

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082219\
 Data File : VU033911.D
 Acq On : 22 Aug 2019 19:55
 Operator : JC/SP
 Sample : K4454-06
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F2B91

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_U\METHOD\SOMULM082219WMA.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	1.148	11	18	56	rBV	2656876	4250473	100.00%	19.017%
2	1.389	87	93	106	rVB2	316495	351851	8.28%	1.574%
3	1.547	136	142	171	rVB	1107775	1295532	30.48%	5.796%
4	1.666	173	179	196	rVB	231652	292994	6.89%	1.311%
5	2.170	330	336	348	rVB	39885	58199	1.37%	0.260%
6	2.254	352	362	373	rBV	476178	698988	16.44%	3.127%
7	2.360	387	395	409	rVB	49074	78954	1.86%	0.353%
8	2.961	572	582	596	rVB	24459	44500	1.05%	0.199%
9	3.138	635	637	641	rBV4	409	365	0.01%	0.002%
10	3.347	699	702	703	rBV3	615	348	0.01%	0.002%
11	3.521	754	756	761	rBV4	235	238	0.01%	0.001%
12	3.624	784	788	791	rVB4	485	373	0.01%	0.002%
13	3.717	813	817	820	rBV3	337	315	0.01%	0.001%
14	3.817	844	848	850	rBV2	413	356	0.01%	0.002%
15	3.871	860	865	868	rBV3	644	737	0.02%	0.003%
16	4.045	916	919	922	rBV3	348	237	0.01%	0.001%
17	4.096	932	935	937	rBV3	425	236	0.01%	0.001%
18	4.148	938	951	1007	rBV	218402	690757	16.25%	3.091%
19	4.620	1079	1098	1125	rBV	372074	884060	20.80%	3.955%
20	4.845	1164	1168	1169	rBV3	992	717	0.02%	0.003%
21	4.862	1170	1173	1179	rVB5	1418	1797	0.04%	0.008%
22	4.958	1201	1203	1205	rBV2	493	303	0.01%	0.001%
23	5.064	1230	1236	1239	rBV3	844	702	0.02%	0.003%
24	5.083	1239	1242	1246	rVV3	413	336	0.01%	0.002%
25	5.315	1288	1314	1350	rBV2	736136	2212164	52.05%	9.897%
26	5.527	1378	1380	1382	rBV3	452	243	0.01%	0.001%
27	5.543	1382	1385	1388	rBV3	515	364	0.01%	0.002%
28	5.643	1414	1416	1420	rBV2	358	337	0.01%	0.002%
29	5.691	1428	1431	1433	rBV3	521	360	0.01%	0.002%
30	5.861	1470	1484	1512	rBV	715756	1422930	33.48%	6.366%
31	6.160	1564	1577	1595	rBV7	25507	59477	1.40%	0.266%
32	6.308	1607	1623	1645	rBV	522369	1051364	24.74%	4.704%
33	6.527	1689	1691	1694	rVB3	769	413	0.01%	0.002%
34	6.546	1695	1697	1701	rVB3	701	373	0.01%	0.002%

