

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VW121123\
 Data File : VW033247.D
 Acq On : 12 Dec 2023 04:53
 Operator : SY/MD
 Sample : 05751-16
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 48 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 YCHF8

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\SFAMVLM120123WMA.M
 Title : VOC Analysis

Signal : TIC: VW033247.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.166	33	39	56	rBV	60490	76903	7.99%	0.916%
2	1.278	67	74	88	rBV	137590	154746	16.08%	1.843%
3	1.532	146	153	170	rVB	96834	116469	12.10%	1.387%
4	2.066	308	319	329	rBV3	330337	565405	58.75%	6.732%
5	2.214	355	365	383	rBV	91329	157277	16.34%	1.873%
6	2.638	493	497	501	rVB3	568	427	0.04%	0.005%
7	2.706	511	518	526	rVB7	1021	1617	0.17%	0.019%
8	2.773	535	539	545	rVB2	542	516	0.05%	0.006%
9	2.889	573	575	581	rVB2	280	249	0.03%	0.003%
10	2.934	582	589	595	rBV2	550	800	0.08%	0.010%
11	3.014	611	614	618	rBB	336	213	0.02%	0.003%
12	3.040	619	622	624	rBV	451	280	0.03%	0.003%
13	3.114	632	645	661	rVV2	10983	23449	2.44%	0.279%
14	3.175	662	664	667	rVB3	499	291	0.03%	0.003%
15	3.198	667	671	675	rVB2	302	332	0.03%	0.004%
16	3.365	721	723	728	rVB2	271	244	0.03%	0.003%
17	3.403	732	735	740	rVB2	203	226	0.02%	0.003%
18	3.465	752	754	757	rVB	298	161	0.02%	0.002%
19	3.590	787	793	795	rBV2	449	443	0.05%	0.005%
20	3.748	839	842	844	rBV2	217	162	0.02%	0.002%
21	3.783	844	853	858	rBV	52907	104333	10.84%	1.242%
22	4.249	976	998	1026	rBV	159005	429834	44.66%	5.118%
23	4.513	1069	1080	1103	rVB3	11457	30590	3.18%	0.364%
24	4.657	1119	1125	1128	rBV3	530	542	0.06%	0.006%
25	4.744	1149	1152	1155	rBV2	348	226	0.02%	0.003%
26	4.770	1158	1160	1164	rVB2	331	195	0.02%	0.002%
27	4.793	1165	1167	1171	rBV2	248	182	0.02%	0.002%
28	4.860	1185	1188	1192	rVB2	353	272	0.03%	0.003%
29	4.886	1192	1196	1198	rBV	294	199	0.02%	0.002%
30	4.956	1198	1218	1252	rBV2	361805	962402	100.00%	11.460%
31	5.532	1386	1397	1429	rBV	295626	609135	63.29%	7.253%
32	5.834	1478	1491	1518	rBV2	189482	393001	40.84%	4.680%
33	5.989	1527	1539	1558	rBV	199304	402960	41.87%	4.798%
34	6.220	1608	1611	1615	rBV2	545	321	0.03%	0.004%
35	6.243	1615	1618	1620	rBV2	387	224	0.02%	0.003%
36	6.281	1627	1630	1632	rBV	361	238	0.02%	0.003%

