

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU010522\
 Data File : VU046675.D
 Acq On : 05 Jan 2022 20:14
 Operator : SY/MD
 Sample : N1009-03
 Misc : 5.35g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGLF9

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_U\Method\SFAMULM010522WMA.M
 Title : VOC Analysis

Signal : TIC: VU046675.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.604	74	82	111	rVB	90323	198164	15.17%	2.456%
2	1.919	172	180	227	rVB	44452	169068	12.94%	2.095%
3	2.552	367	377	420	rVB	215464	386274	29.57%	4.787%
4	2.845	466	468	472	rBV2	248	218	0.02%	0.003%
5	3.009	515	519	521	rVB	168	112	0.01%	0.001%
6	3.044	521	530	543	rBB3	1626	3361	0.26%	0.042%
7	3.099	545	547	548	rBV3	322	102	0.01%	0.001%
8	3.179	561	572	594	rVB	3716	9341	0.71%	0.116%
9	3.324	612	617	621	rBB	183	229	0.02%	0.003%
10	3.517	675	677	679	rBV	146	103	0.01%	0.001%
11	3.559	686	690	694	rBB	132	160	0.01%	0.002%
12	3.684	727	729	732	rBB	148	101	0.01%	0.001%
13	3.707	733	736	740	rBB	135	121	0.01%	0.001%
14	3.729	741	743	747	rBB	141	97	0.01%	0.001%
15	3.973	816	819	822	rBV	166	158	0.01%	0.002%
16	4.543	994	996	999	rBB	150	100	0.01%	0.001%
17	4.671	1017	1036	1099	rBV	50419	317621	24.31%	3.936%
18	5.067	1144	1159	1189	rVB	214335	512353	39.22%	6.350%
19	5.227	1207	1209	1215	rVB2	240	266	0.02%	0.003%
20	5.260	1216	1219	1221	rBB	160	110	0.01%	0.001%
21	5.301	1230	1232	1235	rBB2	240	138	0.01%	0.002%
22	5.597	1321	1324	1327	rBB	150	97	0.01%	0.001%
23	5.723	1342	1363	1388	rBV2	517545	1306493	100.00%	16.192%
24	5.989	1433	1446	1456	rBV6	3451	8996	0.69%	0.111%
25	6.070	1468	1471	1473	rVB	239	118	0.01%	0.001%
26	6.170	1499	1502	1505	rBV	180	169	0.01%	0.002%
27	6.250	1514	1527	1551	rVV	55021	107996	8.27%	1.338%
28	6.465	1591	1594	1597	rBV	127	130	0.01%	0.002%
29	6.530	1606	1614	1623	rVB5	2040	3313	0.25%	0.041%
30	6.607	1626	1638	1648	rBV5	1530	3816	0.29%	0.047%
31	6.694	1650	1665	1692	rVB	273953	580397	44.42%	7.193%
32	7.086	1784	1787	1789	rVB2	242	138	0.01%	0.002%
33	7.102	1790	1792	1795	rBB	232	129	0.01%	0.002%
34	7.192	1813	1820	1824	rBV2	817	1142	0.09%	0.014%
35	7.221	1827	1829	1831	rBV2	472	334	0.03%	0.004%
36	7.276	1844	1846	1849	rBV2	235	152	0.01%	0.002%

