

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121123\
 Data File : VV033242.D
 Acq On : 12 Dec 2023 02:57
 Operator : SY/MD
 Sample : 05751-09
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 YCHB3

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: VV033242.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	34	39	58	rVB	102508	131088	13.61%	1.605%
2	1.278	67	74	101	rBV	234122	354018	36.75%	4.335%
3	1.532	148	153	170	rVB	101124	121241	12.59%	1.485%
4	2.060	309	317	327	rBV	208223	294497	30.57%	3.606%
5	2.211	354	364	392	rBV	226328	391097	40.60%	4.789%
6	2.696	512	515	519	rBV4	832	864	0.09%	0.011%
7	2.790	542	544	547	rVB2	570	279	0.03%	0.003%
8	2.880	570	572	575	rBV	231	161	0.02%	0.002%
9	2.928	584	587	588	rBV	509	234	0.02%	0.003%
10	3.185	662	667	669	rBV	463	427	0.04%	0.005%
11	3.201	669	672	677	rVB	451	323	0.03%	0.004%
12	3.272	690	694	696	rBV2	287	218	0.02%	0.003%
13	3.317	704	708	710	rBV	275	236	0.02%	0.003%
14	3.349	716	718	723	rBV2	191	174	0.02%	0.002%
15	3.433	740	744	747	rBB2	250	172	0.02%	0.002%
16	3.513	764	769	774	rBV2	188	255	0.03%	0.003%
17	3.558	777	783	786	rBV2	265	312	0.03%	0.004%
18	3.577	786	789	793	rVB	235	159	0.02%	0.002%
19	3.658	811	814	817	rVB2	317	222	0.02%	0.003%