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 Title : VOC Analysis

35	6.624	1716	1721	1723	rBV3	610	415	0.01%	0.002%
36	6.656	1728	1731	1737	rVB3	649	711	0.02%	0.003%
37	6.694	1740	1743	1745	rBV	381	257	0.01%	0.001%
38	6.749	1756	1760	1763	rVB3	387	302	0.01%	0.001%
39	6.771	1763	1767	1771	rVB3	724	633	0.01%	0.003%
40	6.800	1771	1776	1779	rBV3	748	803	0.02%	0.004%
41	6.858	1784	1794	1800	rBV8	1756	3480	0.08%	0.016%
42	6.951	1817	1823	1828	rBV3	735	844	0.02%	0.004%
43	6.984	1828	1833	1834	rBV2	306	305	0.01%	0.001%
44	7.042	1848	1851	1855	rBV3	284	245	0.01%	0.001%
45	7.087	1862	1865	1871	rVV3	572	508	0.01%	0.002%
46	7.138	1876	1881	1882	rBV	281	231	0.01%	0.001%
47	7.154	1882	1886	1890	rVV4	261	321	0.01%	0.001%
48	7.215	1899	1905	1910	rVB6	1102	1222	0.03%	0.005%
49	7.247	1910	1915	1919	rBV4	640	628	0.01%	0.003%
50	7.376	1951	1955	1956	rBV	750	523	0.01%	0.002%
51	7.453	1976	1979	1983	rBV4	479	354	0.01%	0.002%
52	7.472	1983	1985	1990	rVB4	1011	728	0.02%	0.003%
53	7.546	1990	2008	2025	rBV	898816	1589177	37.39%	7.110%
54	7.842	2095	2100	2105	rBV6	1663	2090	0.05%	0.009%
55	7.906	2117	2120	2123	rBV3	355	261	0.01%	0.001%
56	8.035	2156	2160	2162	rVB5	523	299	0.01%	0.001%
57	8.093	2175	2178	2183	rVB3	381	250	0.01%	0.001%
58	8.135	2184	2191	2192	rBV4	465	477	0.01%	0.002%
59	8.209	2206	2214	2224	rBV5	5645	9689	0.23%	0.043%
60	8.295	2229	2241	2287	rBV2	624888	1250623	29.42%	5.595%
61	8.594	2332	2334	2337	rBV2	1115	766	0.02%	0.003%
62	8.652	2350	2352	2357	rVB3	789	472	0.01%	0.002%
63	8.752	2381	2383	2387	rVB4	521	312	0.01%	0.001%
64	8.778	2387	2391	2395	rBV4	761	662	0.02%	0.003%
65	8.794	2395	2396	2403	rVB3	878	673	0.02%	0.003%
66	8.865	2416	2418	2422	rBV3	492	354	0.01%	0.002%
67	8.890	2422	2426	2432	rVV6	632	734	0.02%	0.003%
