

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121123\
 Data File : VV033246.D
 Acq On : 12 Dec 2023 04:30
 Operator : SY/MD
 Sample : 05751-15
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 47 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 YCHF7

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: VV033246.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	55	rBV	71189	90080	9.15%	1.055%
2	1.278	67	74	95	rBV	142896	172621	17.53%	2.022%
3	1.532	146	153	168	rVB	103046	119459	12.13%	1.400%
4	2.066	308	319	329	rBV3	333951	573590	58.26%	6.720%
5	2.214	355	365	387	rBV	92929	162931	16.55%	1.909%
6	2.413	423	427	430	rBV4	522	492	0.05%	0.006%
7	2.558	463	472	474	rBV5	3211	4140	0.42%	0.049%
8	2.703	509	517	525	rBV5	1587	2478	0.25%	0.029%
9	2.963	595	598	600	rBV	292	207	0.02%	0.002%
10	3.021	610	616	620	rBV2	323	477	0.05%	0.006%
11	3.040	620	622	625	rVB2	414	208	0.02%	0.002%
12	3.059	625	628	633	rBB	392	354	0.04%	0.004%
13	3.114	633	645	660	rBV	11369	24462	2.48%	0.287%
14	3.201	668	672	678	rVB2	462	414	0.04%	0.005%
15	3.243	682	685	687	rBV2	272	202	0.02%	0.002%
16	3.416	736	739	742	rBB2	281	173	0.02%	0.002%
17	3.535	772	776	780	rBB	181	198	0.02%	0.002%
18	3.609	797	799	805	rVB	375	327	0.03%	0.004%
19	3.648	808	811	814	rBV2	272	258	0.03%	0.003%
20	3.783	841	853	859	rBV	55928	118089	11.99%	1.383%
21	4.246	976	997	1027	rBV	159885	433108	43.99%	5.074%
22	4.513	1066	1080	1099	rBV4	11899	29450	2.99%	0.345%
23	4.651	1120	1123	1129	rBV3	628	569	0.06%	0.007%
24	4.693	1134	1136	1139	rVB2	504	250	0.03%	0.003%
25	4.838	1179	1181	1183	rVB	437	177	0.02%	0.002%
26	4.850	1183	1185	1187	rBV	463	282	0.03%	0.003%
27	4.876	1192	1193	1196	rVB	368	179	0.02%	0.002%
28	4.956	1199	1218	1249	rBV2	368603	984550	100.00%	11.535%
29	5.265	1312	1314	1318	rBV3	433	315	0.03%	0.004%
30	5.532	1386	1397	1433	rBV	290415	605120	61.46%	7.089%
31	5.831	1479	1490	1514	rBV	187601	383334	38.93%	4.491%
32	5.989	1526	1539	1565	rBV	200764	415035	42.15%	4.862%
33	6.436	1675	1678	1679	rBV	355	170	0.02%	0.002%
34	6.519	1699	1704	1710	rBV5	749	722	0.07%	0.008%
35	6.609	1728	1732	1734	rBV	244	168	0.02%	0.002%
36	6.911	1816	1826	1853	rBV	113273	210563	21.39%	2.467%

