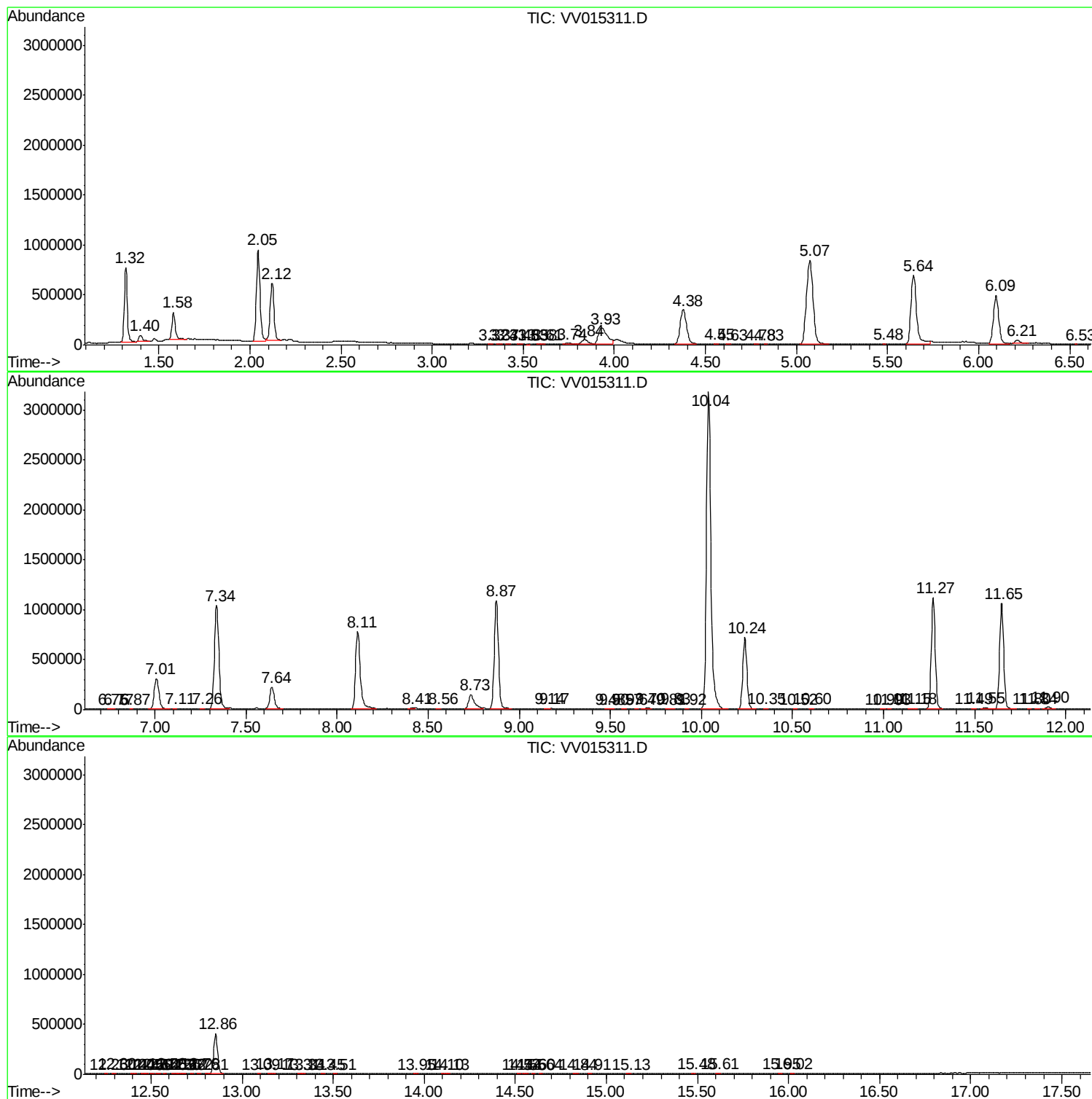
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Instrument :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM033020WMA.M
Quant Title : VOC Analysis

