

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121123\
 Data File : VV033241.D
 Acq On : 12 Dec 2023 02:34
 Operator : SY/MD
 Sample : 05751-08
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 YCHB2

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: VV033241.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.169	35	40	58	rVB	88057	112699	13.33%	1.561%
2	1.278	66	74	98	rBV	238658	403524	47.74%	5.590%
3	2.059	310	317	326	rBV	172410	239803	28.37%	3.322%
4	2.214	355	365	388	rBV	160713	276247	32.68%	3.827%
5	2.500	450	454	456	rBV2	658	542	0.06%	0.008%
6	2.561	464	473	484	rBV2	3483	7089	0.84%	0.098%
7	2.899	574	578	580	rBV2	385	327	0.04%	0.005%
8	2.947	590	593	596	rBV3	296	267	0.03%	0.004%
9	3.297	699	702	707	rVB	192	181	0.02%	0.003%
10	3.323	707	710	712	rVB	370	215	0.03%	0.003%
11	3.342	712	716	719	rBV	324	280	0.03%	0.004%
12	3.436	740	745	750	rBB2	365	437	0.05%	0.006%
13	3.465	750	754	758	rBV2	281	318	0.04%	0.004%
14	3.584	788	791	793	rBV	253	186	0.02%	0.003%
15	3.606	796	798	802	rVB	363	188	0.02%	0.003%
16	3.657	808	814	817	rBV	288	309	0.04%	0.004%
17	3.712	828	831	837	rVB2	420	438	0.05%	0.006%
18	3.783	844	853	871	rBV	43988	111537	13.19%	1.545%
19	4.249	983	998	1026	rVB2	137767	353946	41.87%	4.903%
