

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121123\
 Data File : VV033245.D
 Acq On : 12 Dec 2023 04:06
 Operator : SY/MD
 Sample : 05751-12
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 YCHF6

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: VV033245.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	62	rBV	78279	102563	10.11%	1.162%
2	1.278	67	74	97	rBV	149825	182146	17.96%	2.064%
3	1.532	146	153	167	rVB	101773	119062	11.74%	1.349%
4	2.063	307	318	327	rBV3	327856	553088	54.54%	6.269%
5	2.214	356	365	379	rBV	60192	103722	10.23%	1.176%
6	2.439	432	435	440	rBV5	547	620	0.06%	0.007%
7	2.481	445	448	452	rVB2	720	505	0.05%	0.006%
8	2.500	452	454	456	rBV	505	285	0.03%	0.003%
9	2.564	466	474	486	rVV5	2665	5691	0.56%	0.065%
10	2.625	490	493	500	rBV3	345	430	0.04%	0.005%
11	2.680	508	510	511	rBV	384	194	0.02%	0.002%
12	2.741	525	529	531	rVB	430	211	0.02%	0.002%
13	2.780	537	541	545	rBV	304	273	0.03%	0.003%
14	2.931	585	588	590	rBV2	379	291	0.03%	0.003%
15	2.944	590	592	594	rVV2	439	197	0.02%	0.002%
16	3.034	617	620	623	rBB	430	290	0.03%	0.003%
17	3.114	633	645	660	rVV	9695	21065	2.08%	0.239%
18	3.198	668	671	676	rBV	294	259	0.03%	0.003%
19	3.375	723	726	729	rBV2	327	263	0.03%	0.003%
