

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121123\
 Data File : VV033244.D
 Acq On : 12 Dec 2023 03:43
 Operator : SY/MD
 Sample : 05751-11
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 YCHC6

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: VV033244.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	60	rBV	83603	103673	10.73%	1.220%
2	1.278	66	74	93	rBV2	148297	205823	21.30%	2.422%
3	1.532	146	153	164	rVB	96538	116506	12.06%	1.371%
4	2.060	308	317	325	rBV	211787	307588	31.83%	3.619%
5	2.105	325	331	351	rVB	201640	308218	31.90%	3.627%
6	2.211	354	364	392	rBV	296804	510654	52.85%	6.009%
7	2.982	597	604	605	rVV2	617	573	0.06%	0.007%
8	3.005	609	611	613	rVV	316	152	0.02%	0.002%
9	3.034	613	620	622	rVV3	313	353	0.04%	0.004%
10	3.060	626	628	633	rVB	377	241	0.02%	0.003%
11	3.117	633	646	661	rBV4	5991	12132	1.26%	0.143%
12	3.211	673	675	678	rBV	343	249	0.03%	0.003%
13	3.233	678	682	684	rVB	318	244	0.03%	0.003%
14	3.426	739	742	744	rBV2	266	153	0.02%	0.002%
15	3.462	750	753	757	rBV2	285	181	0.02%	0.002%
16	3.513	767	769	772	rBV	294	185	0.02%	0.002%
17	3.593	791	794	799	rVB2	156	162	0.02%	0.002%
18	3.783	843	853	881	rBV	52108	142653	14.76%	1.679%
19	4.134	959	962	965	rBV3	413	368	0.04%	0.004%
20	4.249	981	998	1027	rBV2	160159	416525	43.11%	4.901%
21	4.404	1043	1046	1054	rBV5	934	1206	0.12%	0.014%
22	4.580	1097	1101	1104	rBV2	363	304	0.03%	0.004%