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

37	7.243	1917	1929	1952	rBV	473245	829718	84.27%	9.721%
38	7.551	2015	2025	2053	rBV	82717	151274	15.36%	1.772%
39	7.690	2065	2068	2071	rBV	474	366	0.04%	0.004%
40	7.751	2085	2087	2090	rBV2	270	182	0.02%	0.002%
41	7.770	2090	2093	2096	rVV	637	334	0.03%	0.004%
42	7.796	2099	2101	2108	rBV	409	441	0.04%	0.005%
43	7.873	2121	2125	2136	rVB4	1654	2281	0.23%	0.027%
44	8.024	2162	2172	2205	rBV	185556	362705	36.84%	4.249%
45	8.307	2253	2260	2275	rVB7	2584	5588	0.57%	0.065%
46	8.410	2290	2292	2296	rVB3	421	242	0.02%	0.003%
47	8.522	2325	2327	2329	rBV2	331	223	0.02%	0.003%
48	8.661	2368	2370	2373	rVB	316	189	0.02%	0.002%
49	8.783	2397	2408	2436	rBV	466676	770726	78.28%	9.030%
50	9.120	2510	2513	2518	rVV2	168	183	0.02%	0.002%
51	9.268	2554	2559	2561	rBV	188	199	0.02%	0.002%
52	9.365	2587	2589	2595	rBV	189	201	0.02%	0.002%
53	9.480	2623	2625	2628	rBV2	258	164	0.02%	0.002%
54	9.593	2656	2660	2663	rBV2	203	203	0.02%	0.002%
55	9.648	2674	2677	2681	rBV2	279	201	0.02%	0.002%
56	9.831	2731	2734	2739	rBV2	227	228	0.02%	0.003%
57	9.914	2753	2760	2762	rBV2	328	291	0.03%	0.003%
58	10.152	2822	2834	2851	rBV	298545	458058	46.52%	5.366%
59	10.265	2864	2869	2873	rVB3	635	660	0.07%	0.008%
60	10.287	2873	2876	2879	rBV	393	199	0.02%	0.002%
61	10.326	2880	2888	2897	rBB6	1783	3050	0.31%	0.036%
62	10.371	2897	2902	2906	rBV2	292	245	0.02%	0.003%
63	10.394	2906	2909	2914	rBV	258	273	0.03%	0.003%
64	10.480	2932	2936	2938	rBV	389	330	0.03%	0.004%
65	10.728	3008	3013	3016	rBV2	277	238	0.02%	0.003%
66	10.837	3043	3047	3051	rBV2	204	206	0.02%	0.002%
67	10.860	3051	3054	3056	rVB	413	193	0.02%	0.002%
68	10.889	3059	3063	3068	rBV2	282	328	0.03%	0.004%
69	11.104	3125	3130	3132	rBV	259	274	0.03%	0.003%
70	11.185	3144	3155	3180	rBV	501770	772036	78.42%	9.045%
71	11.374	3211	3214	3217	rBV2	298	274	0.03%	0.003%
72	11.451	3235	3238	3239	rBV2	352	181	0.02%	0.002%
73	11.561	3257	3272	3295	rVV	537722	830502	84.35%	9.730%
74	11.721	3320	3322	3325	rBV2	650	412	0.04%	0.005%
75	11.763	3333	3335	3338	rBV	354	243	0.02%	0.003%
76	11.831	3353	3356	3359	rBV2	426	356	0.04%	0.004%

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 Title : VOC Analysis

77	11.895	3372	3376	3380	rBV2	314	363	0.04%	0.004%
78	11.972	3394	3400	3403	rBV3	470	487	0.05%	0.006%
79	12.001	3407	3409	3411	rVB2	393	172	0.02%	0.002%
80	12.037	3416	3420	3423	rBV	243	204	0.02%	0.002%
81	12.130	3442	3449	3451	rBV2	302	357	0.04%	0.004%
82	12.191	3465	3468	3470	rBV3	505	339	0.03%	0.004%
83	12.355	3513	3519	3525	rVV3	452	424	0.04%	0.005%
84	12.484	3556	3559	3563	rBV	171	182	0.02%	0.002%
85	12.532	3571	3574	3576	rBV	468	302	0.03%	0.004%
86	12.570	3584	3586	3589	rBV2	324	234	0.02%	0.003%
87	12.654	3610	3612	3618	rBV2	295	337	0.03%	0.004%
88	12.779	3647	3651	3652	rBV2	278	218	0.02%	0.003%
89	13.017	3723	3725	3728	rBV	389	195	0.02%	0.002%
90	13.075	3741	3743	3745	rBV2	372	202	0.02%	0.002%
91	13.268	3801	3803	3805	rBV	251	165	0.02%	0.002%
92	13.323	3816	3820	3823	rBV	305	288	0.03%	0.003%
93	13.355	3826	3830	3831	rBV	278	192	0.02%	0.002%
94	13.429	3851	3853	3855	rBV	332	242	0.02%	0.003%
95	13.683	3930	3932	3934	rBV3	512	262	0.03%	0.003%
96	13.847	3981	3983	3986	rBV2	390	263	0.03%	0.003%
97	14.075	4052	4054	4057	rBV	391	230	0.02%	0.003%
98	14.233	4098	4103	4105	rBV3	398	315	0.03%	0.004%
99	14.332	4133	4134	4137	rBV	399	226	0.02%	0.003%
100	14.609	4217	4220	4221	rBV	397	204	0.02%	0.002%