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 Title : VOC Analysis

37	6.448	1679	1682	1686	rVB2	314	253	0.03%	0.003%
38	6.506	1698	1700	1703	rBV2	271	193	0.02%	0.002%
39	6.603	1725	1730	1732	rBV	324	297	0.03%	0.004%
40	6.667	1746	1750	1754	rBB2	282	304	0.03%	0.004%
41	6.706	1758	1762	1766	rBV2	274	307	0.03%	0.004%
42	6.757	1773	1778	1781	rVB2	181	181	0.02%	0.002%
43	6.911	1815	1826	1851	rBV	112562	209008	21.72%	2.489%
44	7.149	1896	1900	1904	rBV3	488	511	0.05%	0.006%
45	7.243	1918	1929	1953	rBV	464395	806610	83.81%	9.605%
46	7.554	2016	2026	2055	rBV	82049	146412	15.21%	1.743%
47	7.751	2085	2087	2091	rVB2	677	382	0.04%	0.005%
48	7.776	2091	2095	2100	rBV3	536	569	0.06%	0.007%
49	7.818	2105	2108	2111	rBV2	287	193	0.02%	0.002%
50	7.850	2116	2118	2119	rBV2	443	211	0.02%	0.003%
51	7.963	2149	2153	2160	rVB	383	438	0.05%	0.005%
52	8.024	2162	2172	2208	rBV	184075	352490	36.63%	4.197%
53	8.304	2253	2259	2271	rVB6	2446	4486	0.47%	0.053%
54	8.416	2288	2294	2297	rBV2	328	241	0.03%	0.003%
55	8.458	2303	2307	2310	rBV4	490	335	0.03%	0.004%
56	8.509	2320	2323	2325	rBV2	241	198	0.02%	0.002%
57	8.583	2340	2346	2347	rBV	362	381	0.04%	0.005%
58	8.783	2397	2408	2436	rBV	476698	773384	80.36%	9.209%
59	9.088	2501	2503	2507	rVB3	338	204	0.02%	0.002%
60	9.107	2507	2509	2512	rVB2	479	267	0.03%	0.003%
61	9.124	2512	2514	2516	rBV	414	236	0.02%	0.003%
62	9.365	2586	2589	2594	rVB2	186	188	0.02%	0.002%
63	9.500	2627	2631	2633	rBV2	491	356	0.04%	0.004%
64	9.796	2719	2723	2729	rBB2	260	316	0.03%	0.004%
65	9.953	2767	2772	2773	rBV	1089	810	0.08%	0.010%
66	10.050	2798	2802	2809	rVB2	224	254	0.03%	0.003%
67	10.152	2822	2834	2856	rBV	285982	449485	46.70%	5.352%
68	10.329	2882	2889	2898	rVB4	2710	3686	0.38%	0.044%
69	10.419	2914	2917	2922	rBV	262	271	0.03%	0.003%
70	10.506	2940	2944	2946	rBV3	288	242	0.03%	0.003%
71	10.612	2975	2977	2982	rVB2	502	351	0.04%	0.004%
72	10.638	2982	2985	2986	rBV	289	179	0.02%	0.002%
73	10.931	3071	3076	3078	rBV2	412	341	0.04%	0.004%
74	11.133	3136	3139	3144	rBV3	500	458	0.05%	0.005%
75	11.185	3144	3155	3180	rBV	502541	783594	81.42%	9.330%
76	11.503	3252	3254	3258	rBV	262	217	0.02%	0.003%

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 Title : VOC Analysis

77	11.561	3260	3272	3293	rBV	517042	816970	84.89%	9.728%
78	11.985	3400	3404	3406	rBV2	460	348	0.04%	0.004%
79	12.040	3418	3421	3424	rBV2	339	221	0.02%	0.003%
80	12.162	3456	3459	3460	rBV	314	187	0.02%	0.002%
81	12.188	3464	3467	3468	rBV2	449	272	0.03%	0.003%
82	12.239	3480	3483	3487	rBV2	307	203	0.02%	0.002%
83	12.284	3491	3497	3500	rBV	481	368	0.04%	0.004%
84	12.355	3517	3519	3522	rBV	313	174	0.02%	0.002%
85	12.426	3534	3541	3543	rBV2	301	348	0.04%	0.004%
86	12.619	3595	3601	3604	rBV	421	567	0.06%	0.007%
87	12.734	3633	3637	3639	rBV2	283	188	0.02%	0.002%
88	13.043	3726	3733	3735	rBV2	346	361	0.04%	0.004%
89	13.123	3755	3758	3761	rVB	408	264	0.03%	0.003%
90	13.152	3761	3767	3772	rBV2	394	508	0.05%	0.006%
91	13.258	3798	3800	3803	rBV2	307	167	0.02%	0.002%
92	13.313	3815	3817	3821	rBV3	416	304	0.03%	0.004%
93	13.696	3934	3936	3937	rBV	413	209	0.02%	0.002%
94	13.766	3955	3958	3964	rVV	548	514	0.05%	0.006%
95	13.811	3968	3972	3973	rBV	307	238	0.02%	0.003%
96	13.869	3982	3990	3992	rBV2	506	599	0.06%	0.007%
97	13.963	4017	4019	4021	rBV4	376	195	0.02%	0.002%
98	14.033	4036	4041	4043	rVB	610	409	0.04%	0.005%
99	14.094	4056	4060	4063	rBV3	417	400	0.04%	0.005%
100	14.779	4270	4273	4275	rBV	807	507	0.05%	0.006%

