

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV082021\  
 Data File : VV021913.D  
 Acq On : 20 Aug 2021 14:36  
 Operator : SY/MD  
 Sample : M3458-06ME  
 Misc : 6.08g/5.0mL/100uL/5.0mL/MSVOA\_V/MEOH  
 ALS Vial : 12 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 C0AR7ME

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: VV021913.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	111	rVB	118585	171593	12.04%	1.527%
2	2.072	312	321	334	rBV	274219	389773	27.34%	3.469%
3	2.494	445	452	466	rVB2	15571	25530	1.79%	0.227%
4	2.735	525	527	529	rBV2	583	299	0.02%	0.003%
5	2.995	606	608	610	rBV2	448	188	0.01%	0.002%
6	3.018	611	615	618	rBV3	741	716	0.05%	0.006%
7	3.076	627	633	634	rBV2	456	493	0.03%	0.004%
8	3.175	660	664	668	rBV2	241	219	0.02%	0.002%
9	3.201	670	672	679	rVV	200	207	0.01%	0.002%
10	3.297	698	702	703	rBV2	391	239	0.02%	0.002%
11	3.616	798	801	805	rBV	433	339	0.02%	0.003%
12	3.706	826	829	830	rBV2	579	240	0.02%	0.002%
13	3.735	833	838	843	rVV4	638	694	0.05%	0.006%
14	3.815	860	863	868	rVB2	378	265	0.02%	0.002%
15	3.892	877	887	924	rBV	85718	313154	21.97%	2.787%
16	4.346	1009	1028	1056	rBV	208761	555469	38.97%	4.944%
17	4.654	1119	1124	1125	rBV2	903	684	0.05%	0.006%
18	4.883	1192	1195	1199	rVB2	321	199	0.01%	0.002%
19	4.908	1199	1203	1208	rVB4	527	435	0.03%	0.004%
20	4.976	1220	1224	1225	rBV2	490	291	0.02%	0.003%
21	5.040	1228	1244	1277	rBV2	578080	1425492	100.00%	12.688%
22	5.294	1321	1323	1324	rBV	420	201	0.01%	0.002%
23	5.336	1327	1336	1343	rBV6	5380	10953	0.77%	0.097%
24	5.445	1368	1370	1373	rVB2	447	195	0.01%	0.002%
25	5.513	1388	1391	1394	rBV3	403	298	0.02%	0.003%
26	5.535	1396	1398	1402	rVB3	542	289	0.02%	0.003%
27	5.558	1402	1405	1410	rVB3	361	291	0.02%	0.003%
28	5.612	1410	1422	1454	rBV	454867	950357	66.67%	8.459%
29	5.902	1501	1512	1527	rBV	27989	60621	4.25%	0.540%
30	6.069	1551	1564	1596	rVB	300994	646159	45.33%	5.751%
31	6.349	1648	1651	1654	rBV	240	184	0.01%	0.002%
32	6.371	1656	1658	1662	rVB2	418	308	0.02%	0.003%
33	6.622	1734	1736	1737	rBV	527	262	0.02%	0.002%
34	6.638	1737	1741	1743	rBV3	1180	841	0.06%	0.007%
35	6.773	1778	1783	1787	rBV3	522	425	0.03%	0.004%
36	6.918	1826	1828	1830	rBV2	667	305	0.02%	0.003%

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 ClientSampleId :  
 COAR7ME

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 >  
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Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM081621WMA.M  
 Title : VOC Analysis

