

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU080819\
 Data File : VU033667.D
 Acq On : 09 Aug 2019 03:23
 Operator : JC/SP
 Sample : K4161-16
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETOF0

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM080819WMA.M
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.177	22	27	38	rBV4	4426	5300	0.38%	0.050%
2	1.283	51	60	72	rBV	41431	89650	6.39%	0.838%
3	1.392	88	94	106	rVB	216391	221723	15.81%	2.073%
4	1.672	173	181	196	rVB	176417	221110	15.77%	2.068%
5	2.261	353	364	375	rBV	325988	495051	35.30%	4.630%
6	2.425	405	415	435	rBV	34968	67078	4.78%	0.627%
7	2.595	465	468	472	rBV2	443	418	0.03%	0.004%
8	2.630	477	479	485	rVB4	528	353	0.03%	0.003%
9	2.688	495	497	502	rVB4	671	552	0.04%	0.005%
10	2.743	512	514	518	rVB2	538	320	0.02%	0.003%
11	2.765	518	521	525	rBV3	446	325	0.02%	0.003%
12	2.823	525	539	551	rBV2	3961	9960	0.71%	0.093%
13	2.962	577	582	585	rVB3	448	359	0.03%	0.003%
14	2.981	585	588	591	rBV2	319	252	0.02%	0.002%
15	3.077	615	618	623	rBV2	323	268	0.02%	0.003%
16	3.177	646	649	654	rVV4	542	436	0.03%	0.004%
17	3.367	705	708	712	rVB	354	246	0.02%	0.002%
18	3.428	724	727	730	rBV	250	250	0.02%	0.002%
19	3.707	807	814	817	rBV2	283	376	0.03%	0.004%
20	4.029	909	914	917	rBV2	182	237	0.02%	0.002%
21	4.071	924	927	931	rVB2	324	263	0.02%	0.002%
22	4.148	938	951	985	rBV	132952	365519	26.07%	3.418%
23	4.418	1033	1035	1041	rVB3	671	451	0.03%	0.004%
24	4.524	1062	1068	1069	rBV2	421	351	0.03%	0.003%