20	4.567	1094	1097	1099	rVB2	386	226	0.03%	0.003%
21	4.651	1120	1123	1128	rVB4	380	281	0.03%	0.004%
22	4.686	1131	1134	1136	rBV2	303	266	0.03%	0.004%
23	4.857	1182	1187	1192	rVB2	254	294	0.03%	0.004%
24	4.956	1201	1218	1247	rBV2	315494	845341	100.00%	11.710%
25	5.307	1325	1327	1332	rBV3	437	345	0.04%	0.005%
26	5.452	1368	1372	1375	rBV2	275	196	0.02%	0.003%
27	5.535	1382	1398	1426	rBV	272306	570959	67.54%	7.909%
28	5.828	1481	1489	1504	rVB7	6383	13954	1.65%	0.193%
29	5.989	1526	1539	1569	rBV2	171100	359723	42.55%	4.983%
30	6.217	1608	1610	1615	rVB3	383	260	0.03%	0.004%
31	6.246	1615	1619	1621	rBV2	295	277	0.03%	0.004%
32	6.371	1654	1658	1661	rVV	487	379	0.04%	0.005%
33	6.455	1680	1684	1686	rBV	416	244	0.03%	0.003%
34	6.468	1686	1688	1692	rVB2	431	313	0.04%	0.004%
35	6.497	1695	1697	1700	rVB3	494	244	0.03%	0.003%
36	6.680	1752	1754	1758	rBV	266	195	0.02%	0.003%

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 Title : VOC Analysis

37	6.789	1786	1788	1791	rBV2	218	179	0.02%	0.002%
38	6.911	1817	1826	1847	rBV	96056	178531	21.12%	2.473%
39	7.191	1909	1913	1917	rBV3	419	467	0.06%	0.006%
40	7.243	1918	1929	1956	rBV	400923	711019	84.11%	9.850%
41	7.554	2017	2026	2045	rBV	66668	120859	14.30%	1.674%
42	7.747	2083	2086	2088	rVB2	320	211	0.02%	0.003%