37	6.940	1833	1835	1838	rVB	508	212	0.01%	0.002%
38	6.989	1838	1850	1875	rBV	161413	317248	22.26%	2.824%
39	7.194	1910	1914	1916	rBV2	840	637	0.04%	0.006%
40	7.255	1928	1933	1935	rBV5	1014	852	0.06%	0.008%
41	7.317	1939	1952	1970	rBV	650026	1168457	81.97%	10.400%
42	7.564	2027	2029	2031	rBV2	391	244	0.02%	0.002%
43	7.625	2037	2048	2070	rBV	107066	209074	14.67%	1.861%
44	7.847	2111	2117	2121	rBV4	639	686	0.05%	0.006%
45	7.876	2121	2126	2127	rBV4	531	448	0.03%	0.004%
46	7.921	2138	2140	2145	rBV2	298	275	0.02%	0.002%
47	8.024	2165	2172	2173	rBV	170	198	0.01%	0.002%
48	8.107	2185	2198	2233	rBV3	278259	662684	46.49%	5.898%
49	8.423	2294	2296	2299	rVB2	619	256	0.02%	0.002%
50	8.525	2325	2328	2333	rBV2	399	295	0.02%	0.003%
51	8.574	2338	2343	2349	rBV4	608	652	0.05%	0.006%
52	8.677	2372	2375	2378	rBV3	586	370	0.03%	0.003%
53	8.696	2378	2381	2385	rVV2	432	285	0.02%	0.003%
54	8.741	2393	2395	2399	rBV2	384	191	0.01%	0.002%
55	8.857	2419	2431	2457	rVV	672416	1162004	81.52%	10.343%
56	9.114	2508	2511	2513	rBV3	582	400	0.03%	0.004%
57	9.207	2538	2540	2543	rBV2	424	253	0.02%	0.002%
58	9.288	2561	2565	2570	rVB3	457	385	0.03%	0.003%
59	9.339	2577	2581	2583	rVB	349	190	0.01%	0.002%
60	9.374	2589	2592	2596	rVB2	294	244	0.02%	0.002%
61	9.458	2616	2618	2623	rVB3	311	203	0.01%	0.002%
62	9.558	2639	2649	2655	rBV3	1254	1829	0.13%	0.016%
63	9.715	2694	2698	2703	rBV3	257	302	0.02%	0.003%
64	9.754	2708	2710	2714	rVB3	305	220	0.02%	0.002%
65	10.075	2807	2810	2811	rBV	461	264	0.02%	0.002%
66	10.130	2818	2827	2838	rBV4	4018	6408	0.45%	0.057%
67	10.223	2844	2856	2872	rBV	448223	727484	51.03%	6.475%
68	10.442	2923	2924	2926	rBV	353	185	0.01%	0.002%
69	10.551	2953	2958	2959	rBV4	716	685	0.05%	0.006%
70	10.660	2988	2992	2993	rBV2	726	505	0.04%	0.004%
71	10.738	3011	3016	3017	rBV2	412	307	0.02%	0.003%
72	10.889	3057	3063	3066	rVV3	1057	1272	0.09%	0.011%
73	10.924	3066	3074	3083	rVB7	4400	7224	0.51%	0.064%
74	11.127	3134	3137	3138	rBV3	374	209	0.01%	0.002%
75	11.152	3138	3145	3152	rVB5	2369	3423	0.24%	0.030%
76	11.185	3152	3155	3156	rBV2	688	394	0.03%	0.004%

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Integration Parameters: LSCINT.P

Integrator: RTE  
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 Sampling : 1                      Min Area: 0 % of largest Peak  
 Start Thrs: 0.2                   Max Peaks: 100  
 Stop Thrs : 0                     Peak Location: TOP