68	8.939	2439	2441	2443	rVB3	628	226	0.01%	0.001%
69	8.974	2449	2452	2454	rBV3	452	330	0.01%	0.001%
70	9.070	2469	2482	2509	rBV	1078692	1793061	42.18%	8.022%
71	9.289	2548	2550	2553	rBV4	651	353	0.01%	0.002%

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 Title : VOC Analysis

72	9.312	2554	2557	2561	rBV6	1083	992	0.02%	0.004%
73	9.427	2588	2593	2596	rBV2	501	549	0.01%	0.002%
74	9.479	2603	2609	2613	rBV3	464	453	0.01%	0.002%
75	9.665	2664	2667	2671	rVB2	385	273	0.01%	0.001%
76	9.691	2671	2675	2677	rBV2	341	261	0.01%	0.001%
77	9.762	2693	2697	2700	rBV3	814	860	0.02%	0.004%
78	9.942	2751	2753	2757	rBV3	344	237	0.01%	0.001%
79	9.964	2757	2760	2764	rBV5	513	379	0.01%	0.002%
80	10.019	2772	2777	2779	rBV3	696	587	0.01%	0.003%
81	10.154	2805	2819	2825	rBV6	1200	2287	0.05%	0.010%
82	10.183	2825	2828	2831	rBV3	557	362	0.01%	0.002%
83	10.221	2838	2840	2845	rVB3	699	569	0.01%	0.003%
84	10.250	2845	2849	2851	rBV	493	371	0.01%	0.002%
85	10.283	2856	2859	2861	rVV3	581	389	0.01%	0.002%
86	10.308	2865	2867	2874	rVB4	929	663	0.02%	0.003%
87	10.414	2887	2900	2923	rBV	741754	1182957	27.83%	5.293%
88	10.701	2987	2989	2992	rBV2	449	318	0.01%	0.001%
89	10.758	3000	3007	3008	rBV2	1142	1198	0.03%	0.005%
90	10.803	3018	3021	3023	rBV2	493	262	0.01%	0.001%
91	10.819	3024	3026	3029	rVB3	902	460	0.01%	0.002%
92	10.839	3029	3032	3034	rBV2	481	344	0.01%	0.002%
93	10.987	3068	3078	3094	rBV2	14302	28130	0.66%	0.126%
94	11.144	3119	3127	3145	rVV2	10722	19245	0.45%	0.086%
95	11.212	3145	3148	3153	rVB5	699	598	0.01%	0.003%
96	11.254	3159	3161	3163	rVB2	459	232	0.01%	0.001%
97	11.266	3163	3165	3168	rBV3	634	330	0.01%	0.001%
98	11.373	3196	3198	3199	rBV2	695	286	0.01%	0.001%
99	11.466	3215	3227	3254	rBV	978442	1553155	36.54%	6.949%
100	11.842	3332	3344	3373	rBV	908415	1489321	35.04%	6.663%