43	7.776	2092	2095	2098	rVB2	302	192	0.02%	0.003%
44	7.796	2098	2101	2103	rBV	459	275	0.03%	0.004%
45	7.876	2117	2126	2135	rBV4	2042	3686	0.44%	0.051%
46	8.024	2160	2172	2208	rBV	146776	303389	35.89%	4.203%
47	8.342	2269	2271	2274	rBV3	363	175	0.02%	0.002%
48	8.429	2295	2298	2299	rBV2	413	210	0.02%	0.003%
49	8.487	2314	2316	2320	rVB2	273	179	0.02%	0.002%
50	8.538	2328	2332	2335	rBV	479	450	0.05%	0.006%
51	8.577	2341	2344	2348	rBV2	252	180	0.02%	0.002%
52	8.786	2397	2409	2433	rBV	438040	729625	86.31%	10.107%
53	9.027	2479	2484	2486	rBV3	305	167	0.02%	0.002%
54	9.043	2486	2489	2493	rBV3	267	211	0.02%	0.003%
55	9.066	2493	2496	2498	rBV	341	216	0.03%	0.003%
56	9.223	2542	2545	2548	rVB2	372	214	0.03%	0.003%
57	9.242	2548	2551	2555	rBV	248	242	0.03%	0.003%
58	9.278	2558	2562	2565	rBV	379	300	0.04%	0.004%
59	9.297	2565	2568	2574	rVB2	261	243	0.03%	0.003%
60	9.361	2585	2588	2589	rBV	295	187	0.02%	0.003%
61	9.451	2613	2616	2618	rBV	201	168	0.02%	0.002%
62	9.545	2643	2645	2648	rBV2	345	276	0.03%	0.004%
63	9.654	2674	2679	2682	rVB2	212	236	0.03%	0.003%
64	9.882	2747	2750	2753	rBV2	312	262	0.03%	0.004%
65	9.905	2753	2757	2763	rVB2	410	385	0.05%	0.005%
66	9.953	2763	2772	2773	rBV4	1785	1626	0.19%	0.023%
67	10.024	2791	2794	2798	rBV2	513	482	0.06%	0.007%