20	3.407	734	736	740	rVB	326	192	0.02%	0.002%
21	3.500	762	765	768	rBB	270	209	0.02%	0.002%
22	3.783	842	853	859	rBV2	56436	119088	11.74%	1.350%
23	4.246	972	997	1023	rBV	167298	474751	46.81%	5.381%
24	4.616	1110	1112	1114	rVB2	484	201	0.02%	0.002%
25	4.632	1114	1117	1120	rVV2	484	358	0.04%	0.004%
26	4.670	1126	1129	1133	rVB2	330	207	0.02%	0.002%
27	4.690	1133	1135	1140	rVB3	270	214	0.02%	0.002%
28	4.712	1140	1142	1147	rBV3	466	313	0.03%	0.004%
29	4.731	1147	1148	1155	rBV2	319	283	0.03%	0.003%
30	4.760	1155	1157	1160	rBV2	327	220	0.02%	0.002%
31	4.831	1176	1179	1182	rVV3	462	350	0.03%	0.004%
32	4.953	1201	1217	1244	rBV2	382869	1014114	100.00%	11.494%
33	5.169	1282	1284	1288	rBV	608	467	0.05%	0.005%
34	5.362	1342	1344	1348	rVB2	481	241	0.02%	0.003%
35	5.532	1386	1397	1426	rBV	286310	599561	59.12%	6.795%
36	5.831	1478	1490	1521	rBV	293651	604195	59.58%	6.848%

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

37	5.989	1527	1539	1562	rBV	209232	424481	41.86%	4.811%
38	6.194	1602	1603	1607	rVB2	594	304	0.03%	0.003%
39	6.262	1621	1624	1628	rVB2	318	223	0.02%	0.003%
40	6.609	1730	1732	1736	rVB2	558	358	0.04%	0.004%
41	6.632	1736	1739	1742	rBV2	455	380	0.04%	0.004%