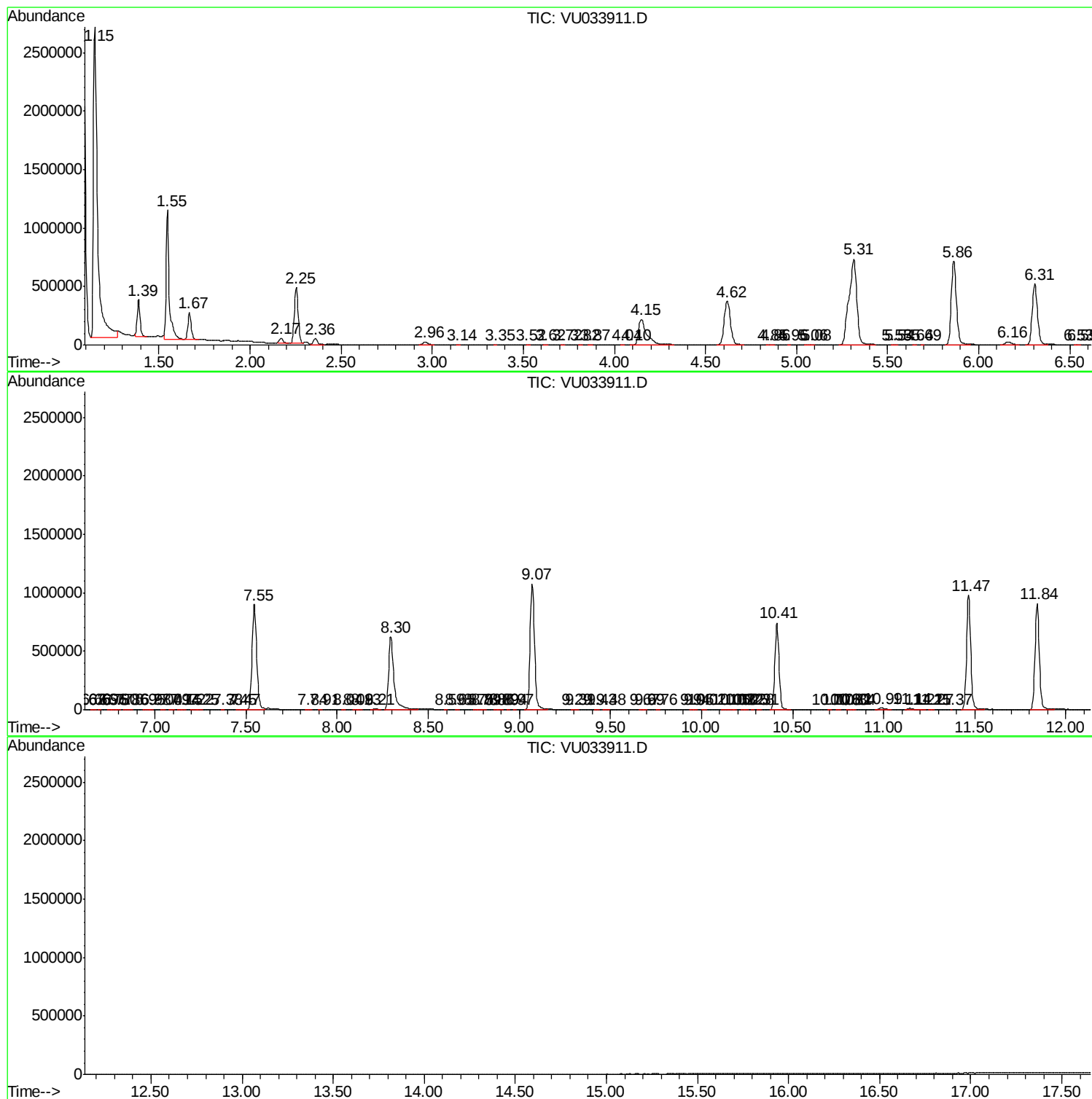
Sum of corrected areas: 22350780

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082219WMA.M
Quant Title : VOC Analysis

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



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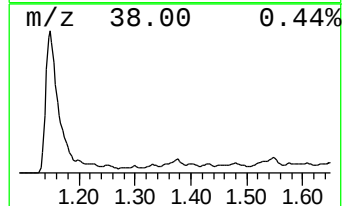
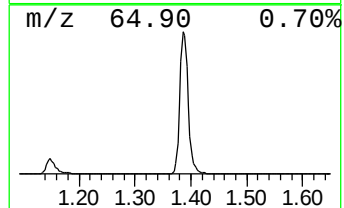
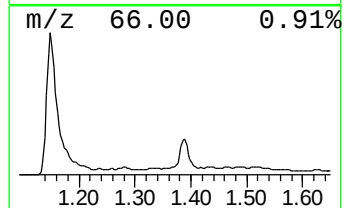
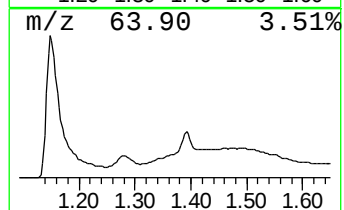
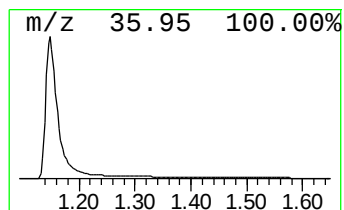
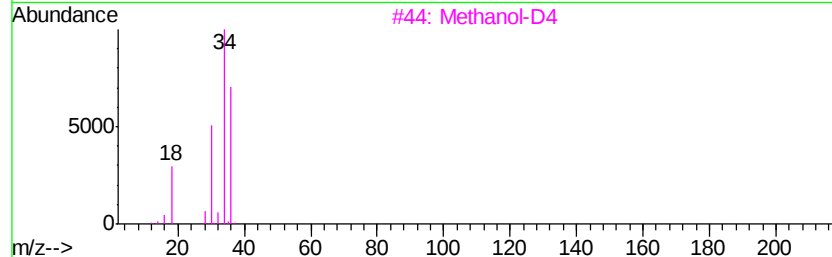