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 Title : VOC Analysis

37	7.305	1853	1855	1858	rBV	132	112	0.01%	0.001%
38	7.333	1861	1864	1865	rVV	258	154	0.01%	0.002%
39	7.359	1869	1872	1876	rBB	136	115	0.01%	0.001%
40	7.568	1922	1937	1969	rBV	138502	309131	23.66%	3.831%
41	7.735	1985	1989	1993	rVB3	334	303	0.02%	0.004%
42	7.800	2001	2009	2015	rBV2	840	1400	0.11%	0.017%
43	7.899	2025	2040	2059	rBV	596605	1116585	85.46%	13.838%
44	8.186	2114	2129	2157	rBV	75634	213177	16.32%	2.642%
45	8.359	2178	2183	2187	rBV	158	199	0.02%	0.002%
46	8.378	2187	2189	2194	rVB	281	239	0.02%	0.003%
47	8.462	2212	2215	2219	rBV2	206	176	0.01%	0.002%
48	8.481	2219	2221	2224	rVB2	238	135	0.01%	0.002%
49	8.687	2261	2285	2318	rBV	213066	719231	55.05%	8.914%
50	8.919	2355	2357	2360	rVB	187	97	0.01%	0.001%
51	8.999	2378	2382	2384	rBV	150	149	0.01%	0.002%
52	9.118	2416	2419	2423	rBV	164	181	0.01%	0.002%
53	9.234	2450	2455	2456	rBV	146	153	0.01%	0.002%
54	9.295	2472	2474	2477	rBB	140	97	0.01%	0.001%
55	9.314	2477	2480	2483	rBV	156	153	0.01%	0.002%
56	9.372	2494	2498	2501	rBV	138	169	0.01%	0.002%
57	9.427	2501	2515	2535	rVV2	59592	143187	10.96%	1.775%
58	9.571	2557	2560	2566	rVV2	253	252	0.02%	0.003%
59	9.629	2573	2578	2580	rBB	157	157	0.01%	0.002%
60	9.700	2593	2600	2607	rBV2	788	1158	0.09%	0.014%
61	9.780	2621	2625	2627	rBV	176	168	0.01%	0.002%
62	9.864	2648	2651	2653	rBV	181	150	0.01%	0.002%
63	9.915	2663	2667	2670	rBB	157	152	0.01%	0.002%
64	10.025	2695	2701	2704	rBB	155	207	0.02%	0.003%
65	10.060	2707	2712	2716	rBV	168	244	0.02%	0.003%
66	10.105	2723	2726	2727	rBV	252	140	0.01%	0.002%
67	10.230	2762	2765	2767	rVB	193	101	0.01%	0.001%
68	10.301	2784	2787	2789	rBV	124	111	0.01%	0.001%
69	10.369	2804	2808	2812	rBV	172	201	0.02%	0.002%
70	10.542	2854	2862	2864	rBV2	581	589	0.05%	0.007%
71	10.581	2871	2874	2878	rBV	156	188	0.01%	0.002%
72	10.671	2892	2902	2911	rBV3	3990	5787	0.44%	0.072%
73	10.774	2919	2934	2951	rVB	419645	713458	54.61%	8.842%
74	10.841	2952	2955	2957	rBV	146	132	0.01%	0.002%
75	10.867	2957	2963	2968	rBV2	852	951	0.07%	0.012%
76	11.121	3032	3042	3048	rBV5	2370	3763	0.29%	0.047%

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 Title : VOC Analysis

77	11.288	3091	3094	3097	rBV2	235	185	0.01%	0.002%
78	11.349	3110	3113	3117	rBV	188	219	0.02%	0.003%
79	11.369	3117	3119	3121	rBV	185	127	0.01%	0.002%
80	11.417	3131	3134	3136	rBV	211	97	0.01%	0.001%
81	11.459	3142	3147	3152	rBV2	1653	2143	0.16%	0.027%
82	11.626	3197	3199	3203	rBV	139	148	0.01%	0.002%
83	11.697	3215	3221	3227	rVB3	1592	2279	0.17%	0.028%
84	11.822	3248	3260	3273	rBV	93675	147248	11.27%	1.825%
85	11.944	3286	3298	3302	rBV3	1284	1887	0.14%	0.023%
86	12.108	3346	3349	3351	rBV2	291	177	0.01%	0.002%
87	12.201	3361	3378	3396	rVB	661539	1060263	81.15%	13.140%
88	12.333	3414	3419	3426	rVB3	940	1096	0.08%	0.014%
89	12.404	3436	3441	3445	rBV3	750	942	0.07%	0.012%
90	12.484	3464	3466	3470	rBV2	402	355	0.03%	0.004%
91	12.520	3474	3477	3479	rBV	281	216	0.02%	0.003%
92	12.565	3488	3491	3494	rBV2	278	218	0.02%	0.003%
93	13.092	3652	3655	3657	rBV	276	123	0.01%	0.002%
94	13.147	3666	3672	3674	rBV	500	517	0.04%	0.006%
95	13.848	3887	3890	3894	rVB	302	273	0.02%	0.003%
96	14.095	3959	3967	3974	rBV2	1517	2224	0.17%	0.028%
97	14.513	4095	4097	4102	rVB2	293	148	0.01%	0.002%
98	14.848	4198	4201	4205	rBV	287	210	0.02%	0.003%
99	15.221	4314	4317	4325	rBV4	850	1138	0.09%	0.014%
100	15.404	4369	4374	4384	rVB5	1438	2063	0.16%	0.026%