23	4.690	1131	1135	1138	rBV3	203	172	0.02%	0.002%
24	4.783	1162	1164	1166	rVB	396	155	0.02%	0.002%
25	4.809	1166	1172	1174	rBV2	311	371	0.04%	0.004%
26	4.957	1200	1218	1239	rBV2	366000	966302	100.00%	11.370%
27	5.323	1329	1332	1339	rVB2	598	549	0.06%	0.006%
28	5.532	1386	1397	1423	rBV	286513	584980	60.54%	6.883%
29	5.838	1480	1492	1515	rVB7	20826	49589	5.13%	0.584%
30	5.989	1523	1539	1562	rBV	195448	410190	42.45%	4.827%
31	6.400	1664	1667	1669	rBV	288	207	0.02%	0.002%
32	6.452	1679	1683	1684	rBV	362	229	0.02%	0.003%
33	6.497	1694	1697	1698	rBV2	317	154	0.02%	0.002%
34	6.510	1698	1701	1702	rBV2	541	278	0.03%	0.003%
35	6.770	1779	1782	1786	rVB2	390	279	0.03%	0.003%
36	6.912	1816	1826	1853	rBV	115036	213513	22.10%	2.512%

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 Title : VOC Analysis

37	7.188	1908	1912	1917	rVB4	607	492	0.05%	0.006%
38	7.243	1917	1929	1952	rBV	471697	815557	84.40%	9.596%
39	7.551	2016	2025	2050	rBV	81178	148194	15.34%	1.744%
40	7.719	2075	2077	2080	rBV2	533	307	0.03%	0.004%
41	7.805	2102	2104	2108	rBV	204	169	0.02%	0.002%
42	7.844	2113	2116	2118	rVV2	432	280	0.03%	0.003%
43	7.876	2121	2126	2135	rVB3	1703	2445	0.25%	0.029%
44	7.973	2153	2156	2158	rVB	301	173	0.02%	0.002%
45	8.024	2163	2172	2209	rBV	183718	354695	36.71%	4.174%
46	8.400	2285	2289	2294	rBV3	384	453	0.05%	0.005%
47	8.506	2319	2322	2326	rBV3	481	336	0.03%	0.004%
48	8.683	2374	2377	2380	rVB2	470	282	0.03%	0.003%