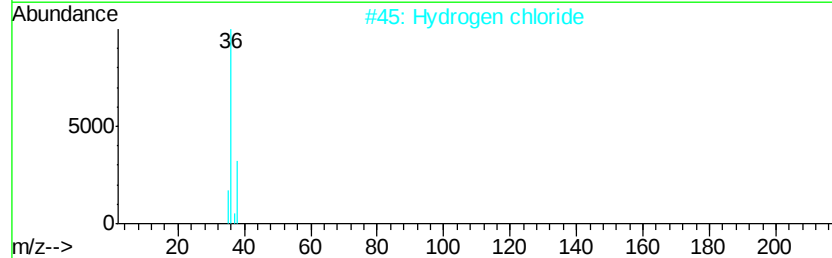
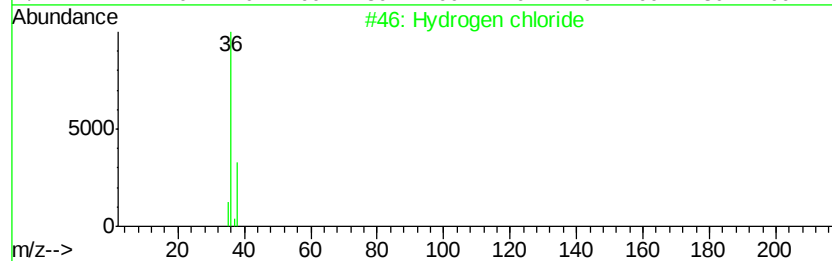
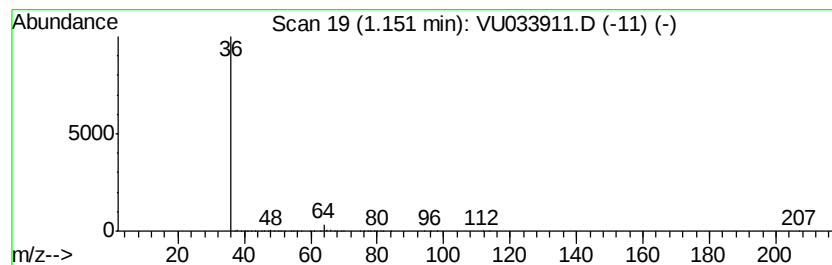
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082219WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.15	149.36 ug/L	4250470	1,4-Difluorobenzene	5.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hydrogen chloride	36	ClH	007647-01-0	2
2		Hydrogen chloride	36	ClH	007647-01-0	2
3		Methanol-D4	36	CD4O	000811-98-3	2
4		Ammonium Chloride	53	ClH4N	012125-02-9	1
5		2-Chloroethylamine	79	C2H6ClN	000689-98-5	1