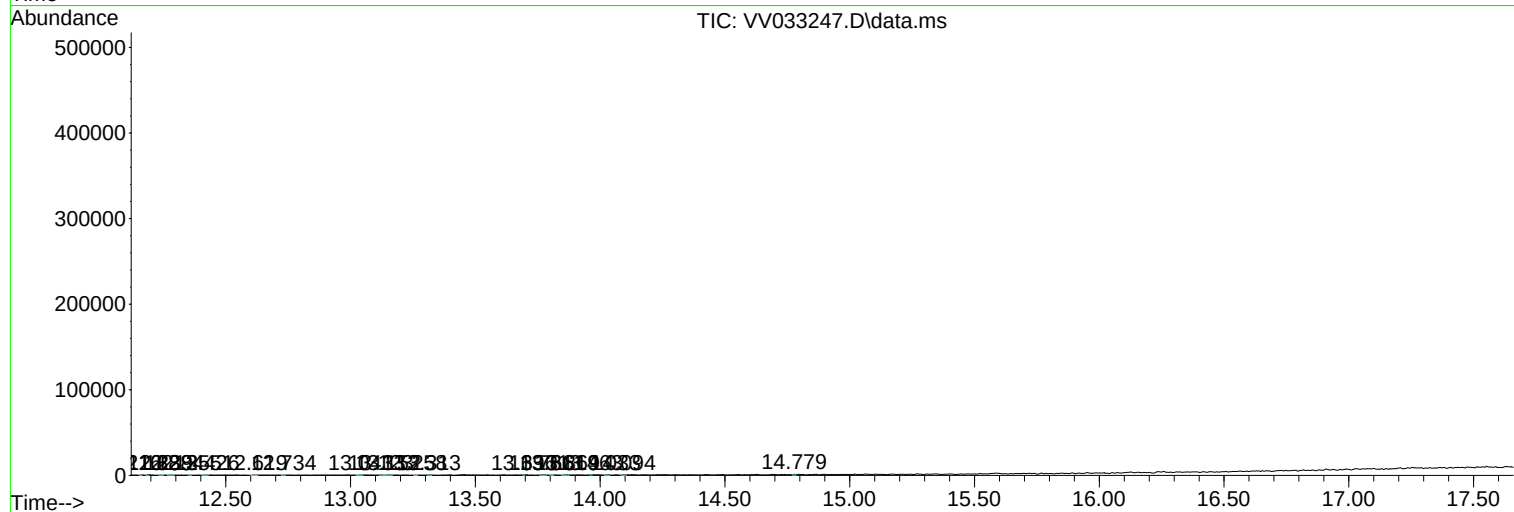
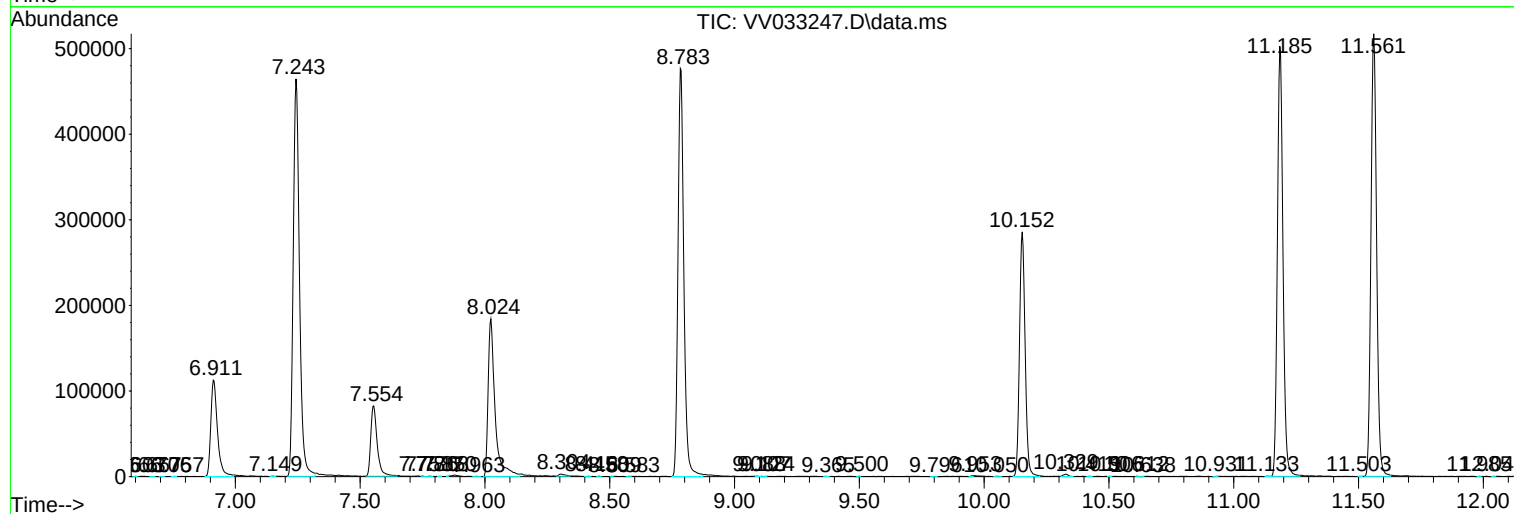