49	8.715	2384	2387	2391	rBV	246	240	0.02%	0.003%
50	8.783	2397	2408	2442	rBV	460655	757334	78.37%	8.911%
51	9.034	2484	2486	2488	rBV	337	182	0.02%	0.002%
52	9.072	2496	2498	2500	rBV	515	263	0.03%	0.003%
53	9.320	2572	2575	2578	rBV2	343	319	0.03%	0.004%
54	9.439	2609	2612	2617	rVB2	235	168	0.02%	0.002%
55	9.468	2617	2621	2623	rBV	241	208	0.02%	0.002%
56	9.484	2623	2626	2629	rBV	457	268	0.03%	0.003%
57	9.529	2635	2640	2644	rBV2	324	213	0.02%	0.003%
58	9.593	2657	2660	2662	rBV	322	171	0.02%	0.002%
59	9.664	2678	2682	2685	rBV	343	267	0.03%	0.003%
60	9.699	2690	2693	2695	rBV2	294	161	0.02%	0.002%
61	9.728	2700	2702	2704	rBV	259	169	0.02%	0.002%
62	9.882	2748	2750	2755	rVB	373	264	0.03%	0.003%
63	9.911	2756	2759	2764	rBV3	558	515	0.05%	0.006%
64	9.940	2764	2768	2769	rBV3	392	274	0.03%	0.003%
65	10.043	2797	2800	2802	rBV	205	154	0.02%	0.002%
66	10.153	2823	2834	2861	rVB	288204	458150	47.41%	5.391%
67	10.323	2881	2887	2895	rBV5	1980	3063	0.32%	0.036%
68	10.403	2909	2912	2914	rBV	333	202	0.02%	0.002%
69	10.452	2925	2927	2932	rVB	288	201	0.02%	0.002%
70	10.490	2936	2939	2944	rBV2	343	380	0.04%	0.004%
71	10.712	3005	3008	3011	rBV2	414	314	0.03%	0.004%
72	10.976	3087	3090	3091	rBV	298	153	0.02%	0.002%
73	11.008	3098	3100	3102	rVB2	381	157	0.02%	0.002%
74	11.120	3134	3135	3140	rVB3	320	213	0.02%	0.003%
75	11.185	3144	3155	3181	rBV	498401	762327	78.89%	8.970%
76	11.561	3260	3272	3295	rBV	530084	826499	85.53%	9.725%