25	4.624	1082	1099	1125	rBV	236139	553115	39.44%	5.173%
26	4.855	1168	1171	1175	rBV5	532	547	0.04%	0.005%
27	4.961	1201	1204	1208	rBV2	540	473	0.03%	0.004%
28	4.984	1208	1211	1216	rVB3	473	281	0.02%	0.003%
29	5.186	1270	1274	1281	rBV2	302	382	0.03%	0.004%
30	5.318	1291	1315	1345	rBV2	473467	1402266	100.00%	13.113%
31	5.489	1366	1368	1372	rVB3	488	281	0.02%	0.003%
32	5.649	1415	1418	1423	rVB3	405	326	0.02%	0.003%
33	5.723	1438	1441	1444	rBV3	337	274	0.02%	0.003%
34	5.775	1454	1457	1460	rVB3	327	236	0.02%	0.002%

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 Title : VOC Analysis

35	5.865	1470	1485	1508	rBV	349557	695281	49.58%	6.502%
36	6.164	1571	1578	1581	rBV5	883	1114	0.08%	0.010%
37	6.177	1581	1582	1586	rVB3	746	415	0.03%	0.004%
38	6.235	1597	1600	1603	rBV2	527	345	0.02%	0.003%
39	6.309	1609	1623	1650	rBV	315094	629742	44.91%	5.889%
40	6.437	1660	1663	1667	rBV3	842	758	0.05%	0.007%
41	6.559	1698	1701	1704	rBV2	317	257	0.02%	0.002%
42	6.698	1740	1744	1749	rVB2	340	323	0.02%	0.003%
43	6.858	1791	1794	1797	rBV2	285	242	0.02%	0.002%
44	6.929	1811	1816	1819	rBV2	257	277	0.02%	0.003%
45	7.209	1891	1903	1933	rBV	163669	299170	21.33%	2.798%
46	7.366	1948	1952	1960	rBV5	1184	1359	0.10%	0.013%
47	7.457	1978	1980	1984	rVB2	389	318	0.02%	0.003%
48	7.547	1994	2008	2029	rBV	635574	1109662	79.13%	10.377%
49	7.833	2086	2097	2116	rBV	117563	204491	14.58%	1.912%
50	8.132	2184	2190	2191	rBV2	370	258	0.02%	0.002%