42	6.712	1759	1764	1766	rBV	201	213	0.02%	0.002%
43	6.783	1782	1786	1788	rBV	277	203	0.02%	0.002%
44	6.841	1802	1804	1809	rBV	336	224	0.02%	0.003%
45	6.911	1815	1826	1848	rBV	118322	220223	21.72%	2.496%
46	7.243	1917	1929	1955	rBV	487269	852087	84.02%	9.657%
47	7.551	2015	2025	2049	rBV	87331	154742	15.26%	1.754%
48	7.815	2104	2107	2108	rBV	433	210	0.02%	0.002%
49	8.024	2162	2172	2190	rBV	194720	353277	34.84%	4.004%
50	8.432	2295	2299	2305	rBV3	449	478	0.05%	0.005%
51	8.564	2333	2340	2341	rBV3	261	207	0.02%	0.002%
52	8.670	2371	2373	2380	rVB	504	342	0.03%	0.004%
53	8.783	2397	2408	2435	rBV	465387	776868	76.61%	8.805%
54	9.034	2482	2486	2489	rVB3	654	618	0.06%	0.007%
55	9.050	2489	2491	2495	rBV	492	381	0.04%	0.004%
56	9.098	2505	2506	2510	rBV3	370	230	0.02%	0.003%
57	9.169	2521	2528	2529	rBV2	395	305	0.03%	0.003%
58	9.236	2545	2549	2551	rBV2	346	304	0.03%	0.003%
59	9.423	2602	2607	2609	rBV2	339	229	0.02%	0.003%
60	9.500	2629	2631	2635	rBV2	428	382	0.04%	0.004%
61	9.606	2662	2664	2671	rVB2	450	341	0.03%	0.004%
62	9.638	2671	2674	2677	rBV	218	200	0.02%	0.002%
63	9.947	2768	2770	2771	rBV	453	208	0.02%	0.002%
64	10.152	2823	2834	2852	rVV	306010	474824	46.82%	5.382%