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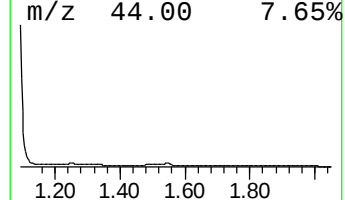
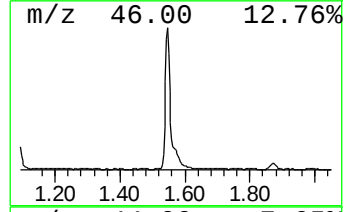
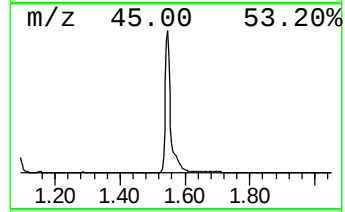
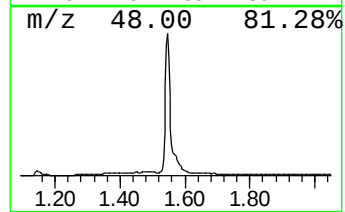
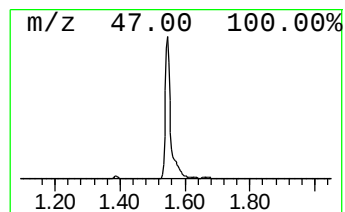
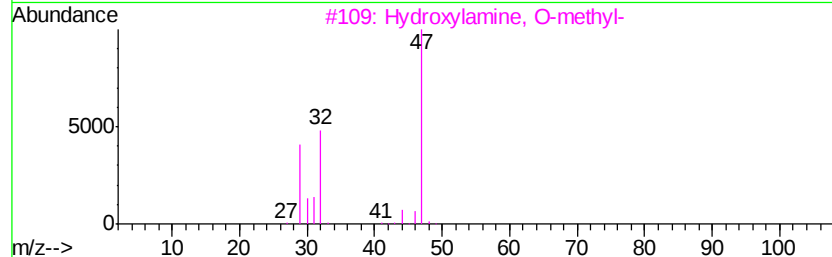
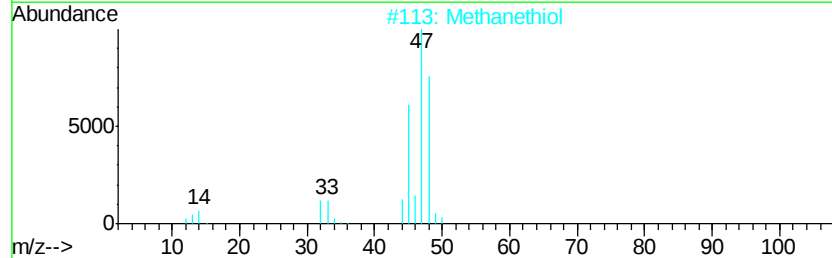
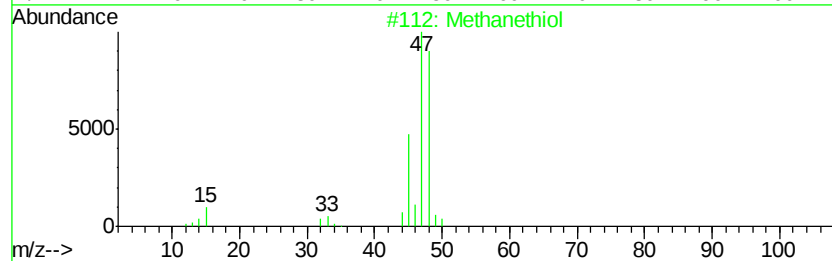
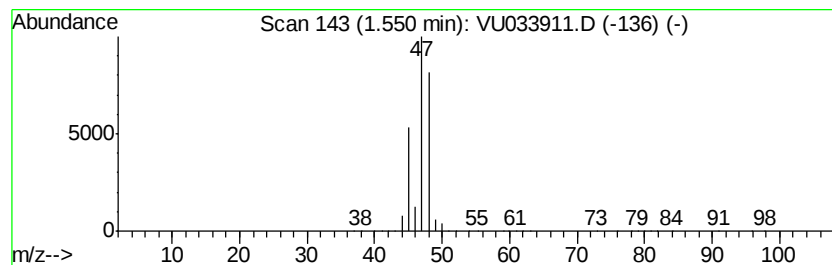
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082219WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Methanethiol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.55	45.52 ug/L	1295530	1,4-Difluorobenzene	5.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methanethiol	48	CH4S	000074-93-1	90
2		Methanethiol	48	CH4S	000074-93-1	83
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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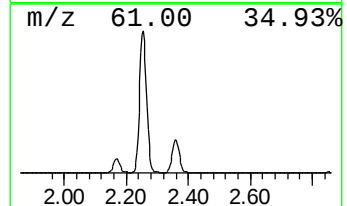
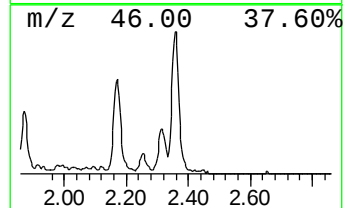
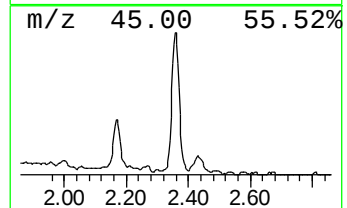