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 Title : VOC Analysis

77	11.751	3330	3331	3335	rBV2	390	245	0.03%	0.003%
78	11.825	3351	3354	3357	rBV3	477	389	0.04%	0.005%
79	12.082	3429	3434	3437	rBV2	337	353	0.04%	0.004%
80	12.297	3498	3501	3505	rVB2	462	380	0.04%	0.004%
81	12.339	3509	3514	3517	rVV2	234	274	0.03%	0.003%
82	12.358	3518	3520	3526	rVB2	338	263	0.03%	0.003%
83	12.403	3531	3534	3535	rBV	327	200	0.02%	0.002%
84	12.455	3547	3550	3552	rBV2	377	179	0.02%	0.002%
85	12.480	3554	3558	3563	rBV	343	280	0.03%	0.003%
86	12.612	3597	3599	3603	rVB	312	180	0.02%	0.002%
87	12.677	3615	3619	3623	rBV	320	349	0.04%	0.004%
88	12.760	3639	3645	3647	rBV	351	327	0.03%	0.004%
89	12.796	3654	3656	3661	rVB	289	157	0.02%	0.002%
90	12.815	3661	3662	3667	rBV2	488	385	0.04%	0.005%
91	12.892	3683	3686	3691	rVB2	349	324	0.03%	0.004%
92	12.921	3691	3695	3697	rBV	371	312	0.03%	0.004%
93	13.368	3831	3834	3837	rBV	354	341	0.04%	0.004%
94	13.451	3857	3860	3864	rBV2	415	366	0.04%	0.004%
95	13.532	3880	3885	3887	rBV3	492	449	0.05%	0.005%
96	13.686	3930	3933	3937	rBV3	571	405	0.04%	0.005%
97	13.718	3940	3943	3946	rBV2	545	359	0.04%	0.004%
98	13.734	3946	3948	3952	rBV2	298	196	0.02%	0.002%
99	14.159	4078	4080	4083	rVB2	547	226	0.02%	0.003%
100	14.181	4085	4087	4089	rBV3	370	223	0.02%	0.003%

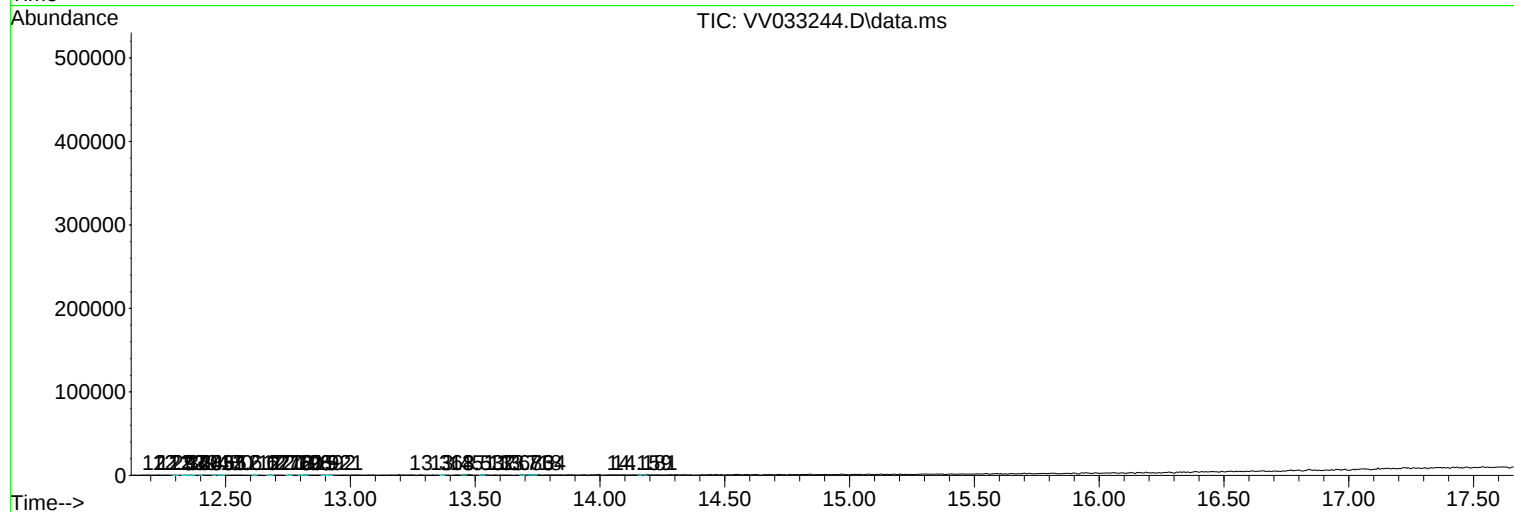
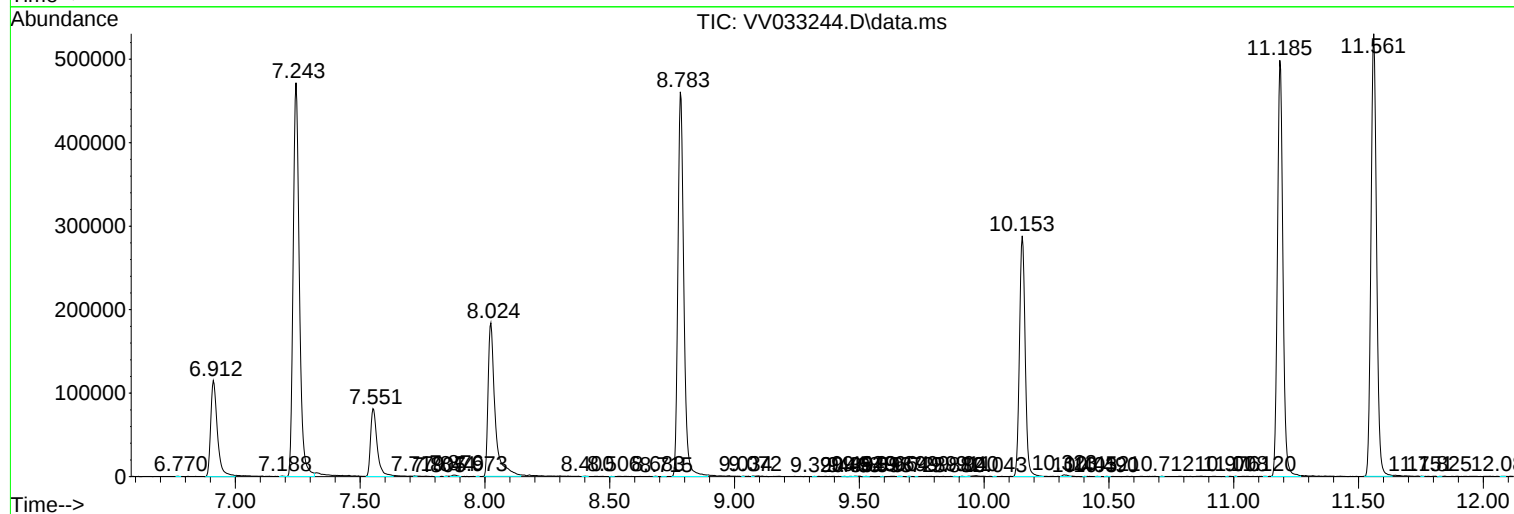
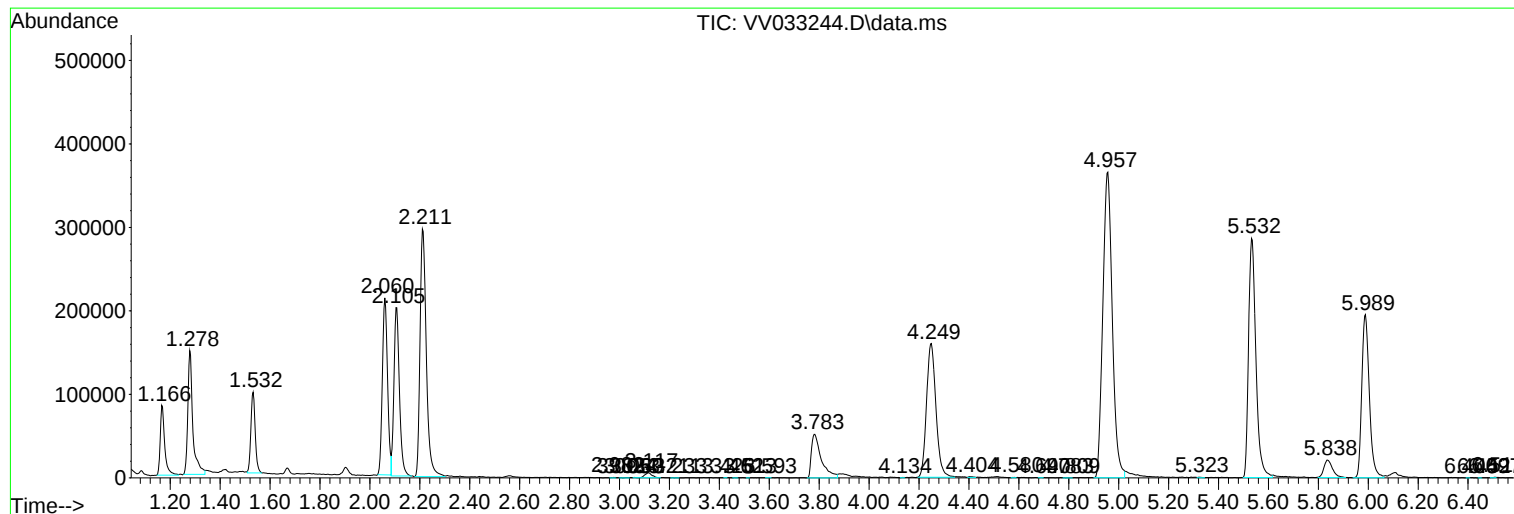