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



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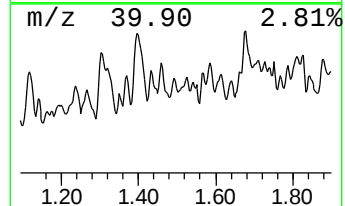
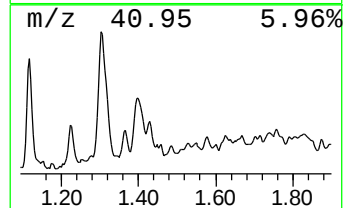
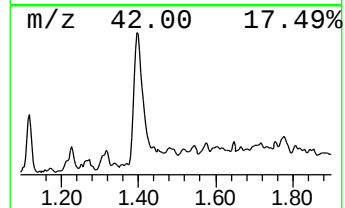
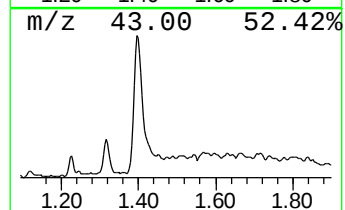
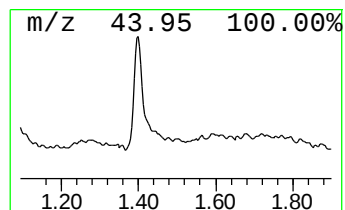
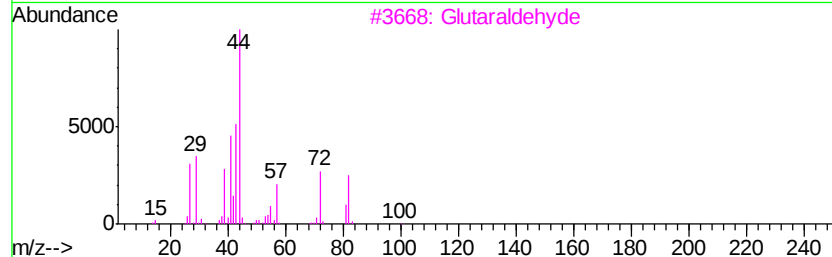
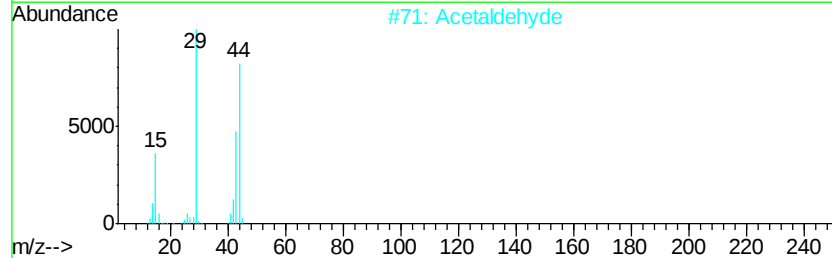
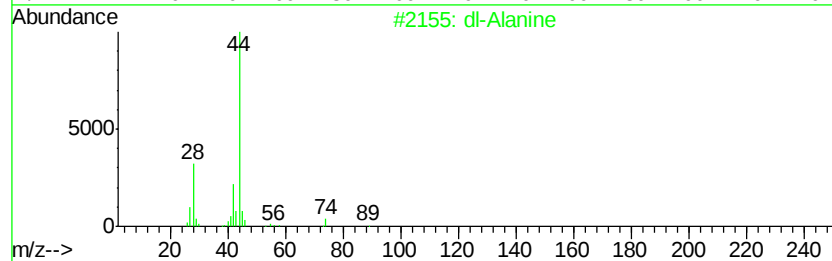
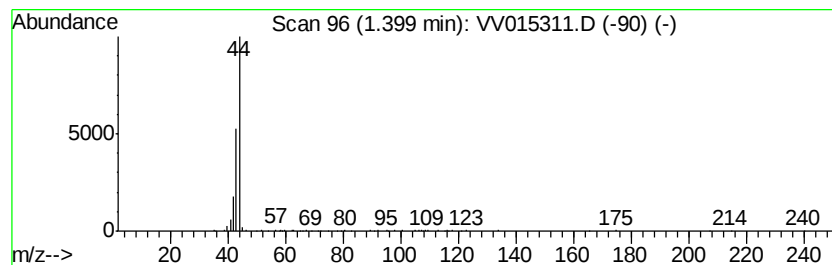
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM033020WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 dl-Alanine Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.40	3.17 ug/L	91998	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	dl-Alanine	89	C3H7NO2	000302-72-7	50
2		Acetaldehydve	44	C2H4O	000075-07-0	9
3		Glutaraldehydve	100	C5H8O2	000111-30-8	9
4		Acetaldehydve	44	C2H4O	000075-07-0	9
5		dl-Alanine	89	C3H7NO2	000302-72-7	7