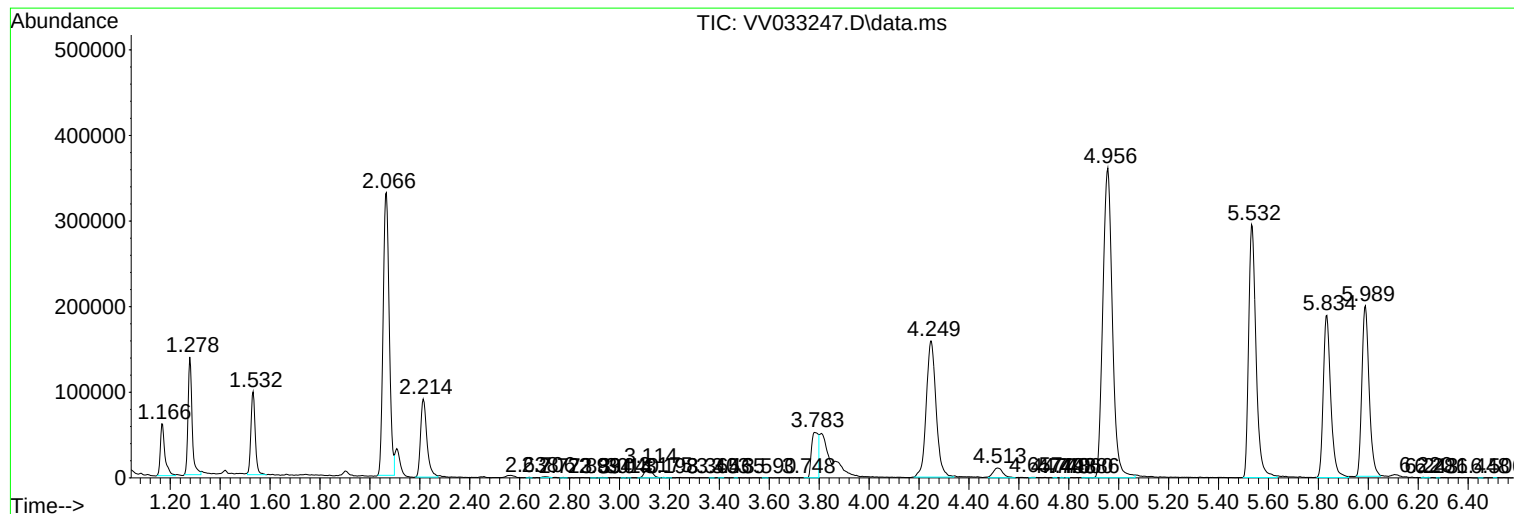
Sum of corrected areas: 8398224