68	10.152	2823	2834	2852	rBV	245671	383986	45.42%	5.319%
69	10.268	2866	2870	2872	rBV2	274	213	0.03%	0.003%
70	10.329	2878	2889	2895	rBV4	3050	4577	0.54%	0.063%
71	10.467	2930	2932	2935	rBV	284	233	0.03%	0.003%
72	10.789	3029	3032	3035	rVB	343	174	0.02%	0.002%
73	10.808	3035	3038	3041	rVB	386	192	0.02%	0.003%
74	10.972	3086	3089	3094	rBV3	488	360	0.04%	0.005%
75	11.033	3105	3108	3112	rVB2	211	178	0.02%	0.002%
76	11.082	3120	3123	3125	rBV2	289	185	0.02%	0.003%

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77	11.185	3144	3155	3177	rBV	475993	745185	88.15%	10.323%
78	11.561	3260	3272	3297	rBV	461524	717449	84.87%	9.939%
79	11.789	3341	3343	3346	rBV2	530	439	0.05%	0.006%
80	11.866	3363	3367	3370	rBV2	423	297	0.04%	0.004%
81	12.069	3428	3430	3437	rVB2	519	437	0.05%	0.006%
82	12.130	3446	3449	3454	rVB2	236	259	0.03%	0.004%
83	12.156	3454	3457	3461	rVB	351	310	0.04%	0.004%
84	12.201	3464	3471	3475	rBV3	811	1091	0.13%	0.015%
85	12.406	3529	3535	3538	rBV2	643	619	0.07%	0.009%
86	12.483	3556	3559	3562	rBV2	289	189	0.02%	0.003%
87	12.500	3562	3564	3569	rBV2	201	210	0.02%	0.003%
88	12.856	3672	3675	3677	rBV	227	169	0.02%	0.002%
89	12.937	3697	3700	3703	rBV2	441	289	0.03%	0.004%
90	12.995	3715	3718	3721	rVB2	450	295	0.03%	0.004%