65	10.329	2879	2889	2896	rBV5	2335	3627	0.36%	0.041%
66	10.410	2912	2914	2920	rVB2	254	217	0.02%	0.002%
67	10.442	2920	2924	2925	rBV	364	281	0.03%	0.003%
68	10.554	2955	2959	2962	rBV2	388	407	0.04%	0.005%
69	10.818	3038	3041	3045	rBV	237	207	0.02%	0.002%
70	10.982	3087	3092	3095	rBB	433	390	0.04%	0.004%
71	11.072	3115	3120	3125	rBV2	188	269	0.03%	0.003%
72	11.185	3144	3155	3177	rBV	502708	780372	76.95%	8.845%
73	11.377	3214	3215	3222	rVB3	378	297	0.03%	0.003%
74	11.480	3244	3247	3251	rBV3	430	420	0.04%	0.005%
75	11.561	3260	3272	3300	rVV	547917	859650	84.77%	9.743%
76	11.847	3356	3361	3365	rBV2	391	417	0.04%	0.005%

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77	11.918	3378	3383	3385	rBV2	285	310	0.03%	0.004%
78	11.979	3397	3402	3405	rBV2	369	394	0.04%	0.004%
79	12.043	3420	3422	3424	rBV2	375	200	0.02%	0.002%
80	12.101	3437	3440	3442	rBV	383	199	0.02%	0.002%
81	12.197	3466	3470	3476	rVB3	639	662	0.07%	0.008%
82	12.230	3476	3480	3484	rBV2	281	337	0.03%	0.004%
83	12.352	3513	3518	3521	rBV2	242	271	0.03%	0.003%
84	12.419	3538	3539	3544	rBV	269	219	0.02%	0.002%
85	12.657	3609	3613	3615	rBV	427	405	0.04%	0.005%
86	12.712	3626	3630	3635	rBV2	223	275	0.03%	0.003%
87	12.779	3649	3651	3654	rBV2	311	234	0.02%	0.003%