51	8.164	2191	2200	2212	rVV2	3566	6527	0.47%	0.061%
52	8.292	2229	2240	2284	rBV	420142	793957	56.62%	7.425%
53	8.582	2326	2330	2334	rVB4	474	359	0.03%	0.003%
54	8.688	2359	2363	2365	rBV3	572	445	0.03%	0.004%
55	8.720	2370	2373	2378	rVB4	367	316	0.02%	0.003%
56	8.936	2438	2440	2445	rVB3	327	264	0.02%	0.002%
57	8.971	2445	2451	2455	rBV2	204	258	0.02%	0.002%
58	9.071	2470	2482	2513	rBV	537239	905466	64.57%	8.468%
59	9.238	2532	2534	2542	rVB3	704	809	0.06%	0.008%
60	9.357	2565	2571	2572	rBV	558	464	0.03%	0.004%
61	9.514	2617	2620	2626	rVB2	329	354	0.03%	0.003%
62	9.614	2647	2651	2655	rVV2	301	323	0.02%	0.003%
63	9.636	2655	2658	2661	rVV2	368	236	0.02%	0.002%
64	9.813	2708	2713	2719	rBV2	275	303	0.02%	0.003%
65	9.871	2727	2731	2733	rBV2	359	288	0.02%	0.003%
66	10.148	2811	2817	2819	rBV2	413	489	0.03%	0.005%
67	10.212	2835	2837	2838	rVV2	567	253	0.02%	0.002%
68	10.225	2838	2841	2845	rVV3	792	628	0.04%	0.006%
69	10.341	2874	2877	2883	rVB2	234	247	0.02%	0.002%
70	10.415	2883	2900	2918	rBV	468800	755377	53.87%	7.064%
71	10.598	2946	2957	2971	rVB4	2906	5158	0.37%	0.048%

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72	10.694	2983	2987	2993	rBV3	361	488	0.03%	0.005%
73	10.762	3004	3008	3011	rVV3	481	449	0.03%	0.004%
74	10.791	3015	3017	3022	rVB2	320	233	0.02%	0.002%
75	10.945	3060	3065	3068	rBV	262	255	0.02%	0.002%
76	10.997	3077	3081	3086	rBV	382	368	0.03%	0.003%
77	11.141	3116	3126	3131	rBV3	528	874	0.06%	0.008%
78	11.180	3135	3138	3144	rVB2	421	428	0.03%	0.004%
