

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082021\
 Data File : VV021918.D
 Acq On : 20 Aug 2021 17:00
 Operator : SY/MD
 Sample : M3458-14ME
 Misc : 6.58g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AW4ME

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\SFAMVLM081621WMA.M
 Title : VOC Analysis

Signal : TIC: VV021918.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.301	75	81	108	rVB	130009	183254	14.73%	1.792%
2	2.072	312	321	334	rBV	270031	384408	30.89%	3.760%
3	2.490	444	451	467	rVB	21252	37683	3.03%	0.369%
4	2.670	505	507	513	rVB3	591	340	0.03%	0.003%
5	2.812	545	551	555	rBV4	490	560	0.05%	0.005%
6	2.931	586	588	594	rVB2	471	344	0.03%	0.003%
7	3.008	605	612	614	rBV3	1101	1186	0.10%	0.012%
8	3.050	623	625	630	rVB2	529	307	0.02%	0.003%
9	3.101	639	641	645	rVV2	291	197	0.02%	0.002%
10	3.275	692	695	698	rBV	328	214	0.02%	0.002%
11	3.381	726	728	731	rVV	452	252	0.02%	0.002%
12	3.403	731	735	738	rVB3	506	382	0.03%	0.004%
13	3.596	793	795	798	rBV2	371	253	0.02%	0.002%
14	3.661	812	815	819	rBV4	393	256	0.02%	0.003%
15	3.738	834	839	842	rBV3	594	369	0.03%	0.004%
16	3.895	877	888	915	rBV2	63084	221775	17.82%	2.169%
17	4.346	1012	1028	1060	rBV	181340	479295	38.52%	4.688%
18	4.577	1099	1100	1104	rBV2	430	298	0.02%	0.003%
19	4.725	1144	1146	1149	rBV3	299	215	0.02%	0.002%
20	4.744	1149	1152	1153	rVV	461	228	0.02%	0.002%
21	4.783	1160	1164	1166	rBV	322	280	0.02%	0.003%
22	4.883	1193	1195	1201	rVB3	364	264	0.02%	0.003%
23	4.915	1201	1205	1207	rBV4	446	278	0.02%	0.003%
24	4.960	1215	1219	1222	rBV2	363	306	0.02%	0.003%
25	4.976	1222	1224	1227	rVB	742	312	0.03%	0.003%
26	5.040	1227	1244	1269	rBV2	502386	1244337	100.00%	12.171%
27	5.291	1320	1322	1324	rBV3	469	226	0.02%	0.002%
28	5.612	1409	1422	1459	rBV	461081	963101	77.40%	9.421%
29	5.866	1499	1501	1502	rBV2	554	253	0.02%	0.002%
30	5.905	1502	1513	1533	rVV4	21876	49424	3.97%	0.483%
31	6.069	1551	1564	1589	rBV	260510	550671	44.25%	5.386%
32	6.387	1659	1663	1664	rBV2	312	214	0.02%	0.002%
33	6.419	1670	1673	1674	rBV	453	225	0.02%	0.002%
34	6.468	1685	1688	1690	rBV	300	196	0.02%	0.002%
35	6.519	1700	1704	1707	rBV4	505	470	0.04%	0.005%
36	6.548	1710	1713	1716	rBV3	302	220	0.02%	0.002%