20	3.693	822	825	828	rBV2	189	194	0.02%	0.002%
21	3.732	835	837	841	rBV2	250	203	0.02%	0.002%
22	3.780	844	852	870	rBV2	50813	130310	13.53%	1.596%
23	4.246	982	997	1034	rVB	158929	412610	42.83%	5.052%
24	4.558	1092	1094	1095	rBV	413	202	0.02%	0.002%
25	4.632	1115	1117	1120	rBV	400	310	0.03%	0.004%
26	4.738	1147	1150	1155	rVB	326	208	0.02%	0.003%
27	4.883	1191	1195	1198	rBV	169	131	0.01%	0.002%
28	4.957	1201	1218	1249	rBV2	361403	963314	100.00%	11.796%
29	5.198	1290	1293	1300	rBV4	702	715	0.07%	0.009%
30	5.423	1361	1363	1366	rBV2	316	192	0.02%	0.002%
31	5.532	1386	1397	1429	rBV	286785	592912	61.55%	7.260%
32	5.831	1479	1490	1505	rBV7	5272	12179	1.26%	0.149%
33	5.989	1526	1539	1558	rBV	196082	406078	42.15%	4.972%
34	6.143	1584	1587	1589	rBV2	897	599	0.06%	0.007%
35	6.368	1654	1657	1661	rVB3	390	316	0.03%	0.004%
36	6.410	1667	1670	1673	rBV	313	220	0.02%	0.003%

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 Title : VOC Analysis

37	6.510	1699	1701	1704	rBV2	453	275	0.03%	0.003%
38	6.555	1713	1715	1721	rVB2	279	171	0.02%	0.002%
39	6.613	1729	1733	1737	rVB2	259	267	0.03%	0.003%
40	6.728	1765	1769	1771	rBV2	278	218	0.02%	0.003%
41	6.831	1796	1801	1804	rBV	142	141	0.01%	0.002%
42	6.854	1805	1808	1811	rBV2	266	146	0.02%	0.002%