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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



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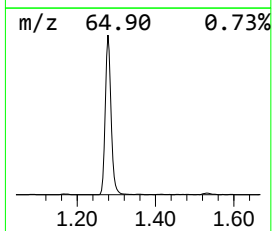
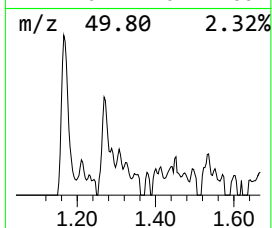
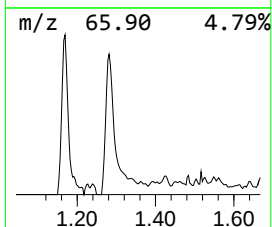
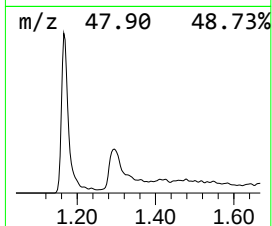
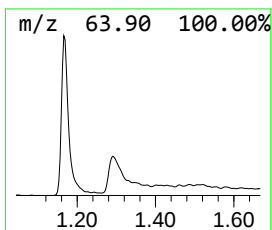
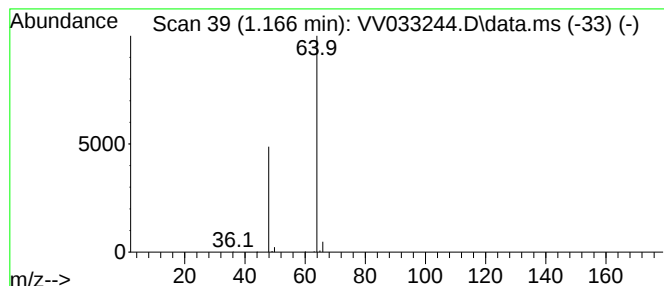
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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	8.86 ug/L	103673	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	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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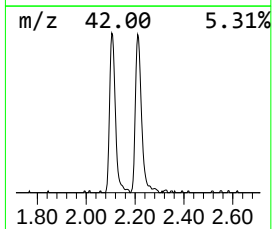
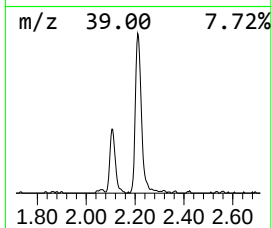
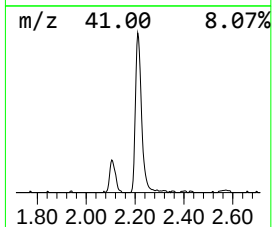
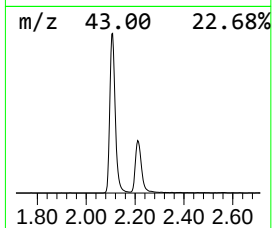
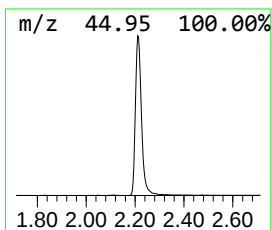
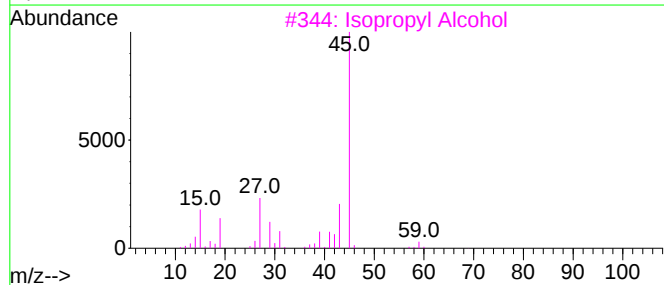
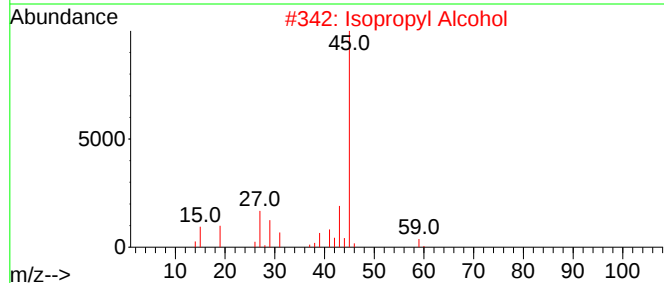
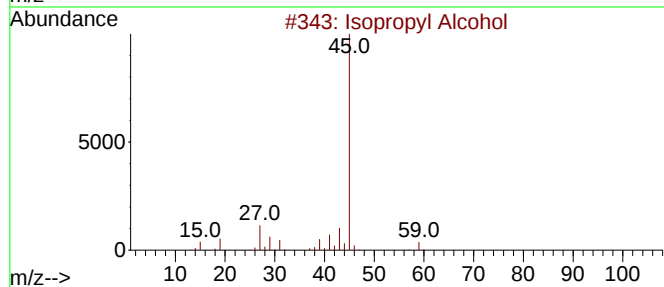
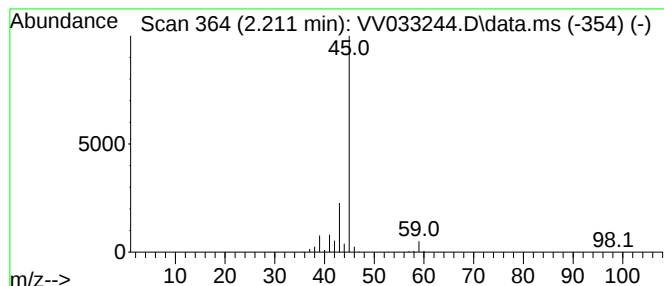
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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	43.65 ug/L	510654	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	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	8.9	ug/L	103673	1	5.535	584980	50.0
Isopropyl Alcohol	2.211	43.6	ug/L	510654	1	5.535	584980	50.0