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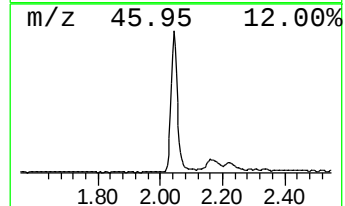
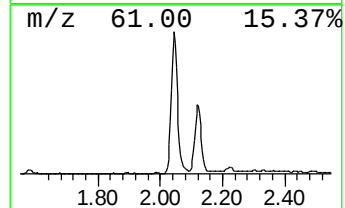
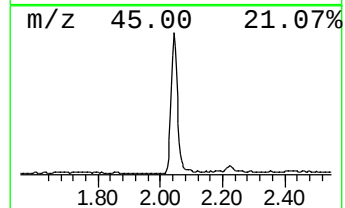
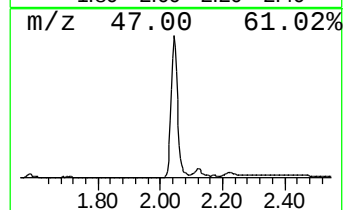
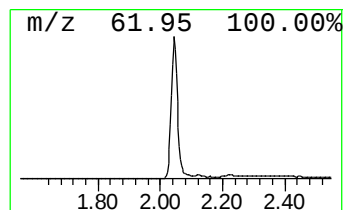
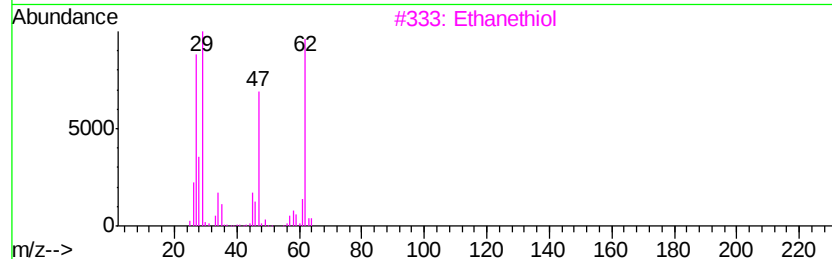
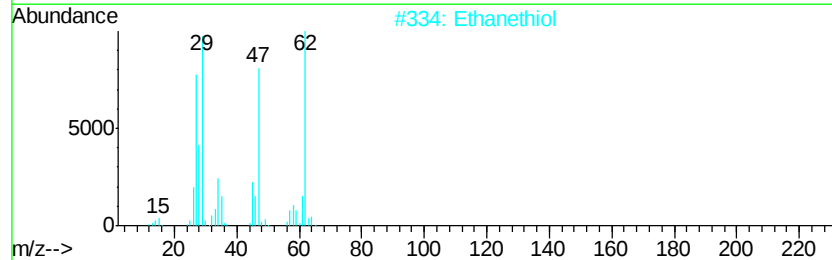
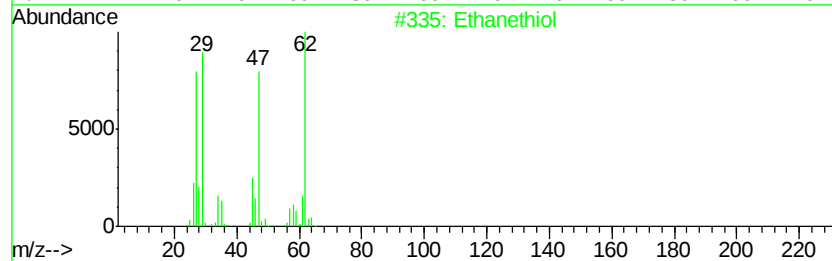
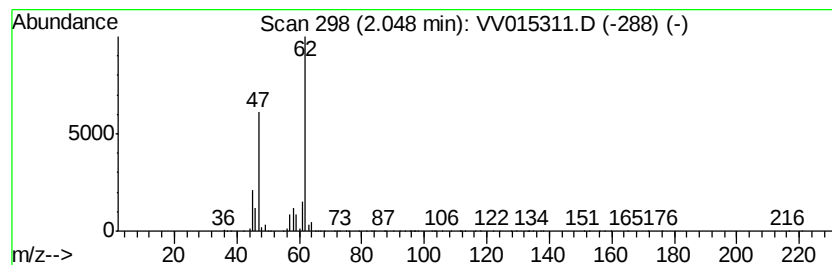
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM033020WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Ethanethiol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.05	44.35 ug/L	1286500	1,4-Difluorobenzene	5.64