43	6.912	1815	1826	1852	rBV2	108821	204768	21.26%	2.507%
44	7.243	1917	1929	1956	rBV	464706	814689	84.57%	9.976%
45	7.551	2016	2025	2047	rBV	79741	143378	14.88%	1.756%
46	7.731	2079	2081	2086	rVB2	257	146	0.02%	0.002%
47	7.789	2093	2099	2100	rBV2	294	176	0.02%	0.002%
48	7.873	2116	2125	2126	rBV4	2547	2386	0.25%	0.029%
49	8.024	2160	2172	2216	rBV	169618	344973	35.81%	4.224%
50	8.410	2289	2292	2296	rVB2	275	181	0.02%	0.002%
51	8.487	2314	2316	2321	rBV2	384	237	0.02%	0.003%
52	8.587	2344	2347	2349	rBV	357	303	0.03%	0.004%
53	8.622	2354	2358	2362	rVV2	306	269	0.03%	0.003%
54	8.641	2362	2364	2368	rVB2	394	236	0.02%	0.003%
55	8.719	2385	2388	2390	rBV	282	173	0.02%	0.002%
56	8.786	2398	2409	2432	rBV	463090	760252	78.92%	9.309%
57	9.002	2472	2476	2480	rBV2	545	467	0.05%	0.006%
58	9.085	2496	2502	2507	rBV3	700	783	0.08%	0.010%
59	9.159	2522	2525	2529	rVB2	382	290	0.03%	0.004%
60	9.178	2529	2531	2532	rBV2	290	153	0.02%	0.002%
61	9.230	2544	2547	2549	rBV2	266	182	0.02%	0.002%
62	9.365	2587	2589	2592	rBV2	258	153	0.02%	0.002%
63	9.474	2618	2623	2625	rBV	204	206	0.02%	0.003%
64	9.493	2625	2629	2633	rVB3	553	573	0.06%	0.007%
65	9.522	2634	2638	2641	rBV2	294	251	0.03%	0.003%
66	9.612	2662	2666	2668	rBV2	325	189	0.02%	0.002%