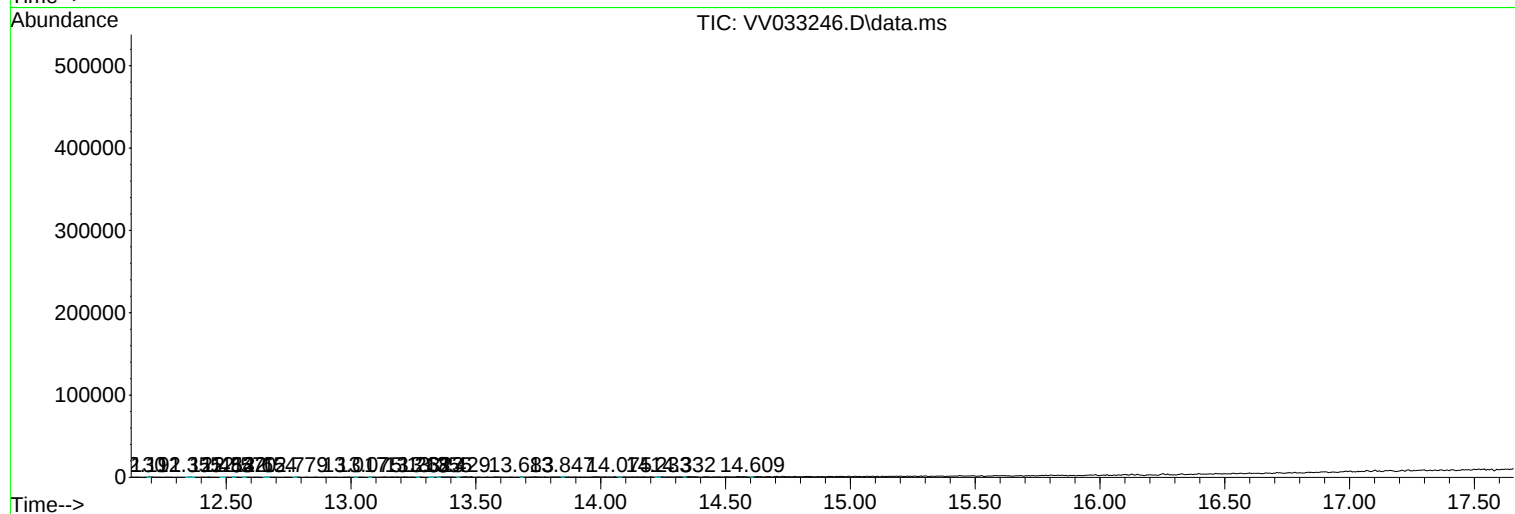
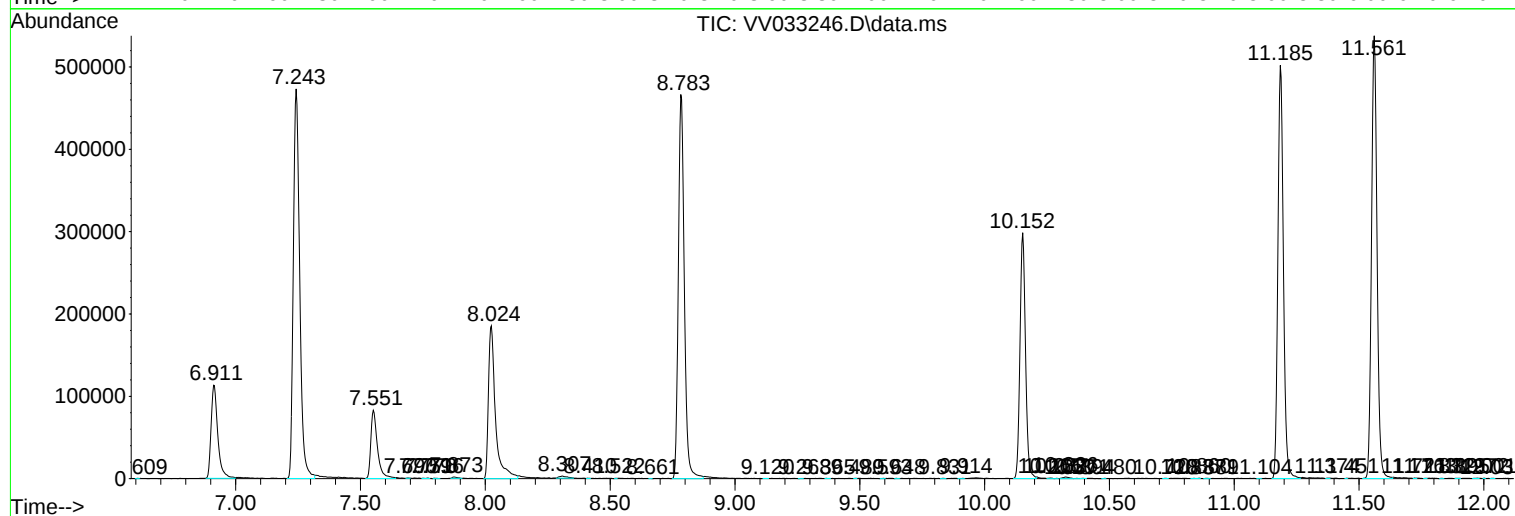