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Integrator: RTE

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 Title : VOC Analysis

37	6.609	1728	1732	1734	rBV3	277	234	0.02%	0.002%
38	6.645	1741	1743	1744	rBV2	740	253	0.02%	0.002%
39	6.706	1760	1762	1768	rVB4	810	696	0.06%	0.007%
40	6.738	1768	1772	1773	rBV	369	260	0.02%	0.003%
41	6.882	1813	1817	1820	rBV2	365	343	0.03%	0.003%
42	6.924	1827	1830	1833	rBV2	675	393	0.03%	0.004%
43	6.989	1836	1850	1871	rBV	135898	269287	21.64%	2.634%
44	7.159	1900	1903	1907	rVB4	376	310	0.02%	0.003%
45	7.178	1907	1909	1911	rBV	493	237	0.02%	0.002%
46	7.226	1922	1924	1927	rVB3	602	265	0.02%	0.003%
47	7.268	1934	1937	1939	rVB2	445	266	0.02%	0.003%
48	7.317	1939	1952	1973	rBV	585740	1043882	83.89%	10.211%
49	7.625	2036	2048	2071	rBV	90663	178924	14.38%	1.750%
50	7.776	2092	2095	2096	rBV2	328	193	0.02%	0.002%
51	7.882	2123	2128	2130	rVB3	386	328	0.03%	0.003%
52	7.915	2136	2138	2141	rBV	465	231	0.02%	0.002%
53	7.934	2141	2144	2147	rBV2	263	203	0.02%	0.002%
54	7.979	2155	2158	2159	rBV	774	337	0.03%	0.003%
55	8.005	2164	2166	2172	rVB2	472	365	0.03%	0.004%
56	8.104	2186	2197	2235	rBV2	229386	525850	42.26%	5.144%
57	8.442	2298	2302	2306	rBV4	656	501	0.04%	0.005%
58	8.689	2376	2379	2382	rBV3	479	419	0.03%	0.004%
59	8.738	2392	2394	2400	rBV2	313	211	0.02%	0.002%
60	8.853	2418	2430	2448	rBV	694100	1185065	95.24%	11.592%
61	9.149	2517	2522	2524	rBV4	1837	1651	0.13%	0.016%
62	9.220	2542	2544	2549	rVB2	532	382	0.03%	0.004%
63	9.307	2568	2571	2574	rBV2	356	237	0.02%	0.002%
64	9.387	2592	2596	2598	rBV	584	283	0.02%	0.003%
65	9.435	2607	2611	2614	rBV2	316	225	0.02%	0.002%
66	9.760	2708	2712	2714	rBV2	343	243	0.02%	0.002%
67	9.966	2774	2776	2780	rVB2	437	222	0.02%	0.002%
68	10.130	2817	2827	2838	rVV5	5860	9872	0.79%	0.097%
69	10.223	2844	2856	2873	rBV	366225	594975	47.81%	5.820%
70	10.451	2923	2927	2930	rBV	379	292	0.02%	0.003%
71	10.474	2930	2934	2938	rBV4	472	452	0.04%	0.004%
72	10.551	2951	2958	2959	rBV	909	974	0.08%	0.010%
73	10.776	3025	3028	3030	rBV	554	360	0.03%	0.004%
74	10.828	3040	3044	3046	rBV2	746	640	0.05%	0.006%
75	10.921	3068	3073	3083	rVB6	5839	8245	0.66%	0.081%
76	10.995	3095	3096	3101	rBV	272	234	0.02%	0.002%

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 ClientSampleId :
 C0AW4ME

Integration Parameters: LSCINT.P

Integrator: RTE

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 Title : VOC Analysis

77	11.040	3101	3110	3116	rVV5	1288	2374	0.19%	0.023%
78	11.194	3152	3158	3164	rVB6	1160	1481	0.12%	0.014%
79	11.252	3164	3176	3206	rBV	801989	1242026	99.81%	12.149%
80	11.628	3281	3293	3316	rBV	634892	999944	80.36%	9.781%
81	11.792	3335	3344	3353	rBV8	2977	4527	0.36%	0.044%
82	11.963	3392	3397	3399	rBV2	264	211	0.02%	0.002%
83	12.004	3407	3410	3413	rVB3	596	440	0.04%	0.004%
84	12.056	3422	3426	3428	rBV3	720	537	0.04%	0.005%
85	12.429	3538	3542	3545	rBV3	498	465	0.04%	0.005%
86	12.464	3550	3553	3554	rBV2	523	288	0.02%	0.003%
87	12.590	3589	3592	3593	rBV	766	498	0.04%	0.005%
88	12.657	3606	3613	3620	rBV5	1578	2105	0.17%	0.021%
89	12.783	3649	3652	3653	rBV2	341	216	0.02%	0.002%
90	12.802	3656	3658	3660	rBV	446	202	0.02%	0.002%
91	12.873	3677	3680	3681	rBV3	385	235	0.02%	0.002%
92	13.088	3745	3747	3751	rBV2	562	280	0.02%	0.003%
93	13.110	3751	3754	3762	rBV2	272	332	0.03%	0.003%
94	13.271	3798	3804	3809	rBV4	1624	2140	0.17%	0.021%
95	13.390	3837	3841	3850	rVB3	707	828	0.07%	0.008%
96	13.432	3852	3854	3857	rVB2	540	227	0.02%	0.002%
97	13.455	3859	3861	3864	rBV2	378	257	0.02%	0.003%
98	13.487	3868	3871	3872	rBV	609	352	0.03%	0.003%
99	13.516	3875	3880	3891	rVB	6624	9611	0.77%	0.094%
100	13.750	3949	3953	3965	rVB5	1991	2920	0.23%	0.029%