88	12.892	3683	3686	3687	rBV	408	248	0.02%	0.003%
89	12.956	3703	3706	3710	rBV2	217	193	0.02%	0.002%
90	13.091	3743	3748	3750	rBV2	336	300	0.03%	0.003%
91	13.448	3856	3859	3861	rBV2	456	302	0.03%	0.003%
92	13.606	3904	3908	3913	rBV2	387	388	0.04%	0.004%
93	13.625	3913	3914	3919	rBV2	404	257	0.03%	0.003%
94	14.053	4044	4047	4052	rBV3	645	518	0.05%	0.006%
95	14.127	4069	4070	4074	rVB	394	224	0.02%	0.003%
96	14.156	4074	4079	4080	rBV2	380	350	0.03%	0.004%
97	14.348	4137	4139	4140	rBV	624	232	0.02%	0.003%
98	14.413	4154	4159	4160	rBV2	710	586	0.06%	0.007%
99	14.548	4198	4201	4203	rBV2	493	326	0.03%	0.004%
100	14.635	4226	4228	4229	rBV2	578	191	0.02%	0.002%

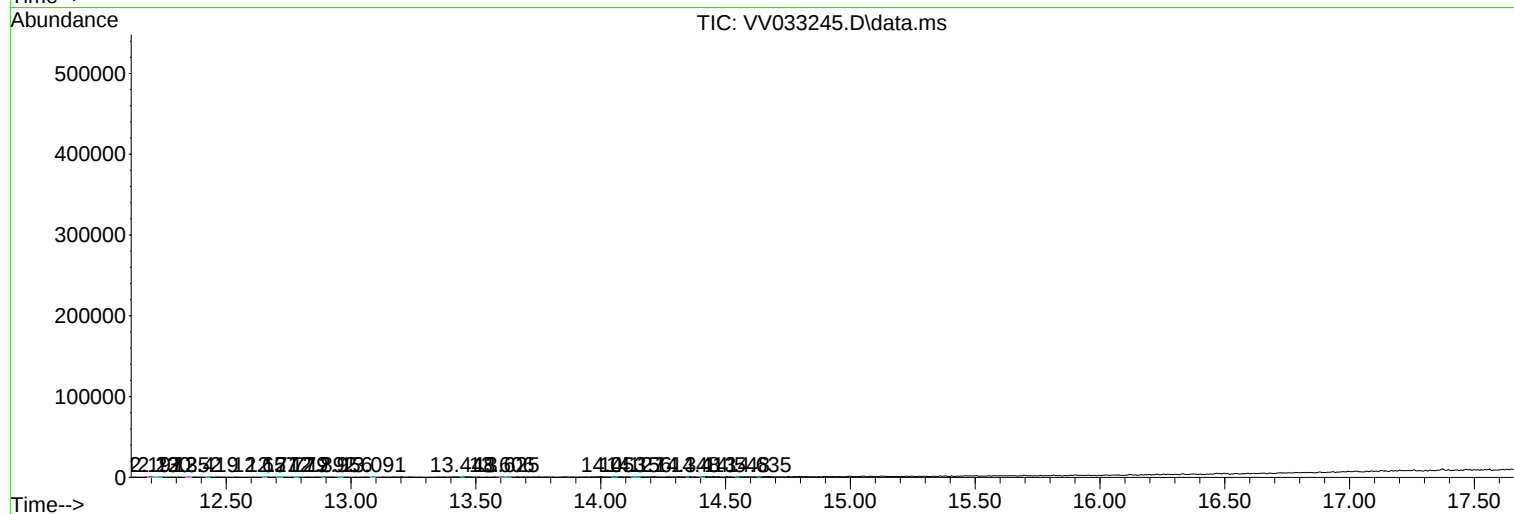
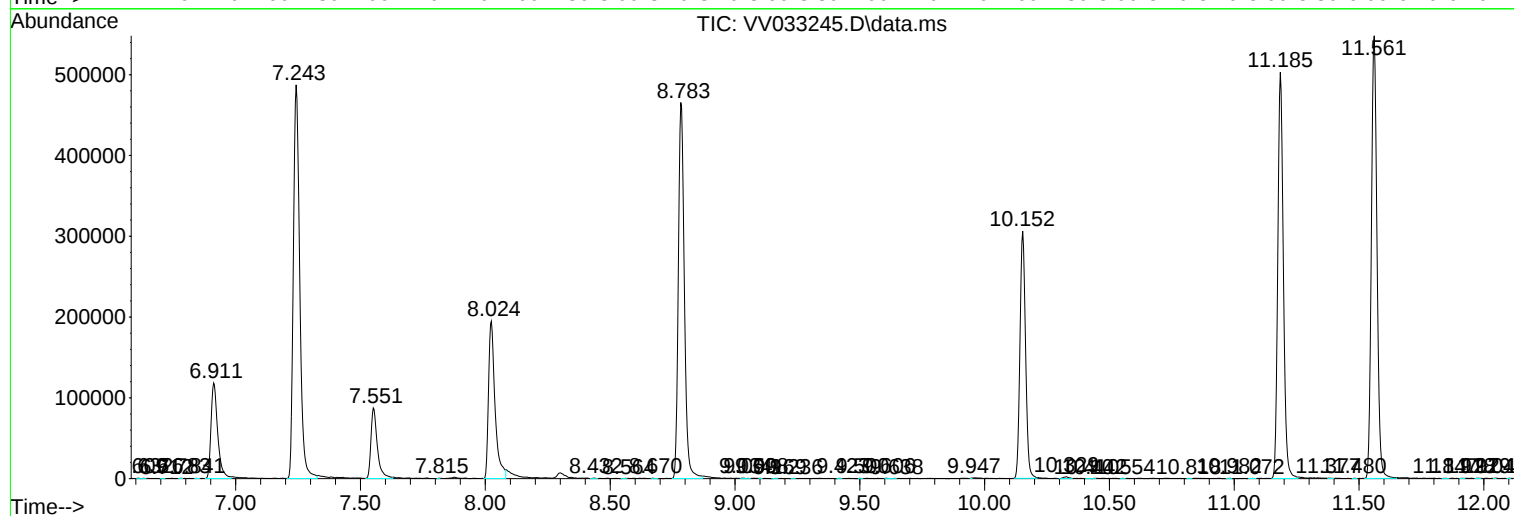
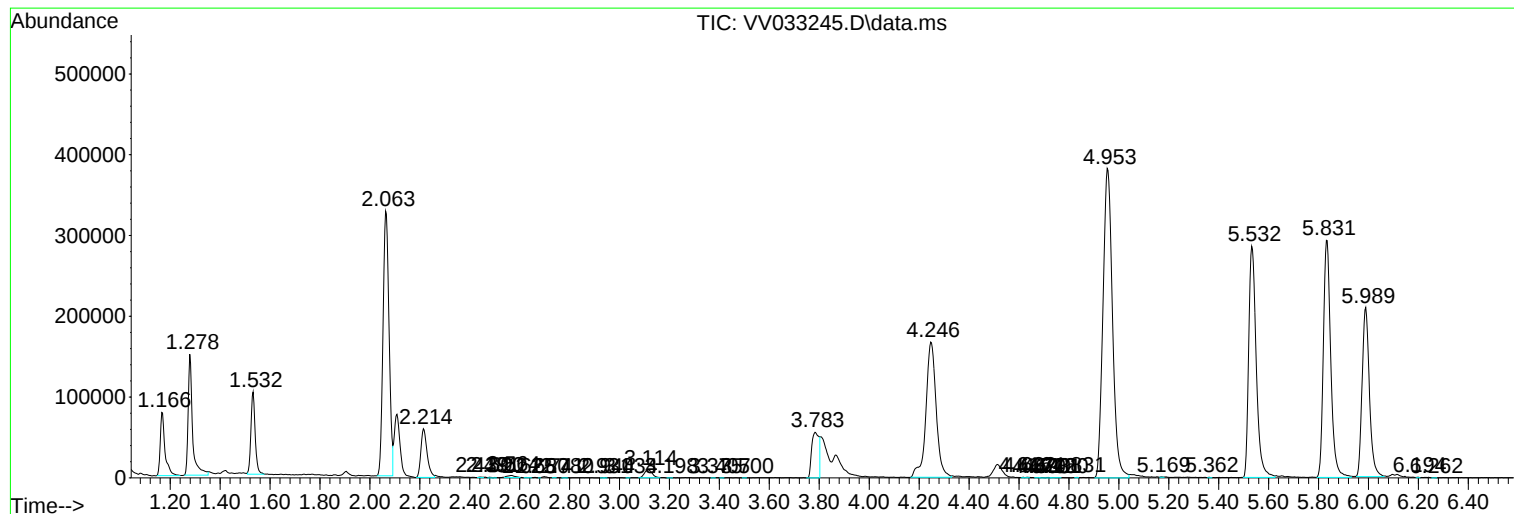
Sum of corrected areas: 8823136

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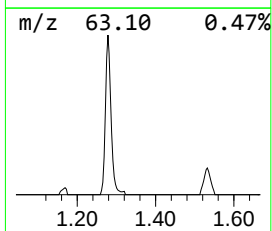
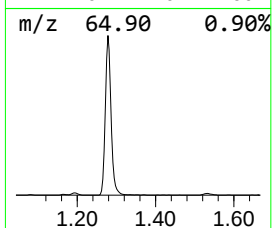
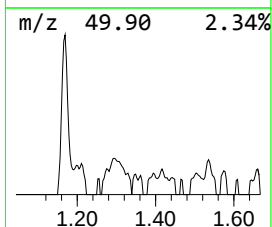
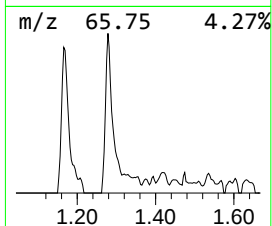
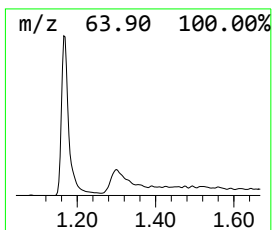
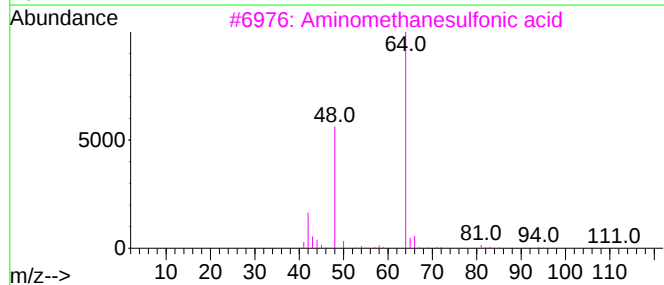
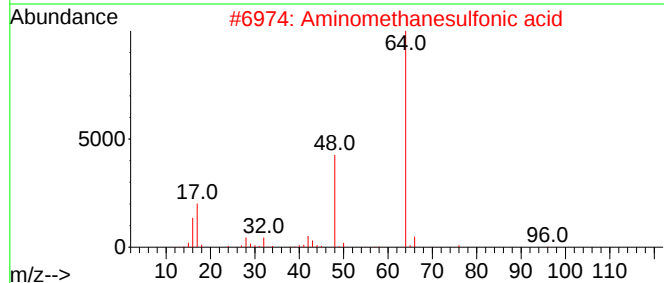
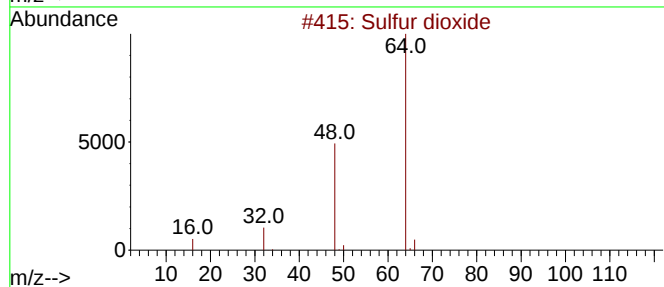