79	11.212	3144	3148	3150	rBV	333	252	0.02%	0.002%
80	11.267	3158	3165	3168	rBV	495	427	0.03%	0.004%
81	11.376	3192	3199	3201	rBV2	560	549	0.04%	0.005%
82	11.405	3203	3208	3209	rBV3	758	602	0.04%	0.006%
83	11.469	3215	3228	3254	rBV	507509	816204	58.21%	7.633%
84	11.710	3300	3303	3307	rVB2	695	492	0.04%	0.005%
85	11.752	3311	3316	3318	rVB3	404	354	0.03%	0.003%
86	11.775	3320	3323	3327	rBV	472	301	0.02%	0.003%
87	11.842	3331	3344	3369	rBV	620434	1009727	72.01%	9.443%
88	12.093	3419	3422	3425	rVB4	452	343	0.02%	0.003%
89	12.135	3431	3435	3440	rBV4	991	1243	0.09%	0.012%
90	12.228	3460	3464	3465	rBV	497	337	0.02%	0.003%
91	12.308	3486	3489	3492	rBV	564	437	0.03%	0.004%
92	12.460	3533	3536	3538	rBV2	384	247	0.02%	0.002%
93	12.623	3579	3587	3591	rBV2	485	646	0.05%	0.006%
94	12.836	3652	3653	3659	rVB3	309	292	0.02%	0.003%
95	12.884	3664	3668	3669	rBV	523	393	0.03%	0.004%
96	12.977	3693	3697	3699	rBV	463	375	0.03%	0.004%
97	13.373	3815	3820	3826	rBV3	336	532	0.04%	0.005%
98	13.723	3925	3929	3932	rBV2	400	351	0.03%	0.003%
99	14.058	4030	4033	4035	rBV2	470	272	0.02%	0.003%
100	14.315	4111	4113	4118	rVB2	518	320	0.02%	0.003%

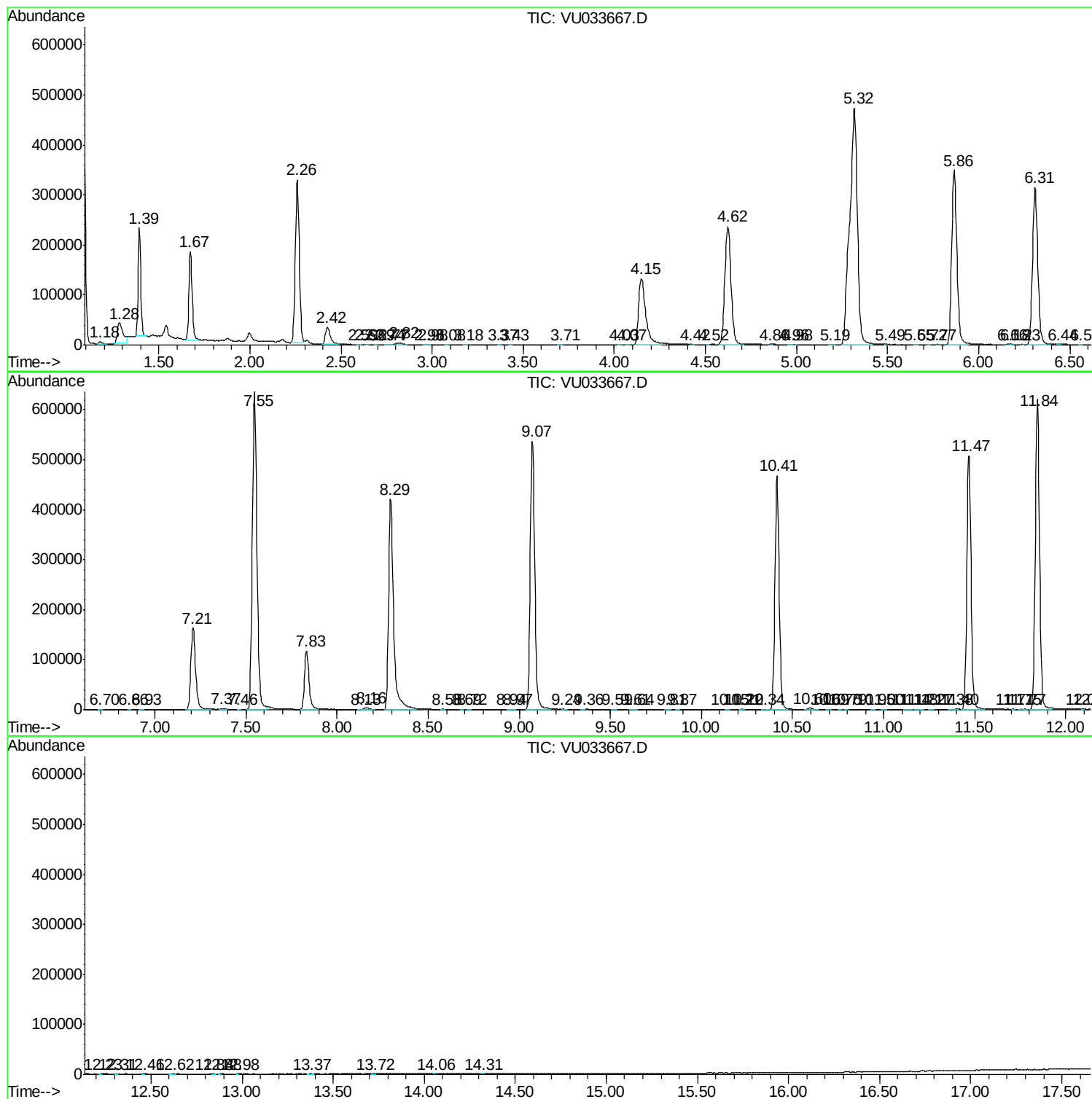
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM080819WMA.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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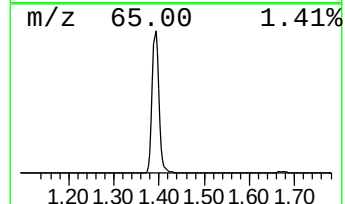
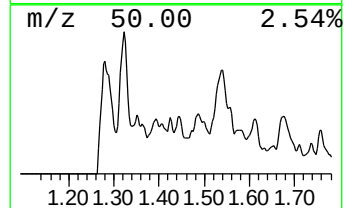
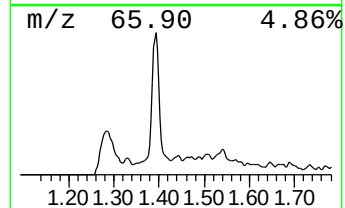