Sum of corrected areas: 10223429

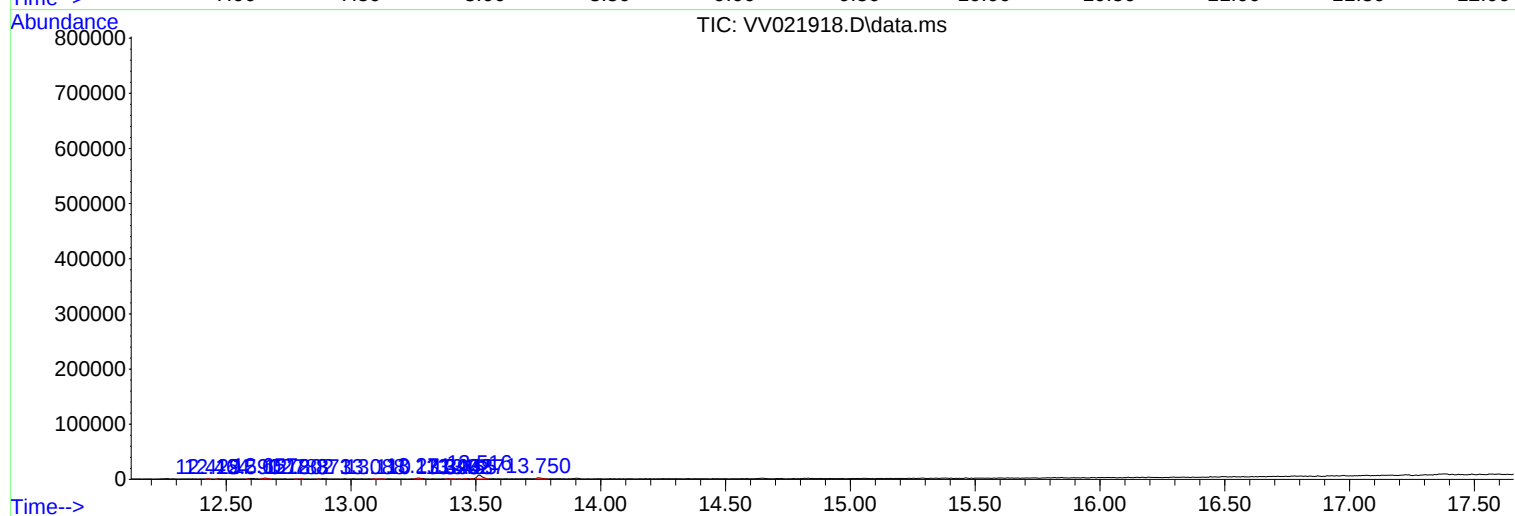
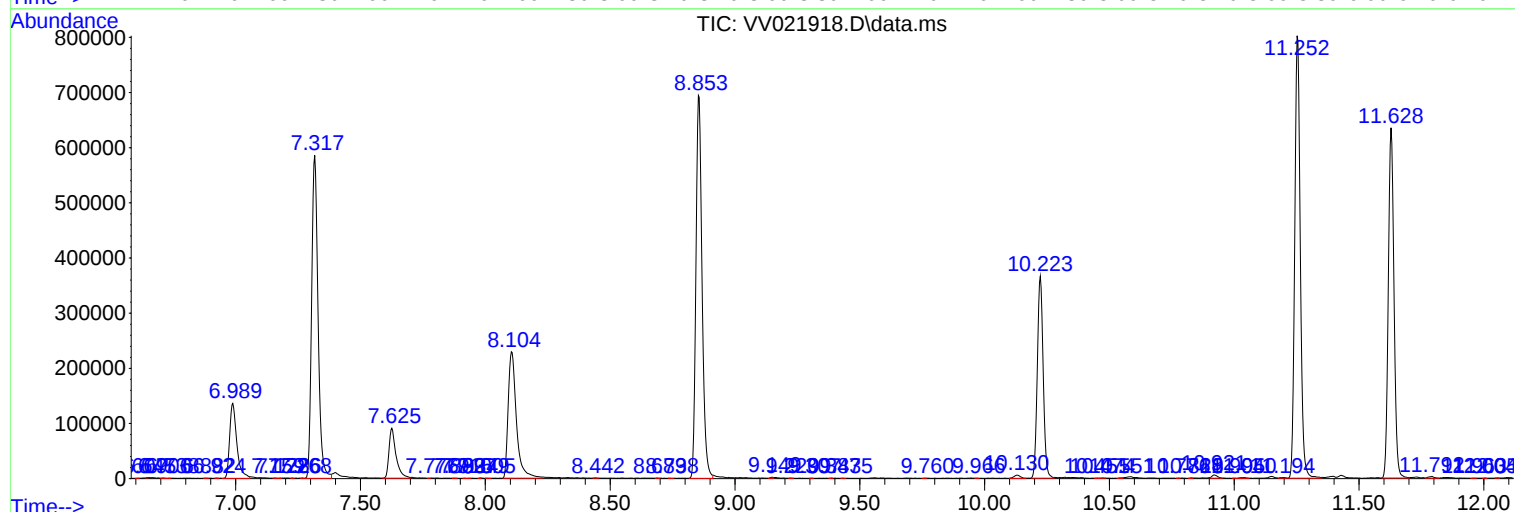
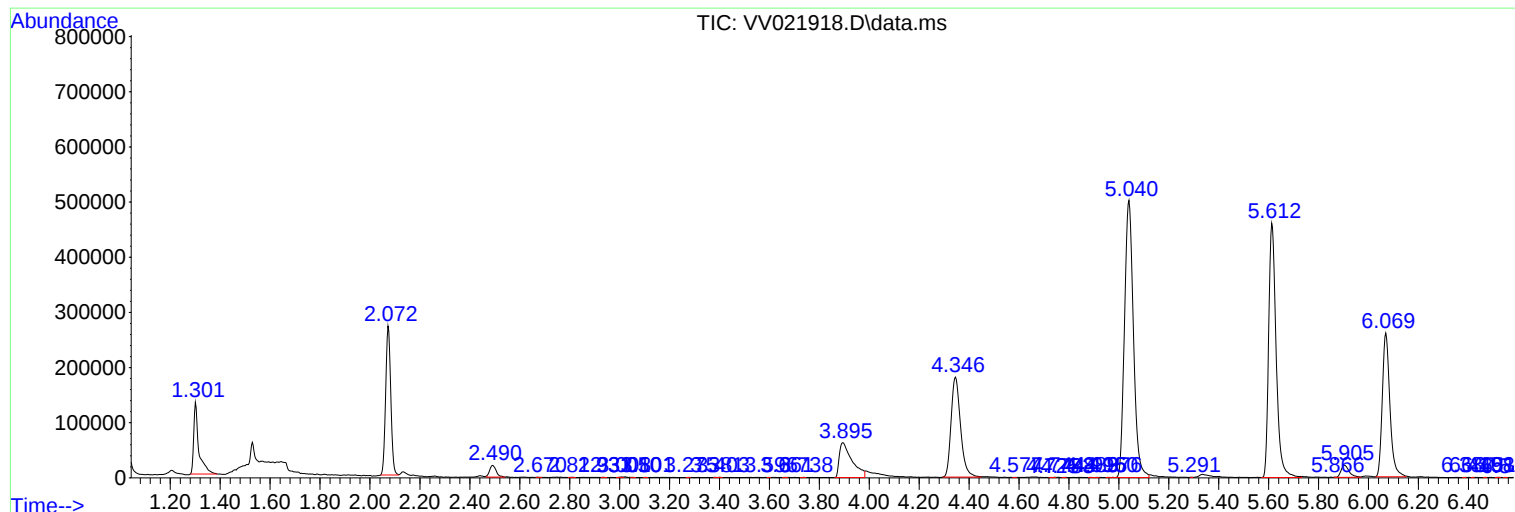
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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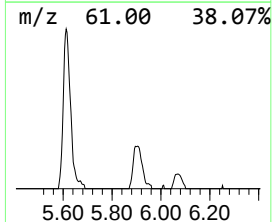
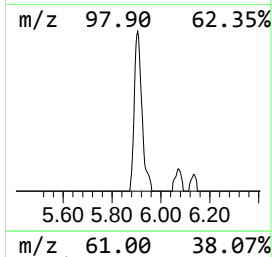
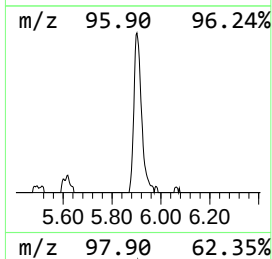