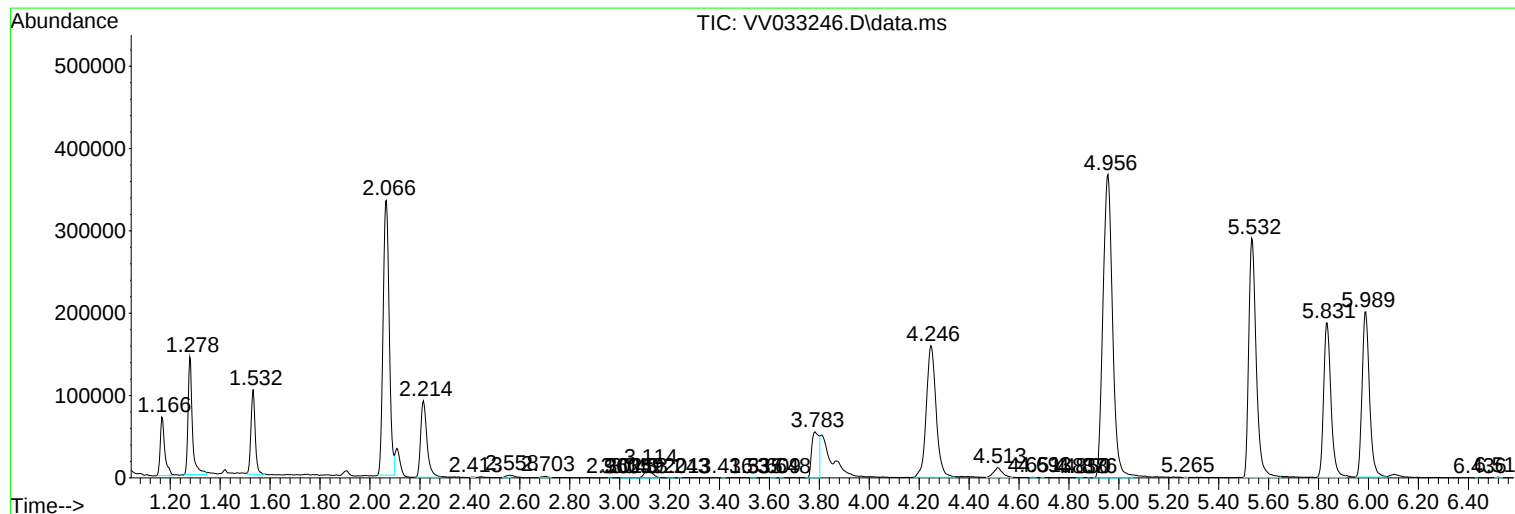
Sum of corrected areas: 8535552