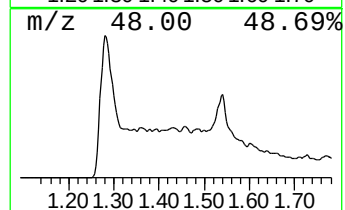
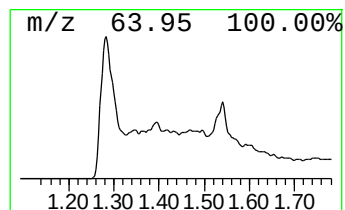
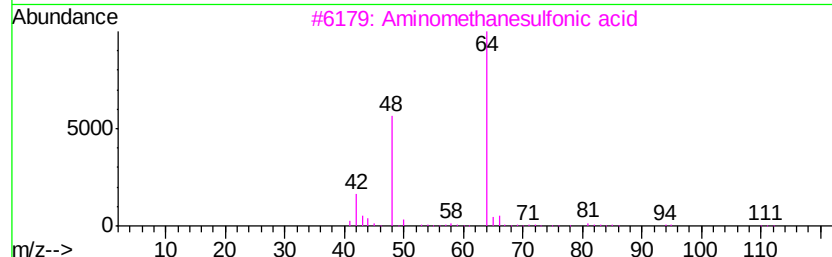
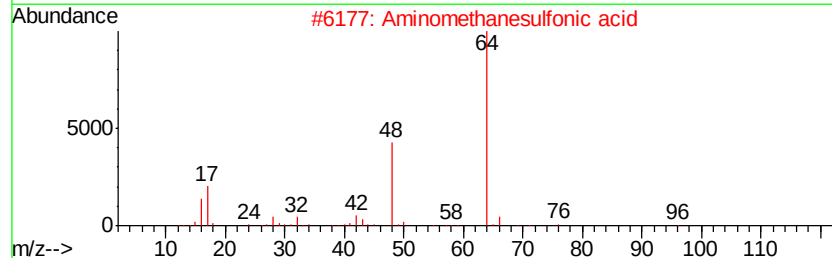
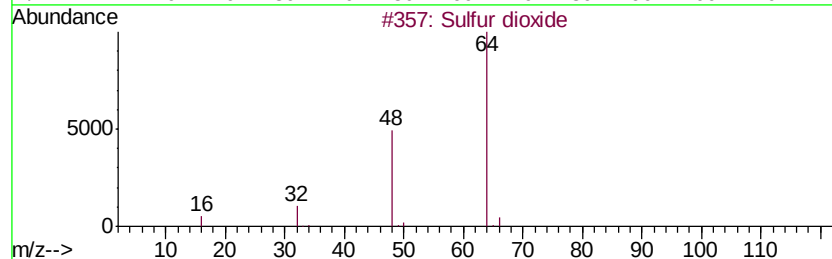
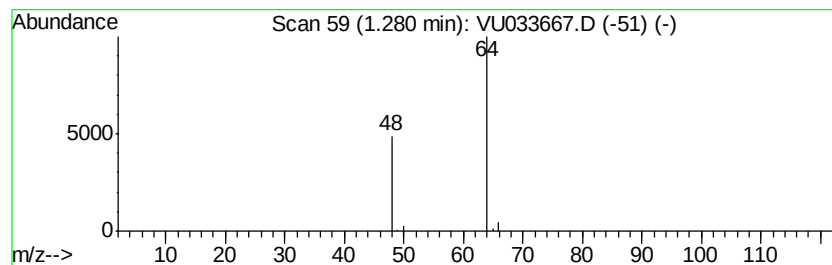
Instrument :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM080819WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.28	6.45 ug/L	89650	1,4-Difluorobenzene	5.86
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		Ethene, 1,1-difluoro-	64 C2H2F2	000075-38-7 5



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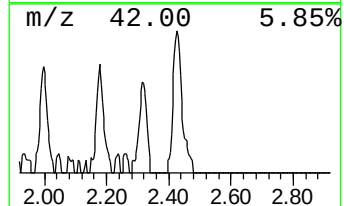
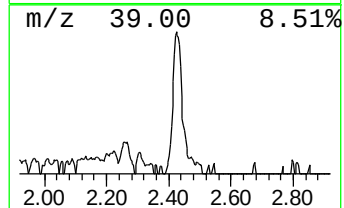
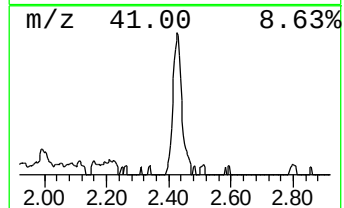
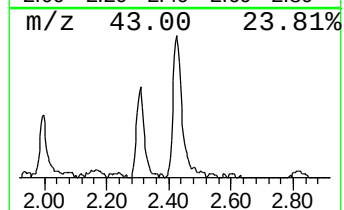
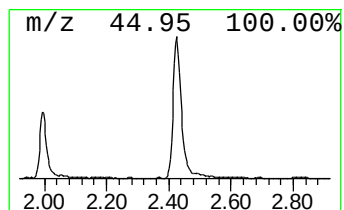
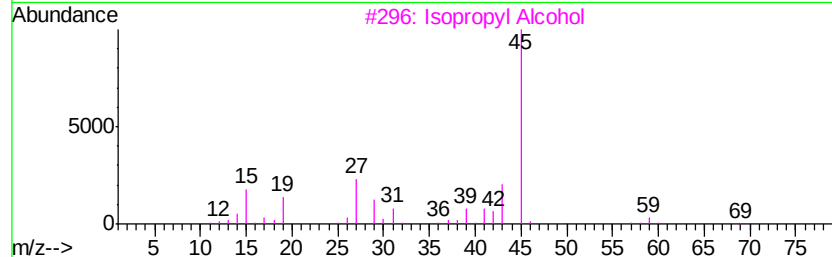
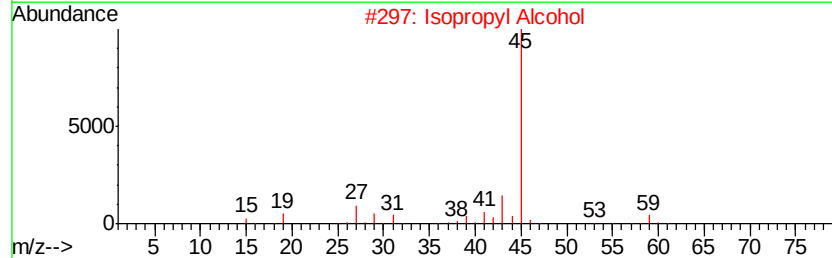
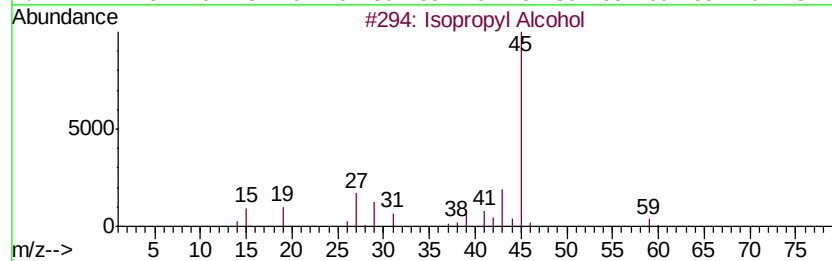
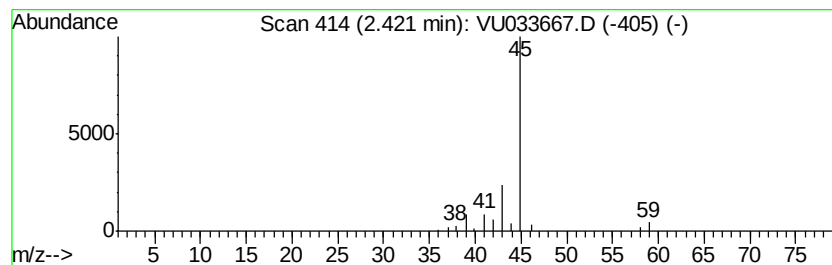
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Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.42	4.82 ug/L	67078	1,4-Difluorobenzene	5.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl Alcohol	60	C3H8O	000067-63-0	74
2		Isopropyl Alcohol	60	C3H8O	000067-63-0	43
3		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5		Formamide	45	CH3NO	000075-12-7	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.28	6.5	ug/L	89650	1	5.86	695281	50.0
Isopropyl Alcohol	2.42	4.8	ug/L	67078	1	5.86	695281	50.0