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77	11.252	3165	3176	3198	rBV	773839	1211770	85.01%	10.786%
78	11.516	3254	3258	3260	rBV	303	227	0.02%	0.002%
79	11.628	3281	3293	3318	rBV	744947	1171724	82.20%	10.429%
80	11.837	3356	3358	3360	rBV	583	374	0.03%	0.003%
81	11.895	3374	3376	3381	rVV2	441	206	0.01%	0.002%
82	11.934	3384	3388	3390	rBV	301	193	0.01%	0.002%
83	12.024	3414	3416	3420	rVB2	404	213	0.01%	0.002%
84	12.049	3420	3424	3425	rBV2	627	396	0.03%	0.004%
85	12.085	3432	3435	3437	rBV2	555	410	0.03%	0.004%
86	12.175	3460	3463	3465	rBV2	430	231	0.02%	0.002%
87	12.294	3497	3500	3502	rBV	393	227	0.02%	0.002%
88	12.397	3529	3532	3535	rBV2	211	186	0.01%	0.002%
89	12.429	3539	3542	3544	rVB3	426	189	0.01%	0.002%
90	12.599	3589	3595	3600	rBV7	1045	1264	0.09%	0.011%
91	12.648	3607	3610	3613	rBV2	487	370	0.03%	0.003%
92	12.680	3618	3620	3622	rBV2	553	231	0.02%	0.002%
93	12.963	3706	3708	3711	rVB2	608	333	0.02%	0.003%
94	13.210	3783	3785	3788	rBV2	342	239	0.02%	0.002%
95	13.278	3802	3806	3810	rBV3	502	403	0.03%	0.004%
96	13.339	3821	3825	3828	rBV3	438	381	0.03%	0.003%
97	13.477	3865	3868	3871	rBV2	505	408	0.03%	0.004%
98	13.512	3873	3879	3886	rBV4	4356	6500	0.46%	0.058%
99	13.905	3996	4001	4008	rVB4	2165	2395	0.17%	0.021%
100	15.024	4347	4349	4352	rBV2	821	450	0.03%	0.004%