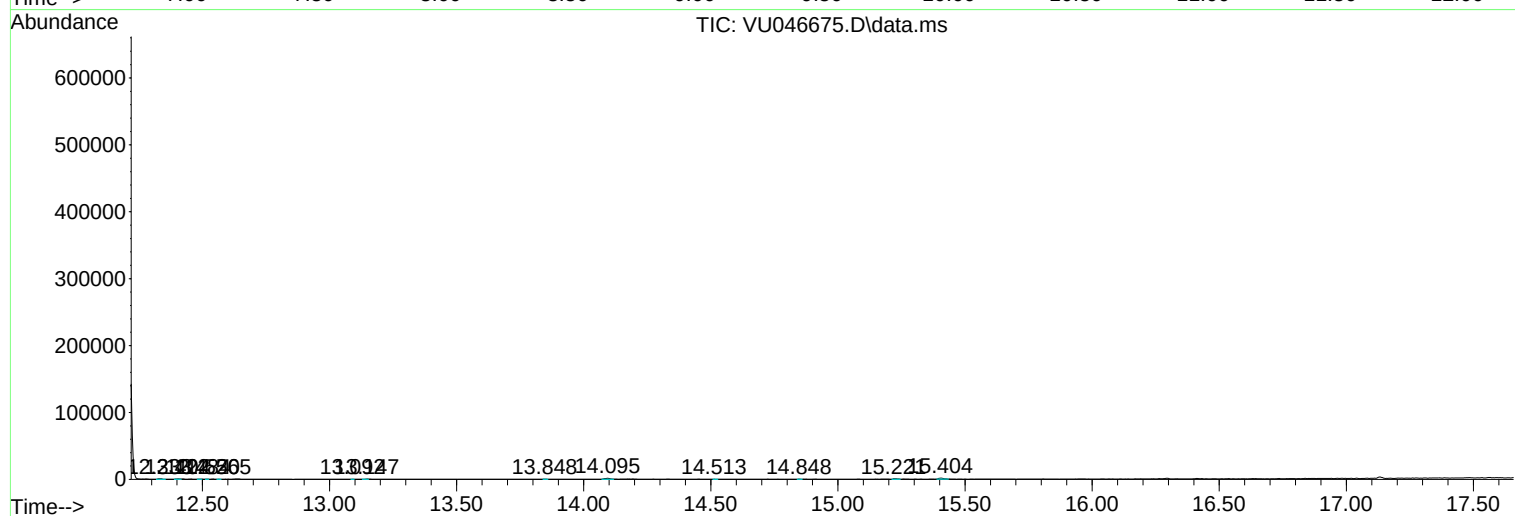
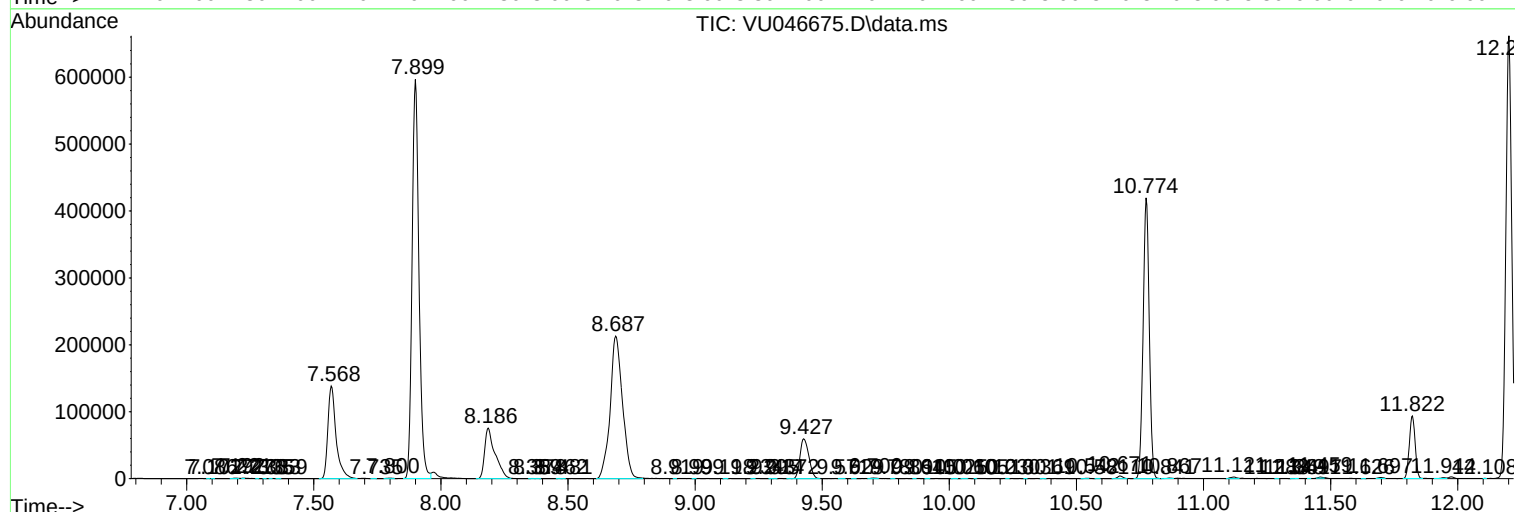