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	91
4		Ethanethiol	62	C2H6S	000075-08-1	91
5		Ethanethiol	62	C2H6S	000075-08-1	91



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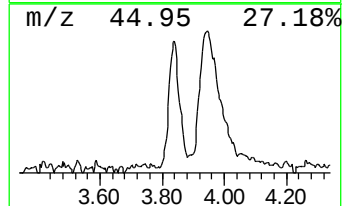
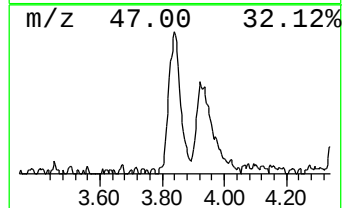
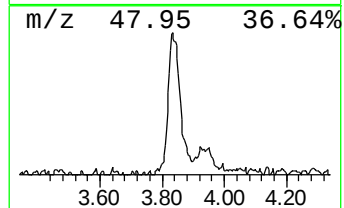
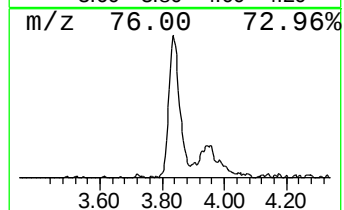
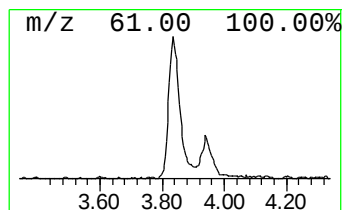
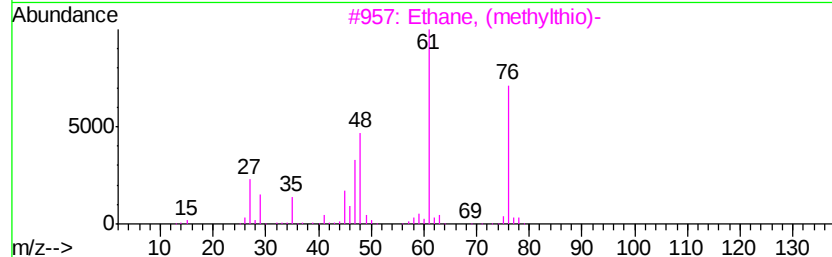
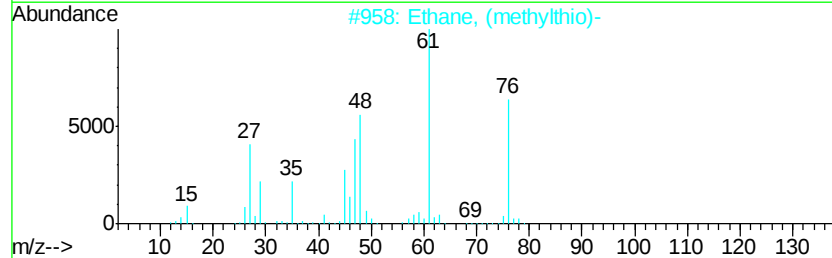
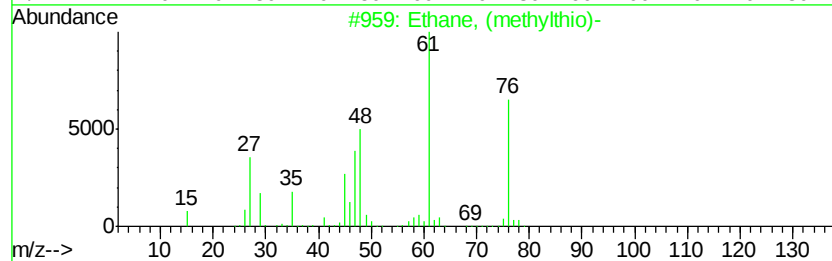
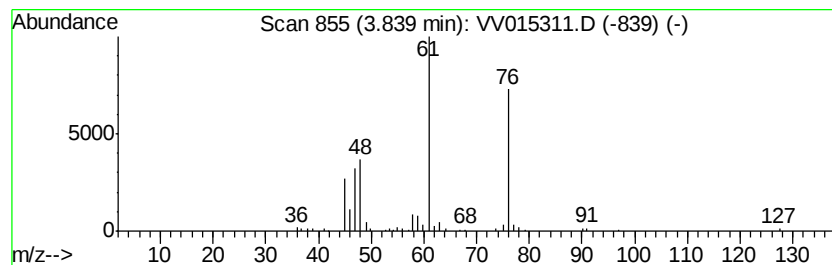
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM033020WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Ethane, (methylthio)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.84	3.99 ug/L	115660	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethane, (methylthio)-	76	C3H8S	000624-89-5	90
2		Ethane, (methylthio)-	76	C3H8S	000624-89-5	90
3		Ethane, (methylthio)-	76	C3H8S	000624-89-5	90
4		Trimethylphosphine	76	C3H9P	000594-09-2	64
5		Trimethylphosphine	76	C3H9P	000594-09-2	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV033120\
Data File : VV015311.D
Acq On : 31 Mar 2020 14:11
Operator : SY/MD
Sample : L1975-12
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
ETTH5