67	9.667	2681	2683	2687	rBV2	335	255	0.03%	0.003%
68	9.719	2698	2699	2702	rVV2	272	132	0.01%	0.002%
69	9.802	2722	2725	2728	rVB2	516	359	0.04%	0.004%
70	9.828	2728	2733	2734	rBV	409	336	0.03%	0.004%
71	9.960	2766	2774	2780	rBV5	2519	4091	0.42%	0.050%
72	10.153	2823	2834	2857	rBV	285795	448974	46.61%	5.498%
73	10.323	2880	2887	2896	rBV4	2206	3475	0.36%	0.043%
74	10.452	2924	2927	2929	rBV2	283	199	0.02%	0.002%
75	10.664	2991	2993	2997	rBV	446	412	0.04%	0.005%
76	10.789	3030	3032	3035	rBV	234	175	0.02%	0.002%

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 Title : VOC Analysis

77	10.834	3043	3046	3048	rBV2	405	295	0.03%	0.004%
78	10.972	3086	3089	3092	rVB2	260	185	0.02%	0.002%
79	11.043	3107	3111	3115	rBV2	304	236	0.02%	0.003%
80	11.185	3142	3155	3183	rBV	506439	779538	80.92%	9.546%
81	11.400	3218	3222	3228	rVB2	499	511	0.05%	0.006%
82	11.436	3228	3233	3236	rBV2	322	273	0.03%	0.003%
83	11.561	3259	3272	3291	rBV	533503	827461	85.90%	10.132%
84	11.735	3324	3326	3328	rBV	429	175	0.02%	0.002%
85	11.989	3402	3405	3408	rBV	154	143	0.01%	0.002%
86	12.037	3412	3420	3424	rBV4	749	978	0.10%	0.012%
87	12.191	3462	3468	3479	rVB3	935	1338	0.14%	0.016%
88	12.316	3505	3507	3509	rBV	316	180	0.02%	0.002%