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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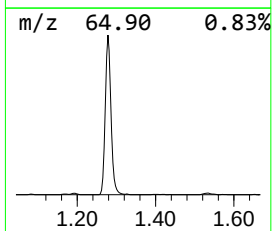
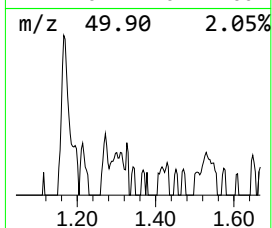
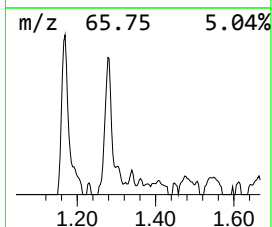
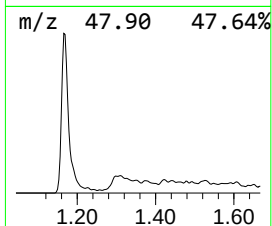
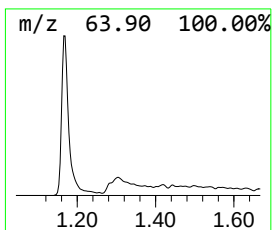
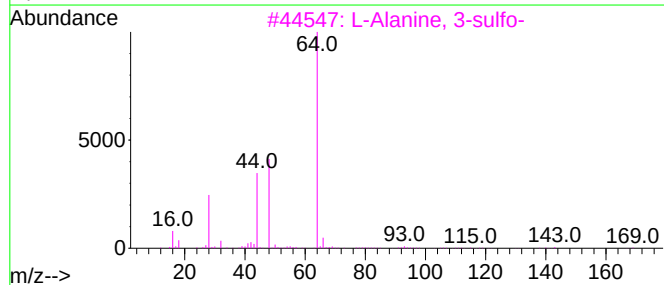
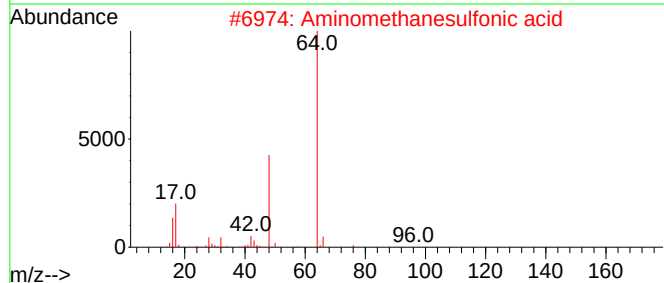
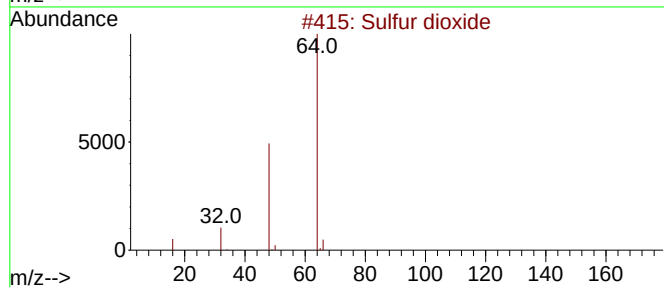
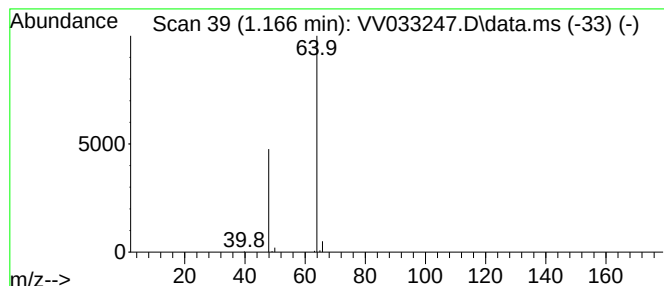
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.166	6.31 ug/L	76903	1,4-Difluorobenzene	5.532