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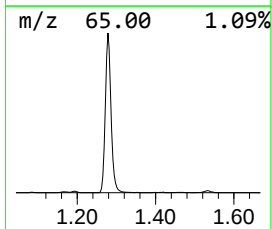
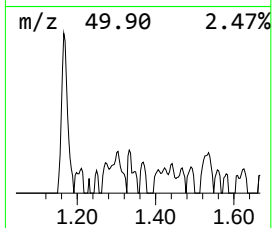
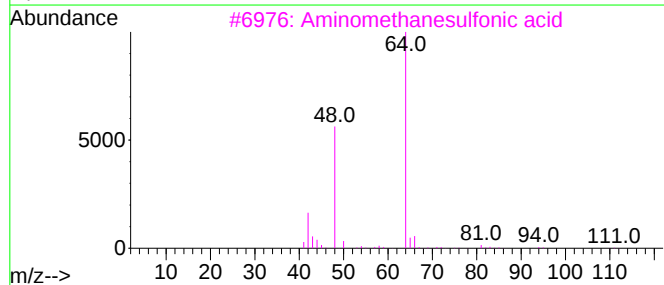
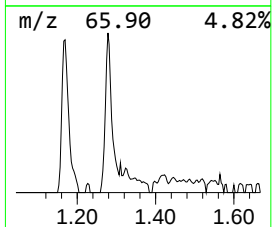
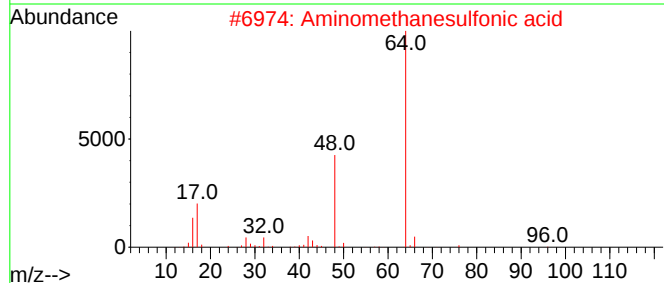
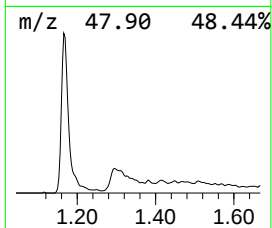
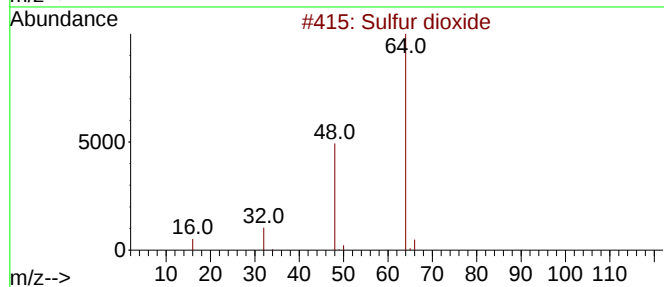
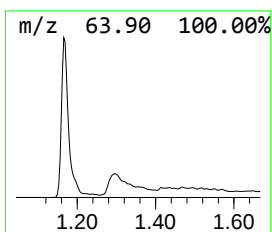
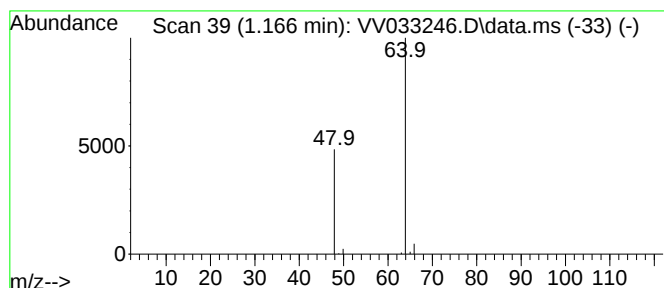
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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	7.44 ug/L	90080	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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Sulfur dioxide	64	O2S	007446-09-5	5