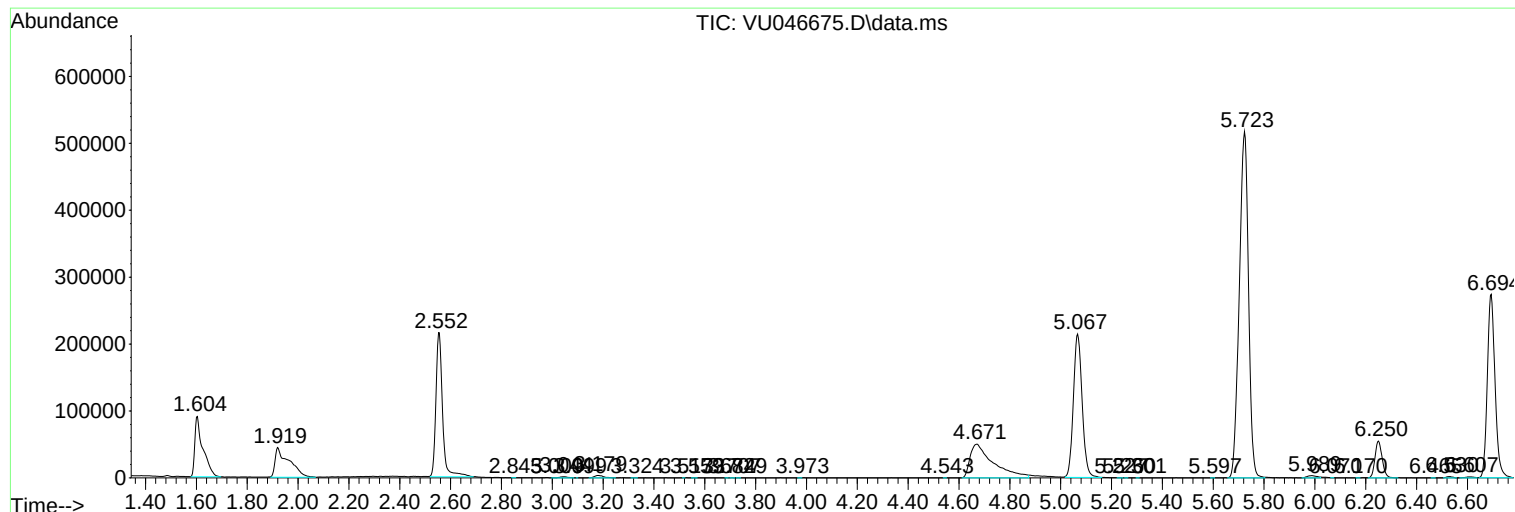
Sum of corrected areas: 8068965