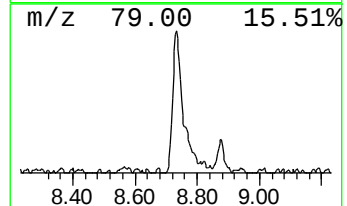
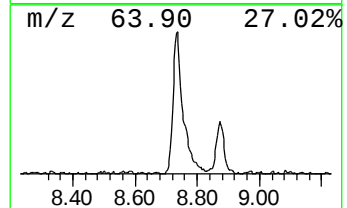
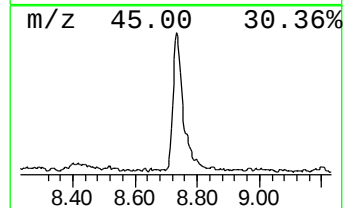
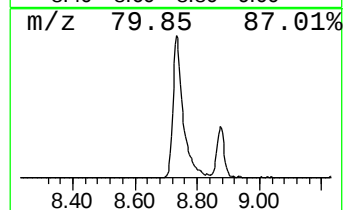
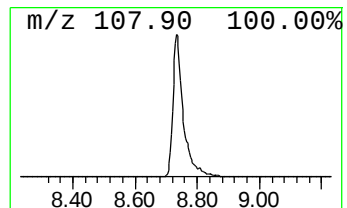
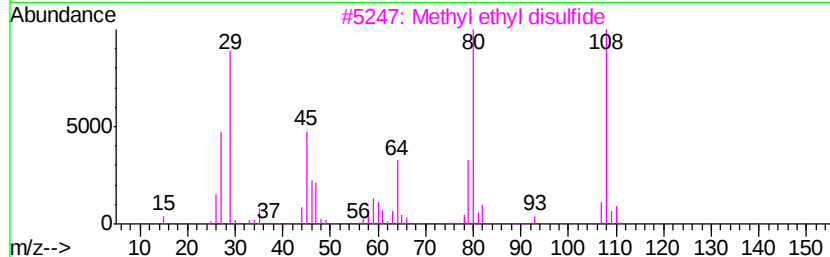
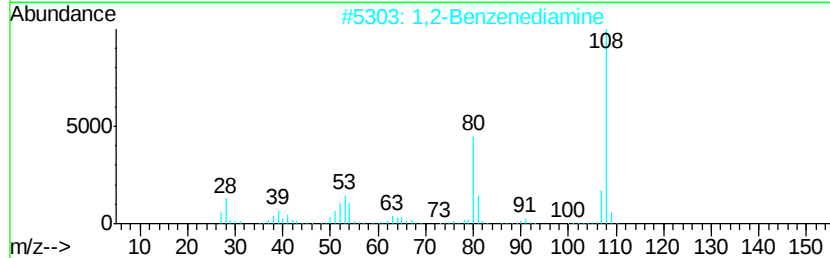
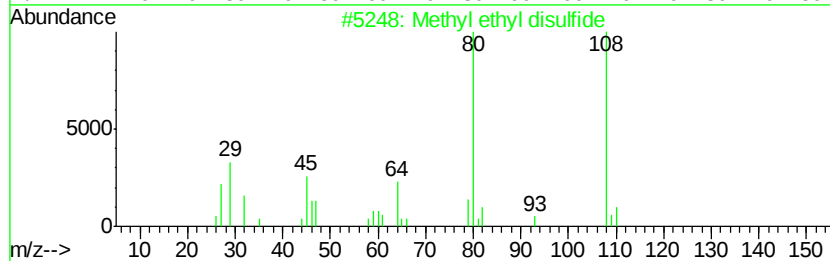
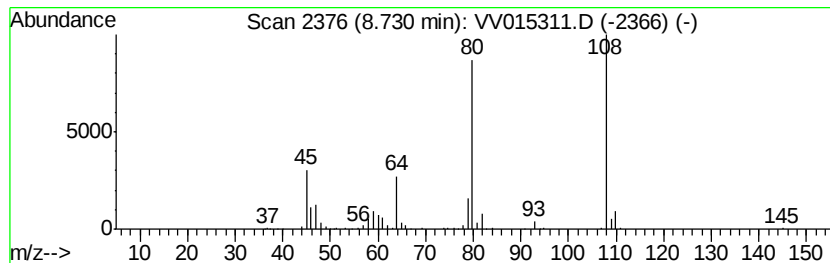
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Quant Title : VOC Analysis