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Sulfur dioxide	64	O2S	007446-09-5	4
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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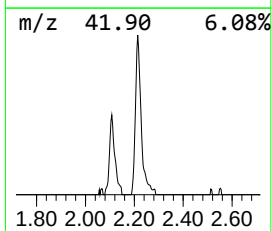
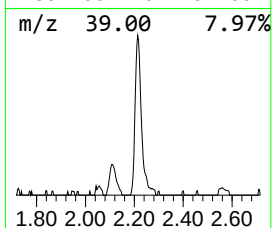
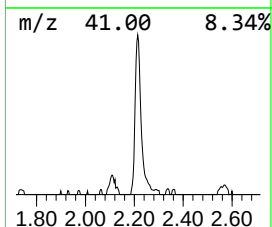
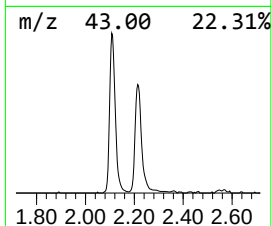
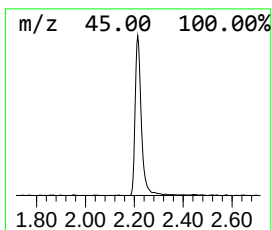
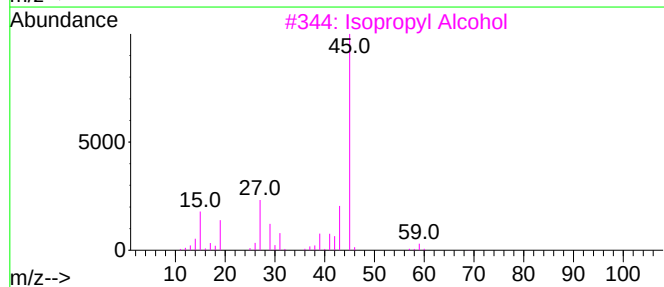
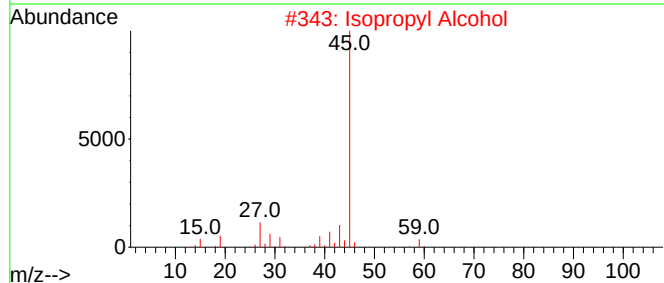
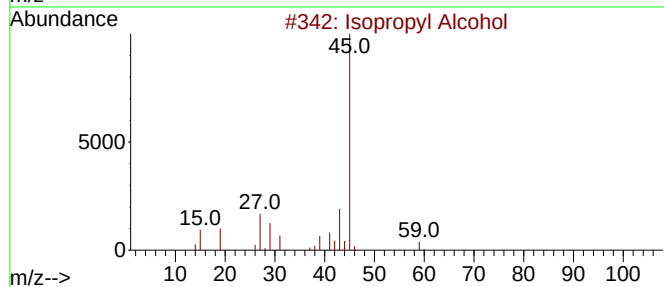
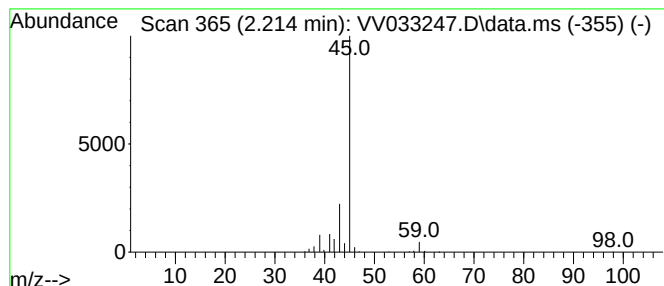
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Isopropyl Alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.214	12.91 ug/L	157277	1,4-Difluorobenzene	5.532

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol			60	C3H8O	000067-63-0	83
2	Isopropyl Alcohol			60	C3H8O	000067-63-0	78
3	Isopropyl Alcohol			60	C3H8O	000067-63-0	78
4	Isopropyl Alcohol			60	C3H8O	000067-63-0	64
5	Isopropyl Alcohol			60	C3H8O	000067-63-0	64



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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.166	6.3	ug/L	76903	1	5.532	609135	50.0
Isopropyl Alcohol	2.214	12.9	ug/L	157277	1	5.532	609135	50.0