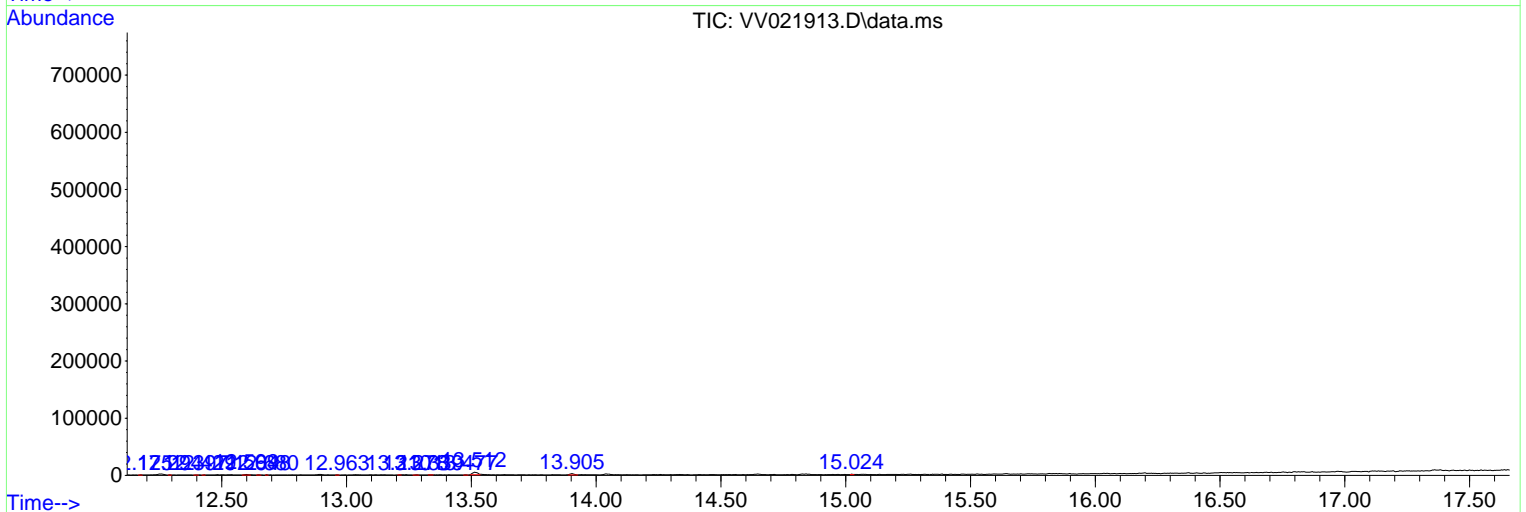
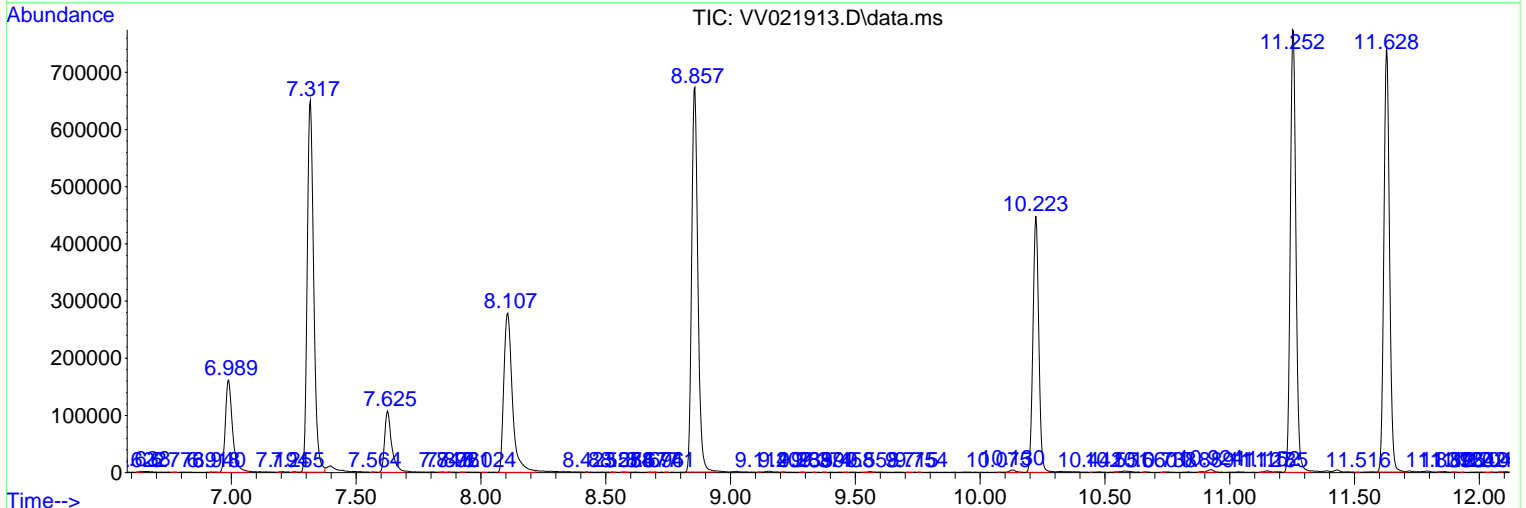
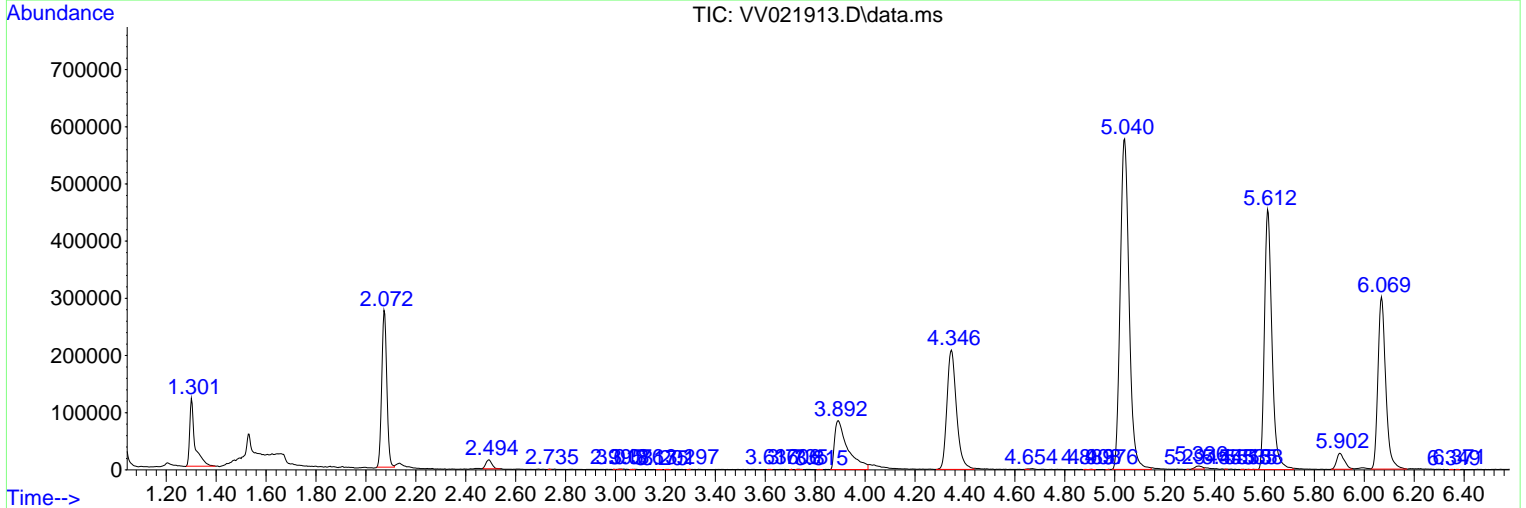
Sum of corrected areas: 11234982