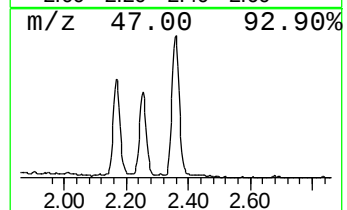
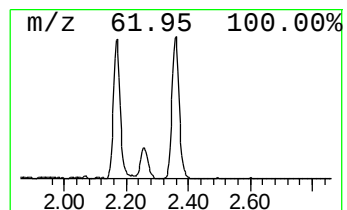
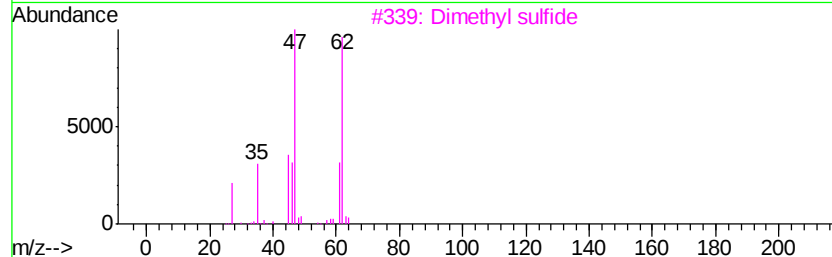
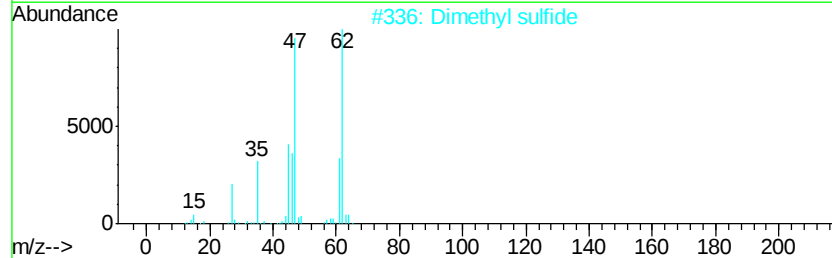
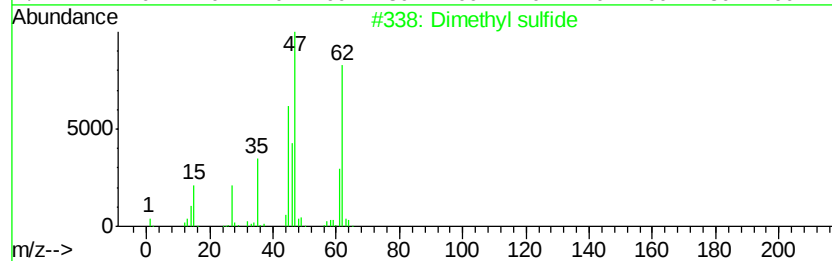
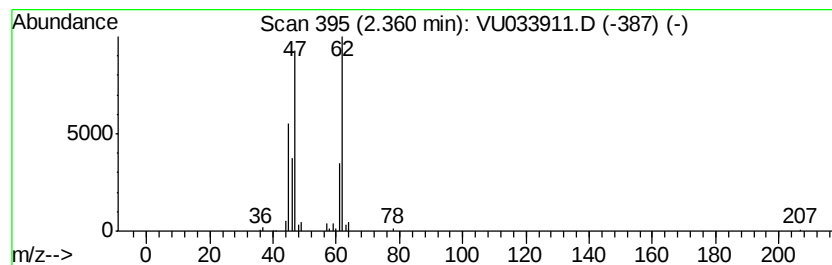
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Dimethyl sulfide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.36	2.77 ug/L	78954	1,4-Difluorobenzene	5.86

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	90
5		Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	83



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Data File : VU033911.D
Acq On : 22 Aug 2019 19:55
Operator : JC/SP
Sample : K4454-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F2B91

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082219WMA.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
unknown-01	1.15	149.4	ug/L	4250470	1	5.86	1422930	50.0
Methanethiol	1.55	45.5	ug/L	1295530	1	5.86	1422930	50.0
Dimethyl sulfide	2.36	2.8	ug/L	78954	1	5.86	1422930	50.0