91	13.098	3747	3750	3752	rBV	405	313	0.04%	0.004%
92	13.313	3814	3817	3822	rVB	447	294	0.03%	0.004%
93	13.464	3854	3864	3869	rBV2	921	1464	0.17%	0.020%
94	13.541	3881	3888	3890	rBV3	414	591	0.07%	0.008%
95	13.622	3910	3913	3916	rBV2	363	326	0.04%	0.005%
96	13.664	3923	3926	3928	rBV2	345	235	0.03%	0.003%
97	13.721	3940	3944	3946	rBV3	386	389	0.05%	0.005%
98	13.895	3994	3998	4000	rBV2	278	213	0.03%	0.003%
99	14.387	4150	4151	4154	rBV2	311	187	0.02%	0.003%
100	14.908	4309	4313	4314	rBV2	710	507	0.06%	0.007%

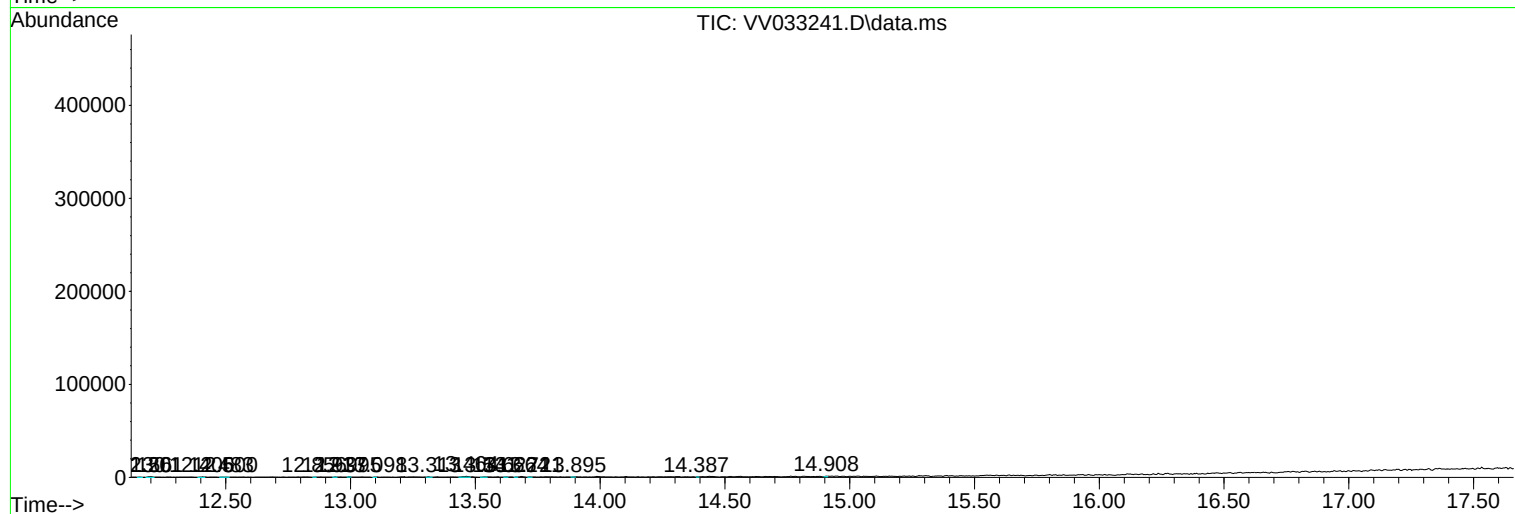
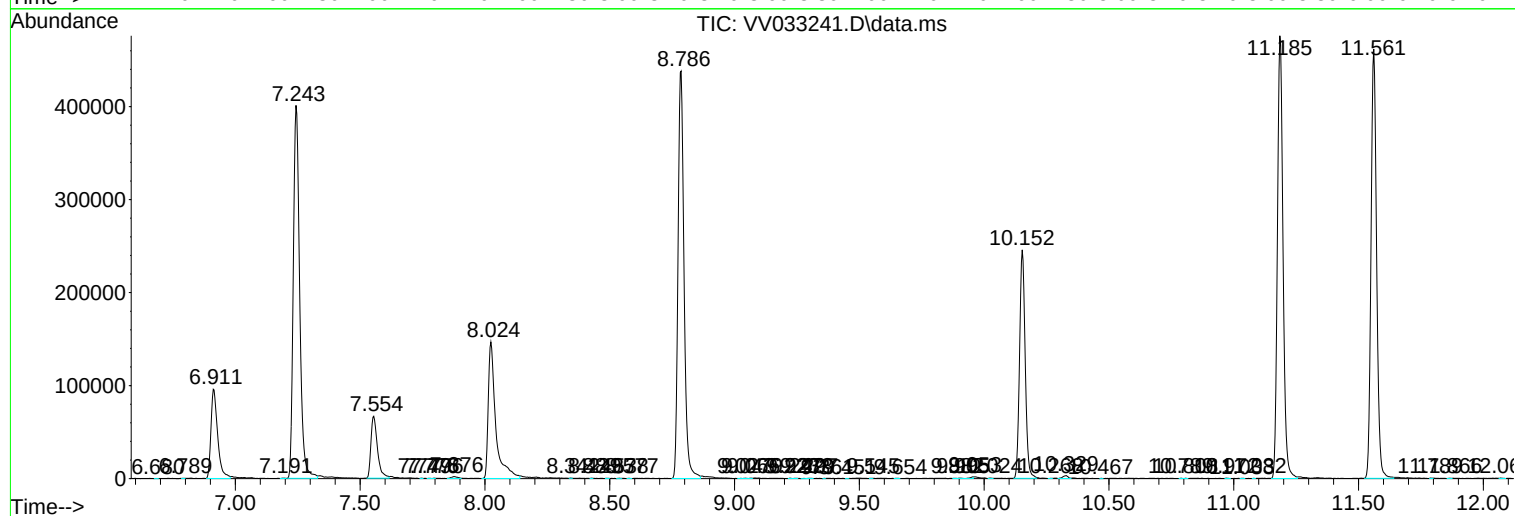
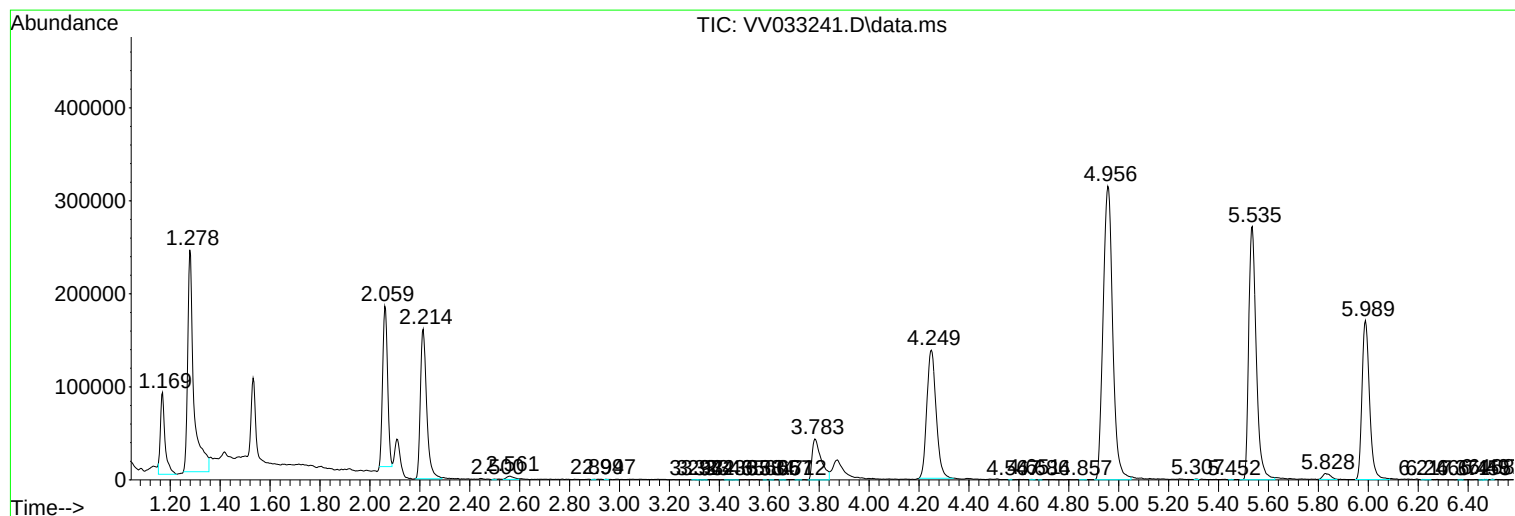
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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



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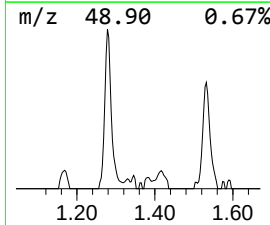
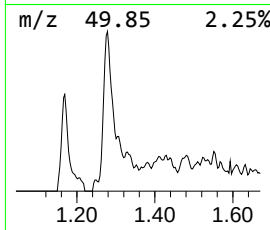
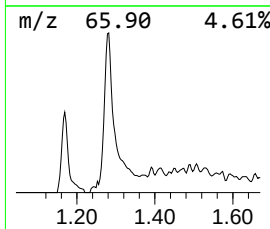
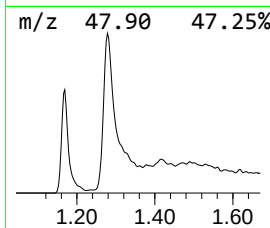
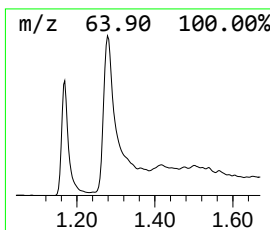
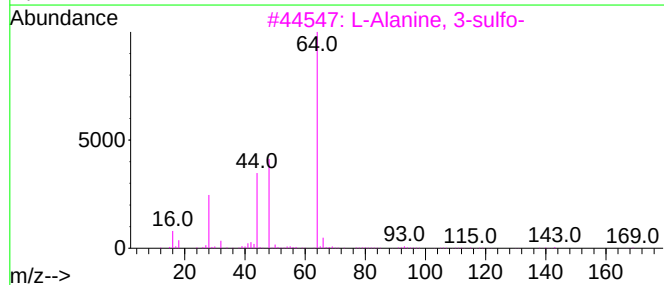
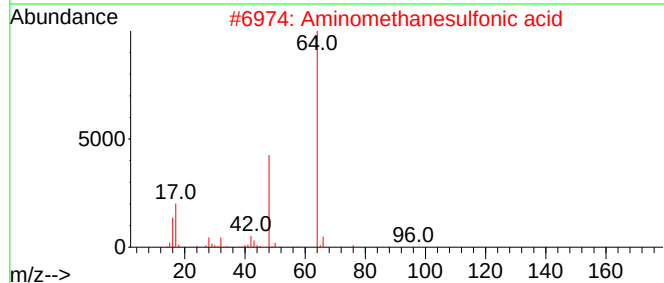
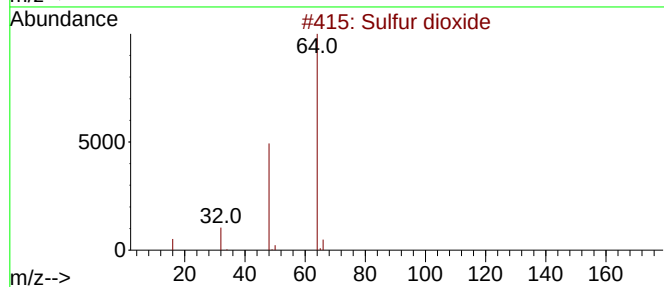
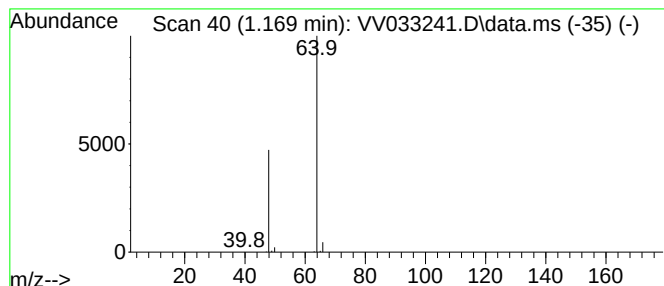
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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.