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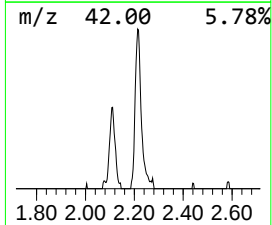
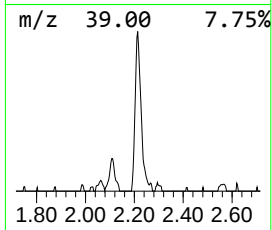
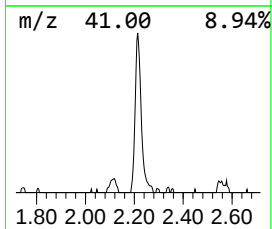
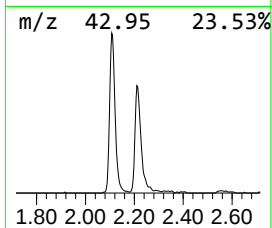
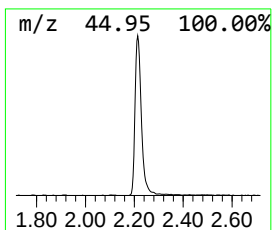
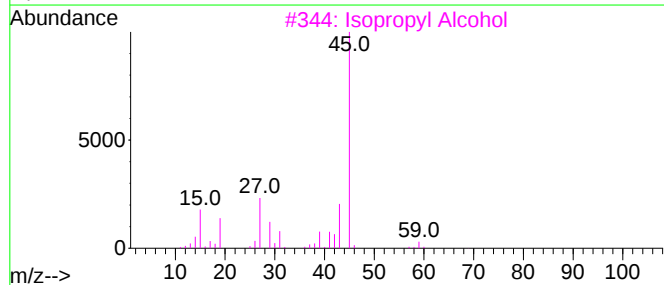
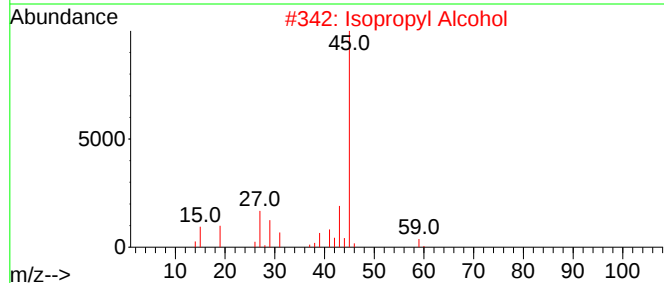
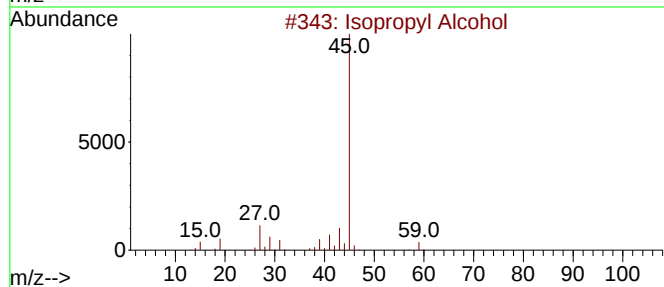
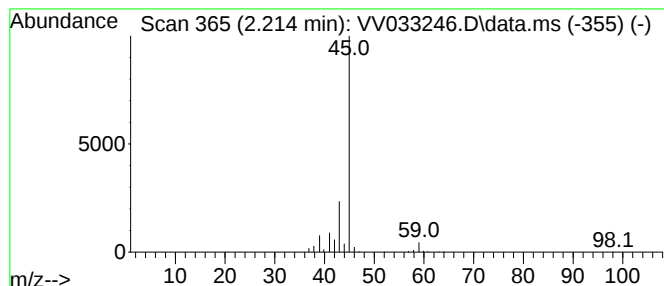
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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	13.46 ug/L	162931	1,4-Difluorobenzene	5.532

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol			60	C3H8O	000067-63-0	78
2	Isopropyl Alcohol			60	C3H8O	000067-63-0	78
3	Isopropyl Alcohol			60	C3H8O	000067-63-0	72
4	Isopropyl Alcohol			60	C3H8O	000067-63-0	64
5	Isopropyl Alcohol			60	C3H8O	000067-63-0	56



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Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.166	7.4	ug/L	90080	1	5.532	605120	50.0
Isopropyl Alcohol	2.214	13.5	ug/L	162931	1	5.532	605120	50.0