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM010522WMA.M
Quant Title : VOC Analysis

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



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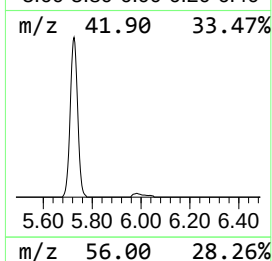
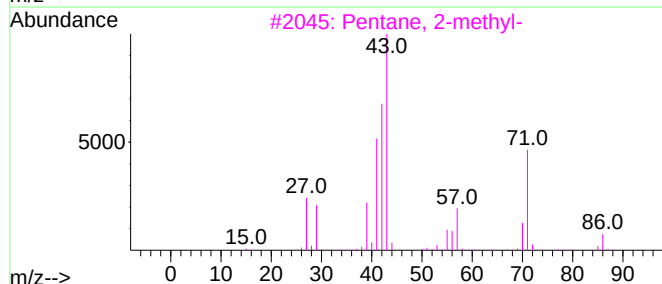
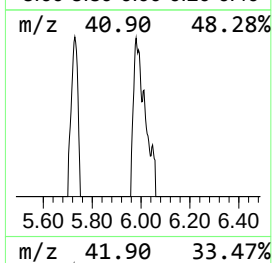
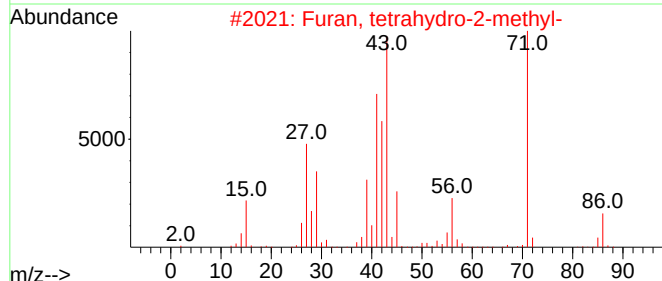
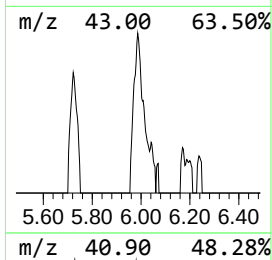
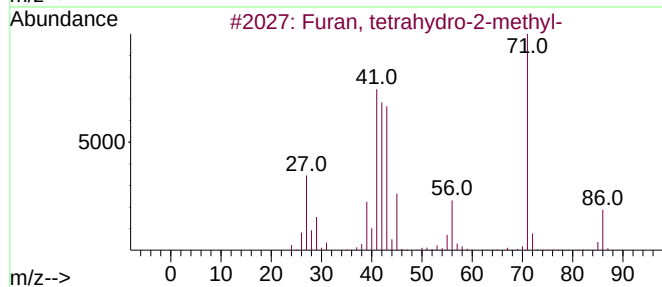
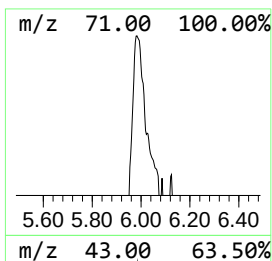
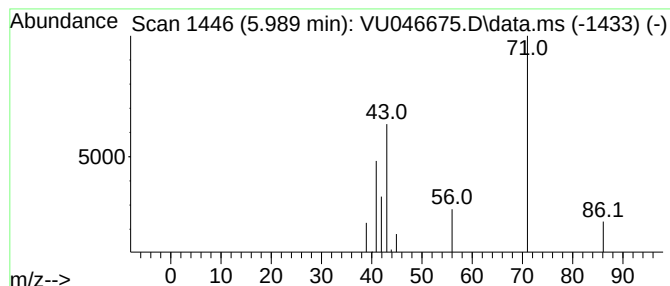
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM010522WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.989	4.16 ug/L	8996	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	38
2			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	9
3			Pentane, 2-methyl-	86	C6H14	000107-83-5	9
4			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	9
5			Prenol	86	C5H10O	000556-82-1	7



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	5.989	4.2	ug/L	8996	1	6.250	107996	50.0