1.169	9.87 ug/L	112699	1,4-Difluorobenzene	5.535

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Sulfur dioxide	64	O2S	007446-09-5	4



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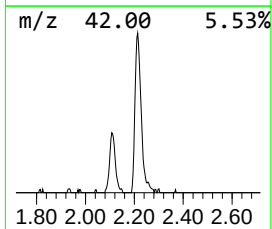
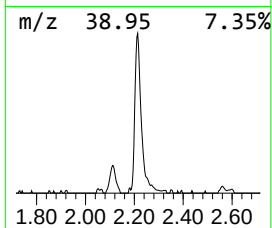
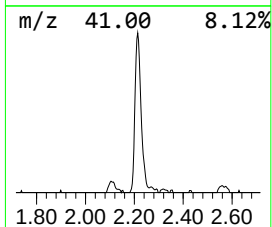
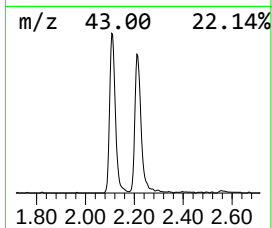
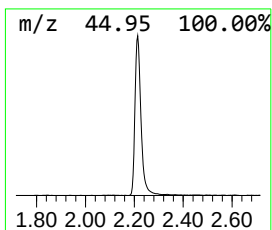
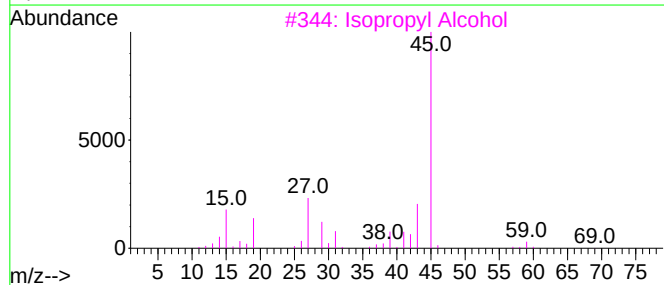
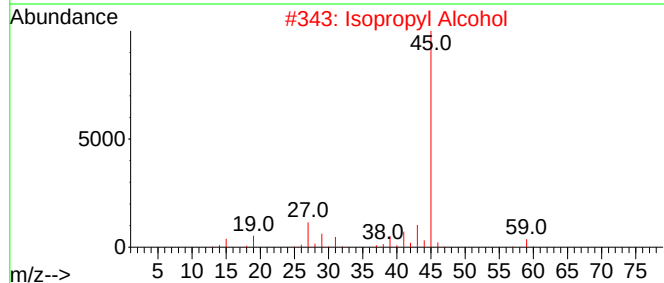
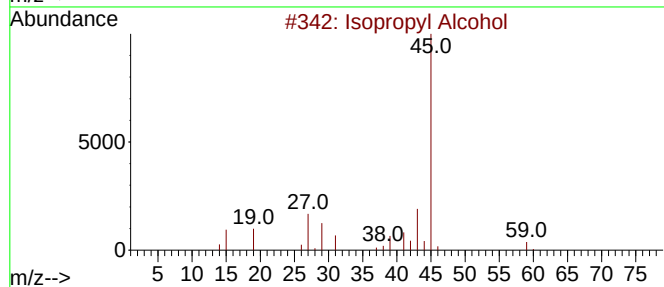
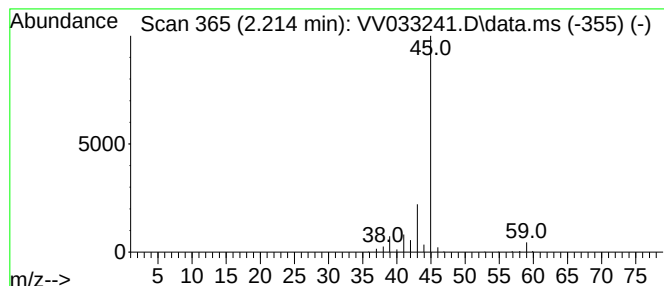
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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.
2.214	24.19 ug/L	276247	1,4-Difluorobenzene	5.535

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	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	1.169	9.9	ug/L	112699	1	5.535	570959	50.0
Isopropyl Alcohol	2.214	24.2	ug/L	276247	1	5.535	570959	50.0