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

Peak Number 5 Methyl ethyl disulfide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.73	9.45 ug/L	328722	Chlorobenzene-d5	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methyl ethyl disulfide	108	C3H8S2	020333-39-5	91
2		1,2-Benzenediamine	108	C6H8N2	000095-54-5	80
3		Methyl ethyl disulfide	108	C3H8S2	020333-39-5	78
4		1,3-Benzenediamine	108	C6H8N2	000108-45-2	64
5		Nicotinyl alcohol	109	C6H7NO	000100-55-0	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV033120\
Data File : VV015311.D
Acq On : 31 Mar 2020 14:11
Operator : SY/MD
Sample : L1975-12
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
ETTH5

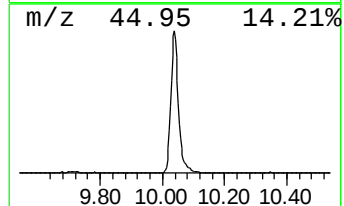
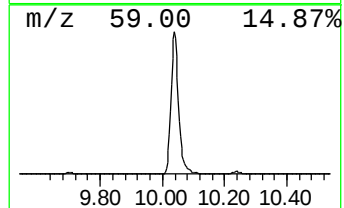
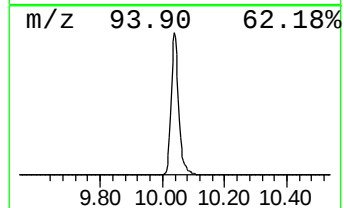
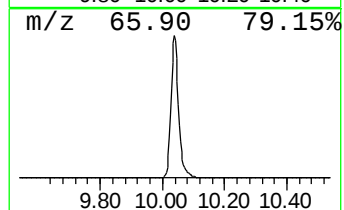
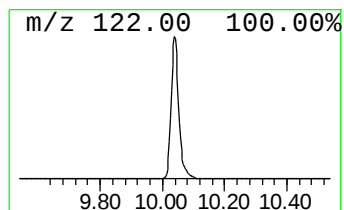
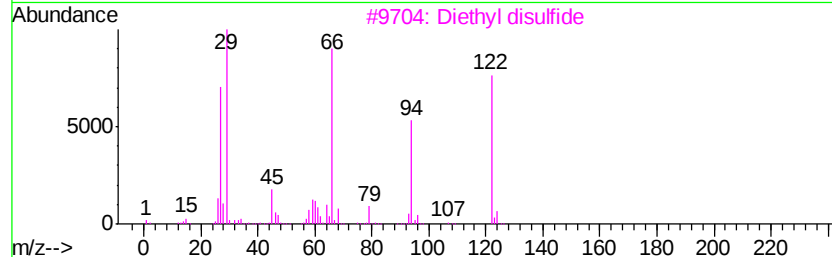
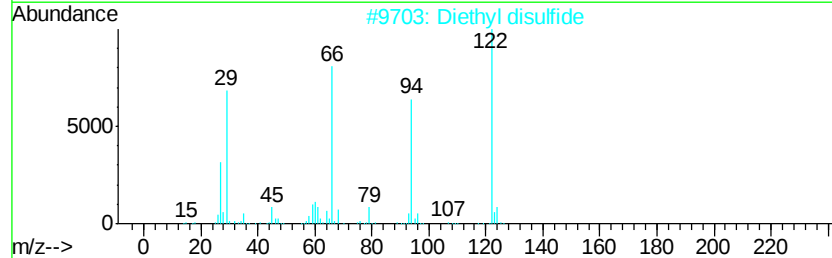
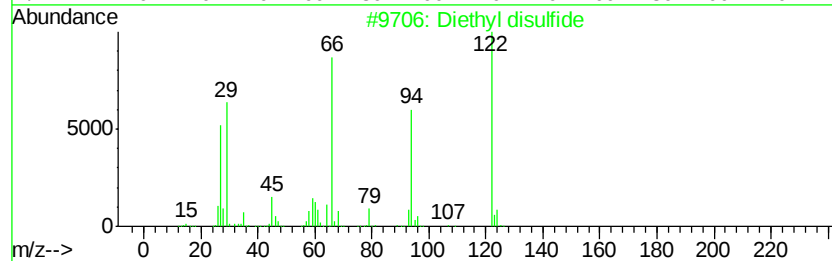
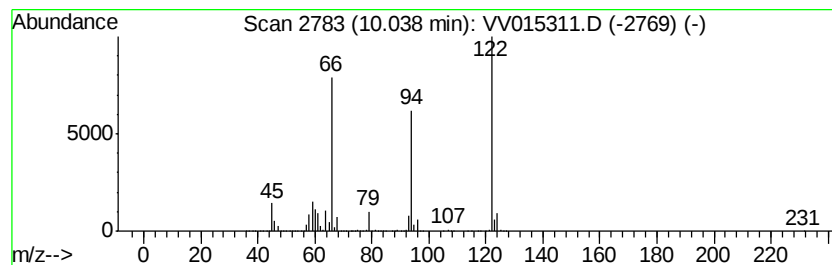
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM033020WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 Diethyl disulfide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.04	155.92 ug/L	5422030	Chlorobenzene-d5	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Diethyl disulfide	122	C4H10S2	000110-81-6	95
2		Diethyl disulfide	122	C4H10S2	000110-81-6	94
3		Diethyl disulfide	122	C4H10S2	000110-81-6	91
4		Diethyl sulfone	122	C4H10O2S	000597-35-3	64
5		6-exo-Methyl-5-endo-norbornenol	124	C8H12O	041414-52-2	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV033120\
 Data File : VV015311.D
 Acq On : 31 Mar 2020 14:11
 Operator : SY/MD
 Sample : L1975-12
 Misc : 5.0mL/MSVOA V/WATER
 ALS Vial : 1 Sample Multiplier: 1