89	12.423	3538	3540	3543	rVB	298	130	0.01%	0.002%
90	12.776	3647	3650	3651	rBV	292	165	0.02%	0.002%
91	12.844	3668	3671	3672	rBV	290	136	0.01%	0.002%
92	12.963	3703	3708	3710	rBV2	420	409	0.04%	0.005%
93	13.098	3747	3750	3755	rBV2	349	265	0.03%	0.003%
94	13.217	3782	3787	3788	rBV3	652	423	0.04%	0.005%
95	13.294	3808	3811	3813	rBV2	380	230	0.02%	0.003%
96	13.394	3839	3842	3843	rBV	340	231	0.02%	0.003%
97	13.641	3916	3919	3923	rBV	441	284	0.03%	0.003%
98	13.747	3948	3952	3955	rBV3	467	494	0.05%	0.006%
99	14.403	4152	4156	4157	rBV2	511	342	0.04%	0.004%
100	14.554	4199	4203	4205	rBV	463	397	0.04%	0.005%

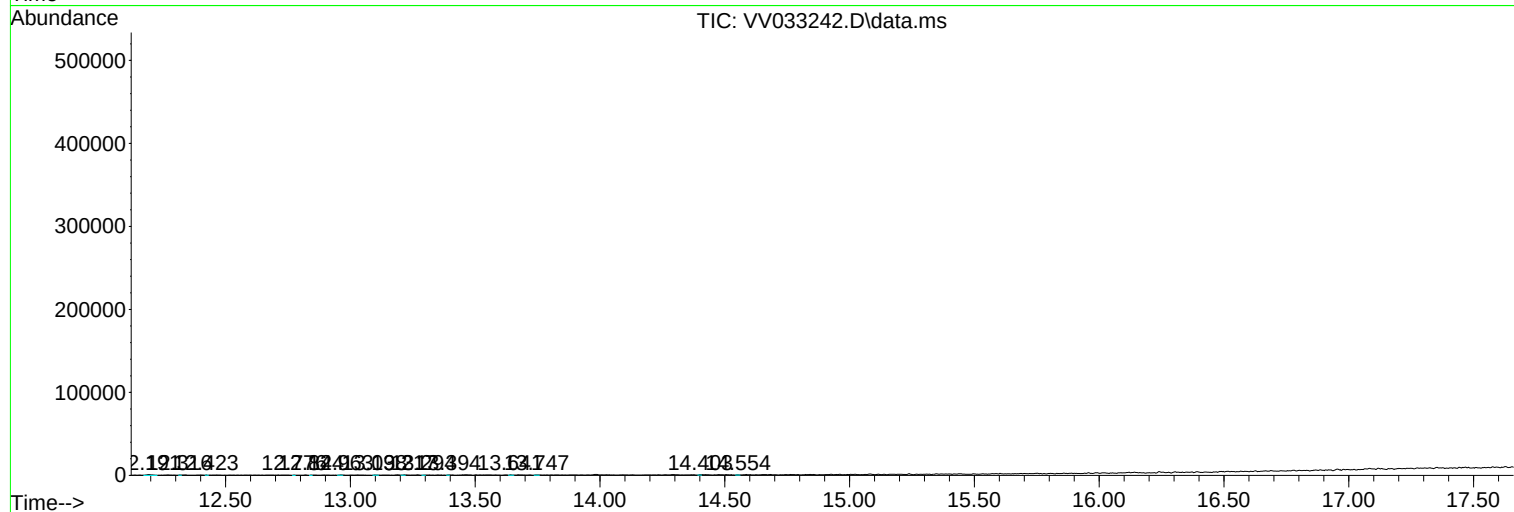
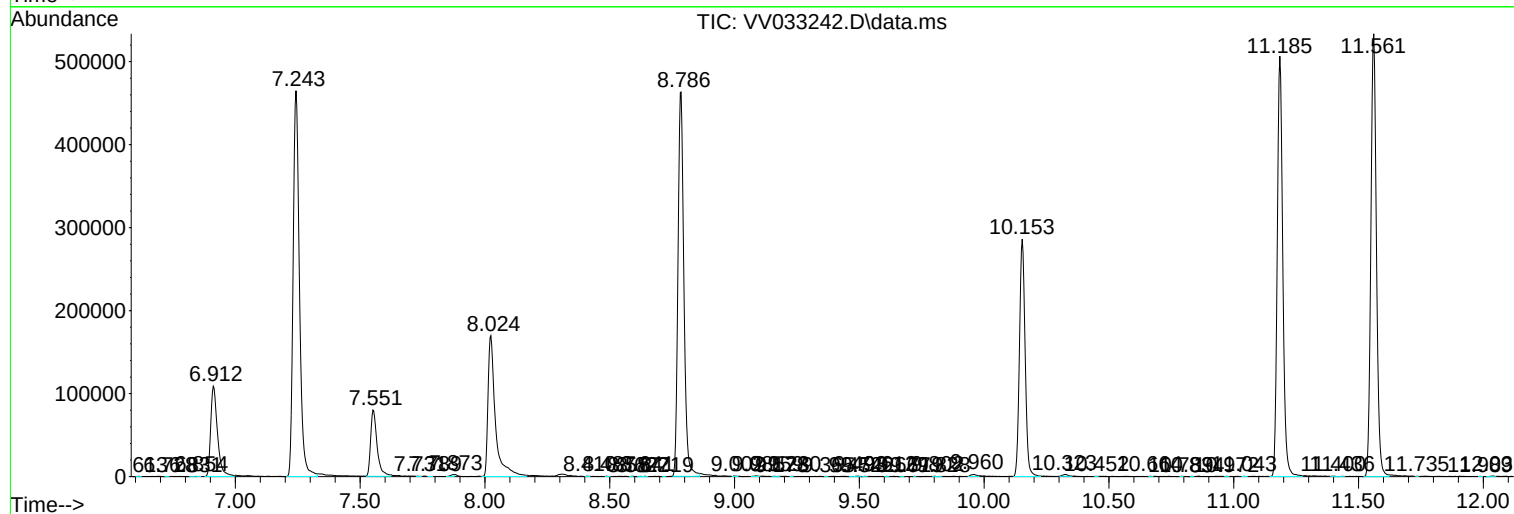
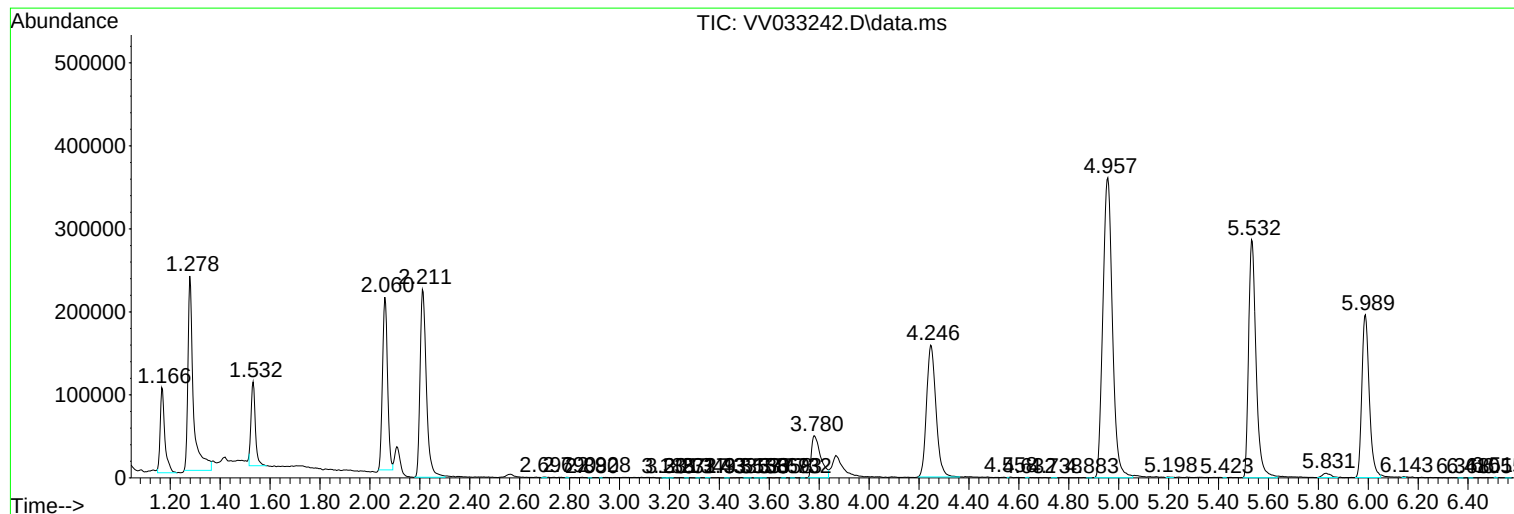
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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



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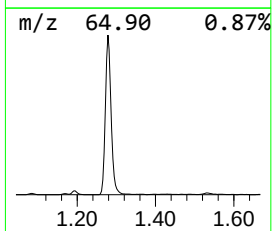
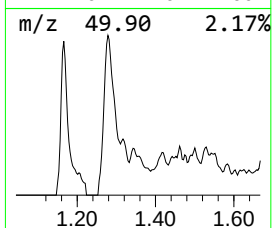
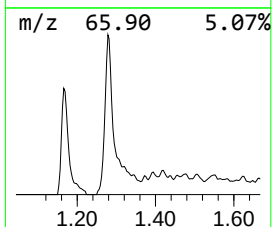
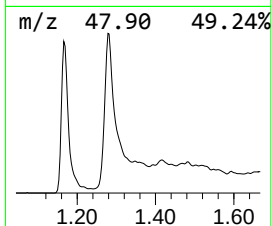
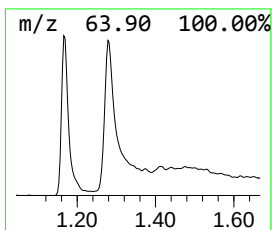
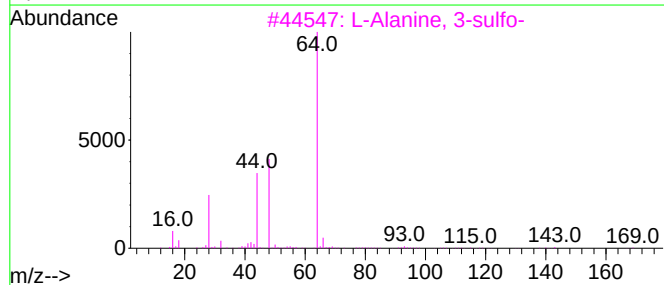
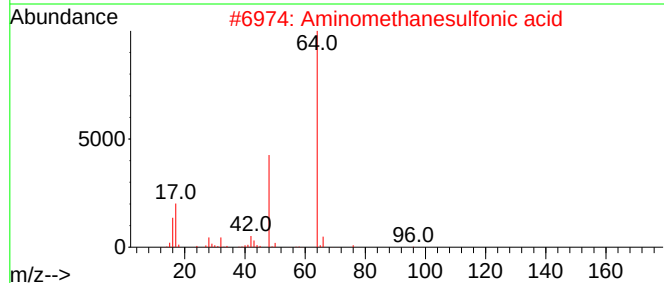
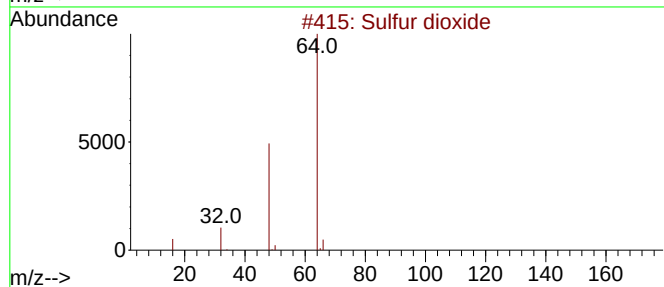
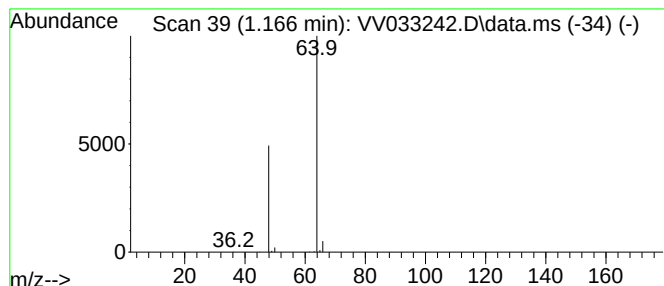