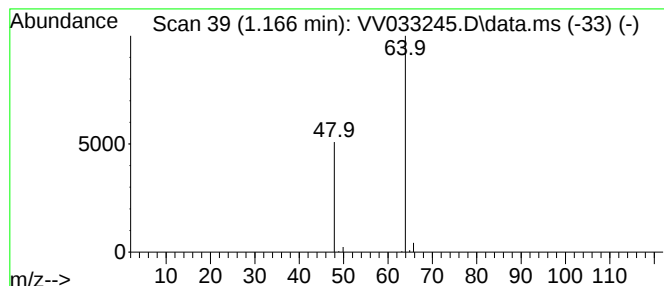
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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	8.55 ug/L	102563	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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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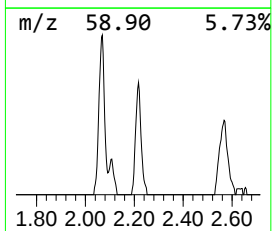
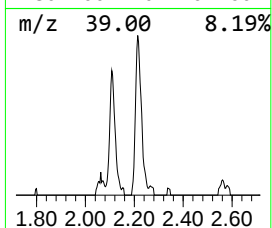
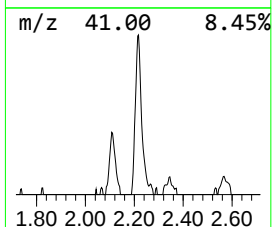
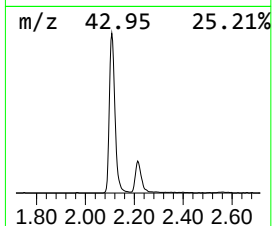
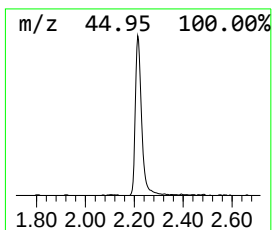
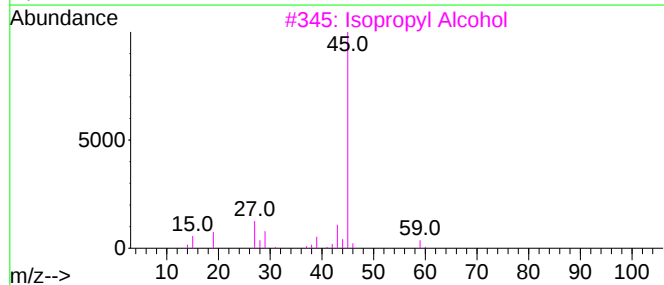
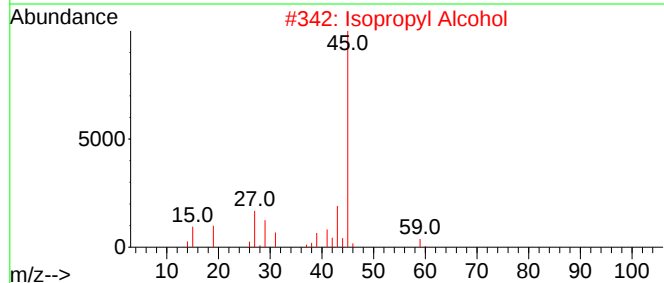
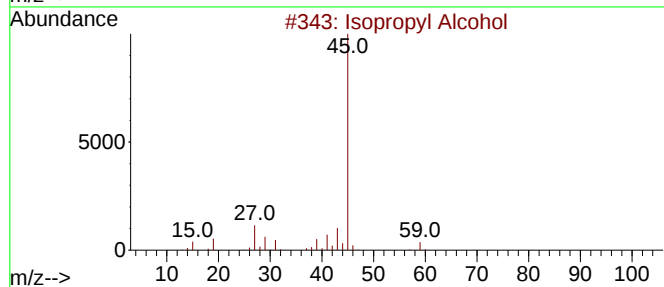
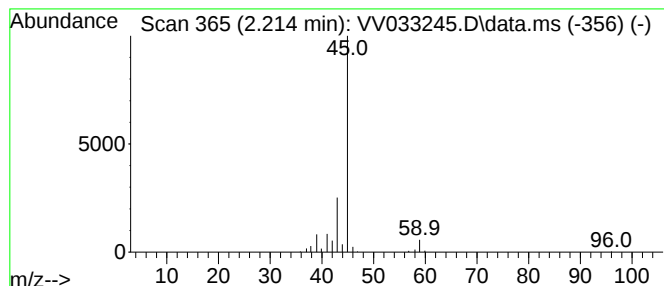
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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	8.65 ug/L	103722	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	64
4			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	56
5			Isopropyl Alcohol	60	C3H8O	000067-63-0	56



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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	8.6	ug/L	102563	1	5.532	599561	50.0
Isopropyl Alcohol	2.214	8.7	ug/L	103722	1	5.532	599561	50.0