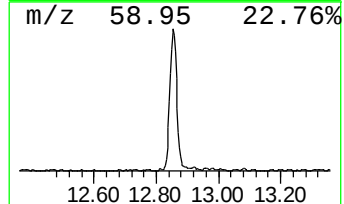
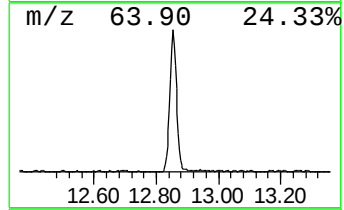
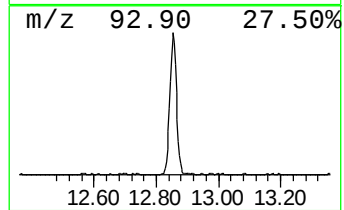
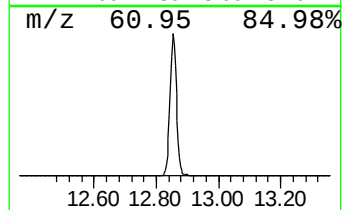
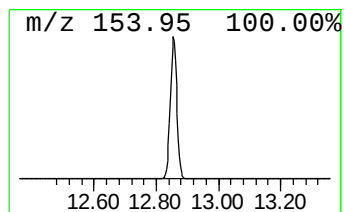
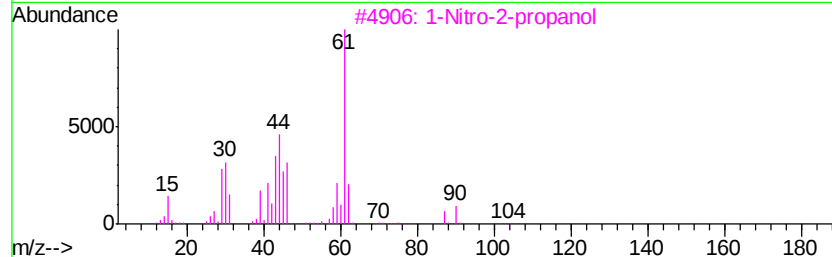
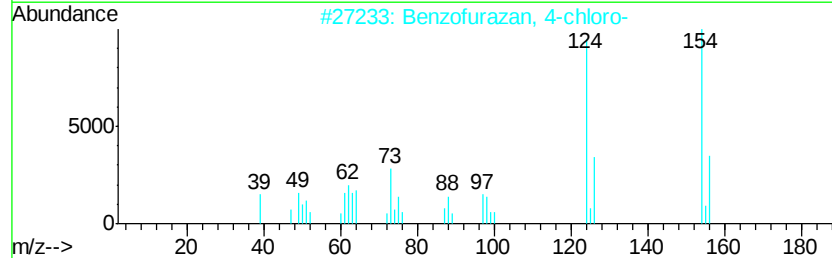
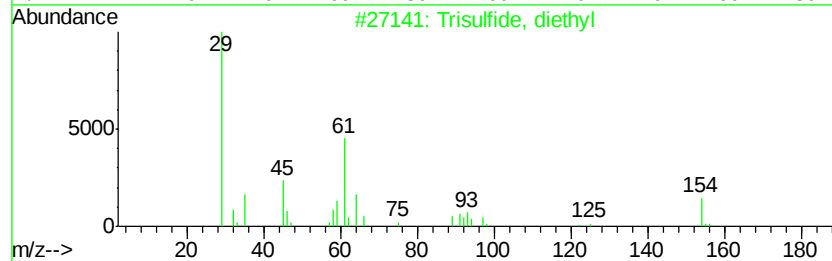
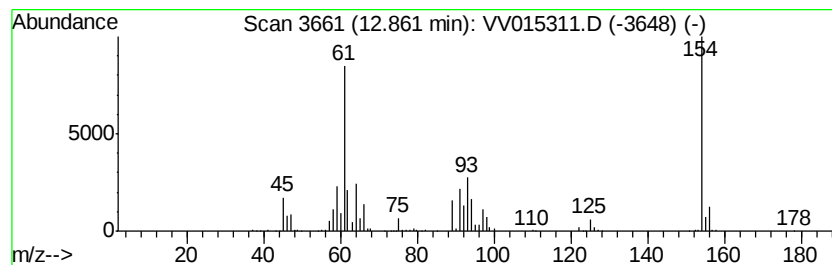
Instrument :
 MSVOA_V
 ClientSampleId :
 ETTH5

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM033020WMA.M
 Quant Title : VOC Analysis

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

 Peak Number 7 Trisulfide, diethyl Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.86	17.82 ug/L	604991	1,4-Dichlorobenzene-d4		11.27	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trisulfide, diethyl	154	C4H10S3	003600-24-6	64
2		Benzofurazan, 4-chloro-	154	C6H3ClN2O	007116-16-7	37
3		1-Nitro-2-propanol	105	C3H7NO3	003156-73-8	23
4		5-Chloro-benzofurazan	154	C6H3ClN2O	019155-86-3	16
5		4-Nitro-2-picoline N-oxide	154	C6H6N2O3	005470-66-6	14



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV033120\
Data File : VV015311.D
Acq On : 31 Mar 2020 14:11
Operator : SY/MD
Sample : L1975-12
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
ETTH5

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM033020WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
dl-Alanine	1.40	3.2	ug/L	91998	1	5.64	1450500	50.0
Ethanethiol	2.05	44.4	ug/L	1286500	1	5.64	1450500	50.0
Ethane, (methylth...	3.84	4.0	ug/L	115660	1	5.64	1450500	50.0
Methyl ethyl disu...	8.73	9.4	ug/L	328722	2	8.87	1738780	50.0
Diethyl disulfide	10.04	155.9	ug/L	5422030	2	8.87	1738780	50.0
Trisulfide, diethyl	12.86	17.8	ug/L	604991	3	11.27	1697460	50.0