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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	11.05 ug/L	131088	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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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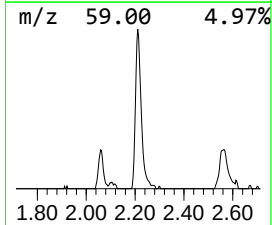
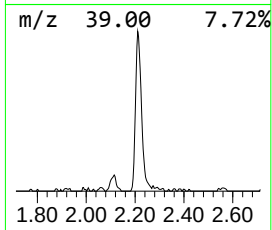
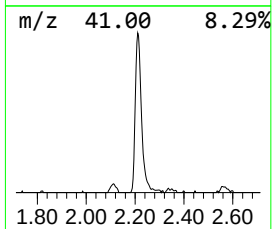
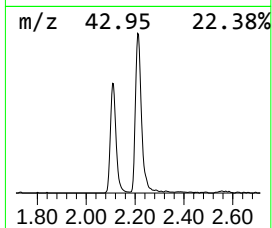
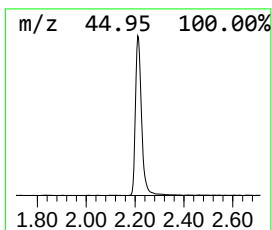
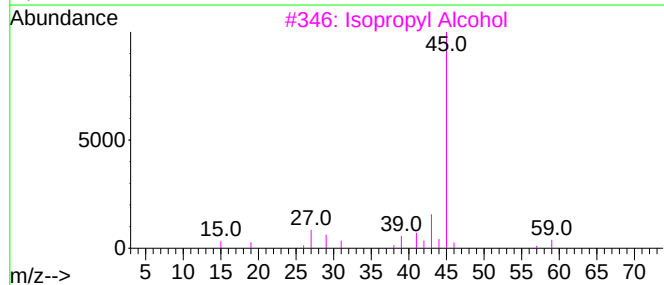
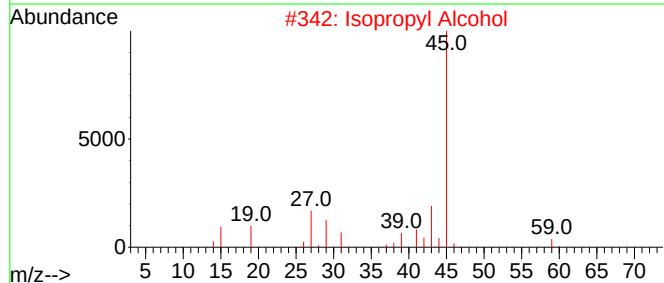
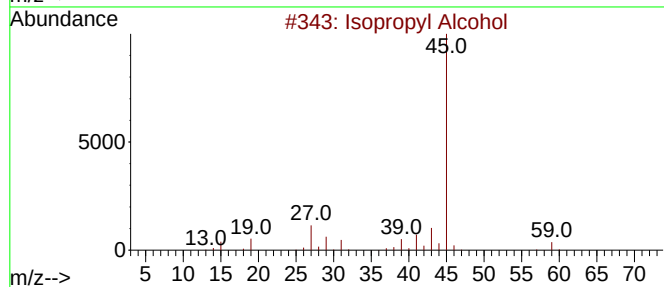
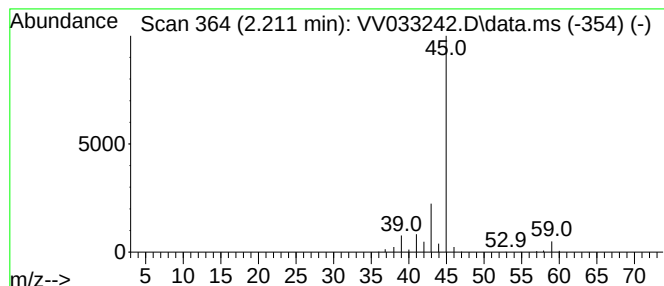
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.211	32.98 ug/L	391097	1,4-Difluorobenzene	5.532

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol			60	C3H8O	000067-63-0	86
2	Isopropyl Alcohol			60	C3H8O	000067-63-0	78
3	Isopropyl Alcohol			60	C3H8O	000067-63-0	64
4	Isopropyl Alcohol			60	C3H8O	000067-63-0	56
5	Isopropyl Alcohol			60	C3H8O	000067-63-0	9



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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	11.1	ug/L	131088	1	5.532	592912	50.0
Isopropyl Alcohol	2.211	33.0	ug/L	391097	1	5.532	592912	50.0