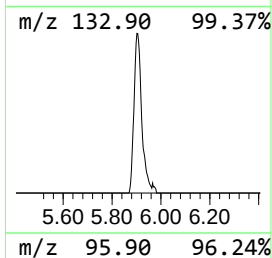
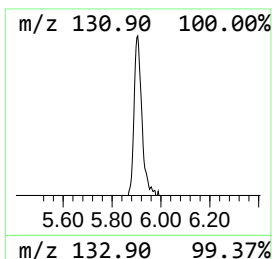
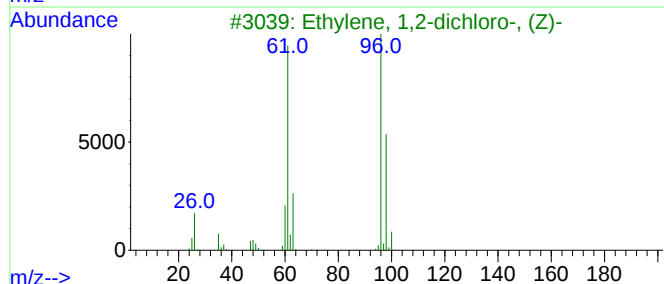
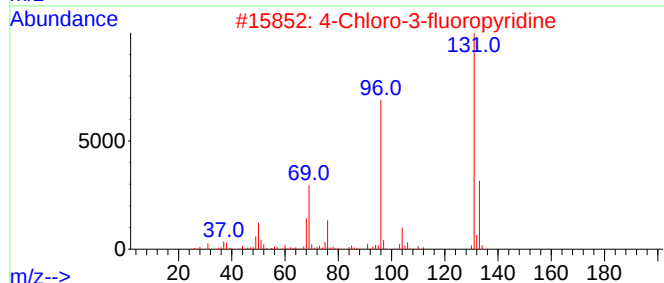
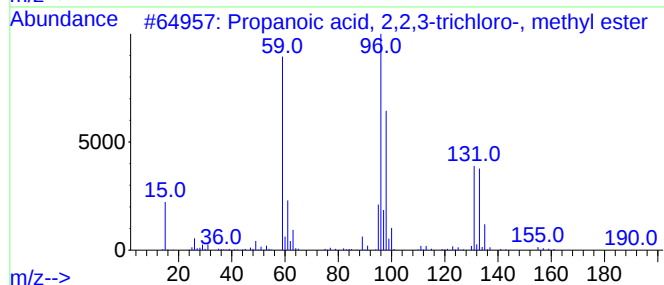
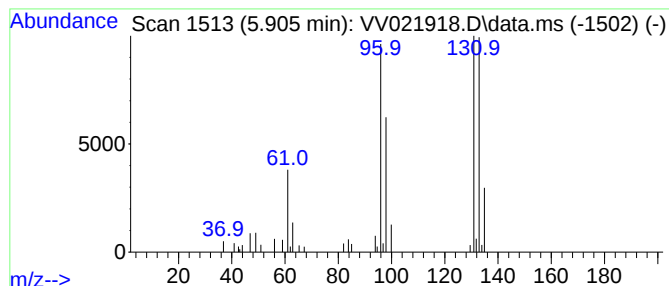
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Propanoic acid, 2,2,3-trich... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.905	2.57 ug/L	49424	1,4-Difluorobenzene	5.612

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	72
2			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	43
3			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
4			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	38
5			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	5.905	2.6	ug/L	49424	1	5.612	963101	50.0