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Instrument :  
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 ClientSampled :  
 COAR7ME

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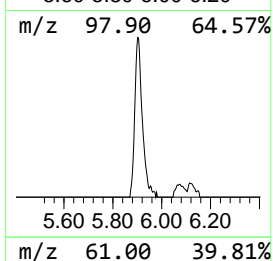
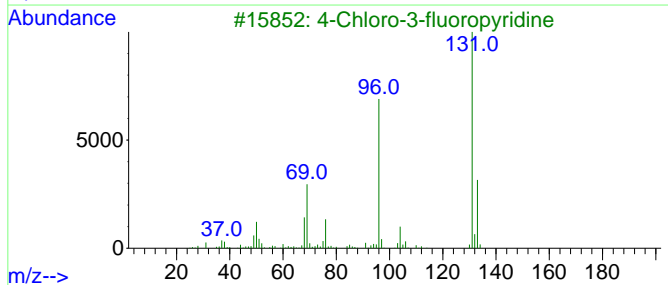
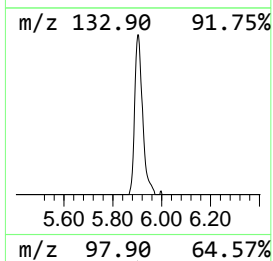
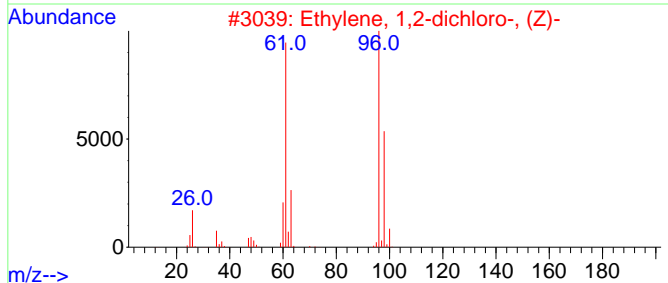
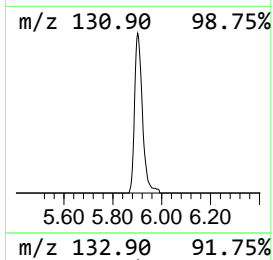
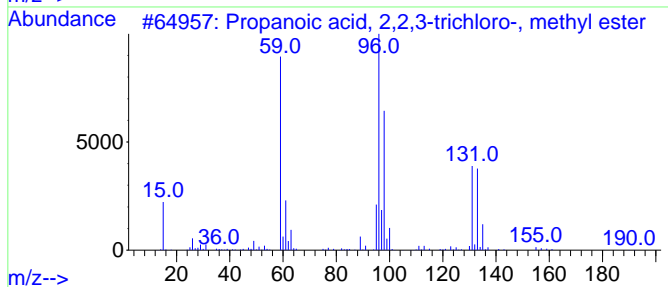
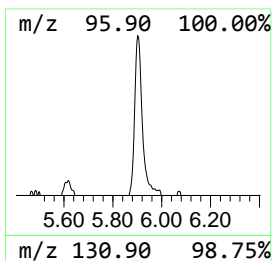
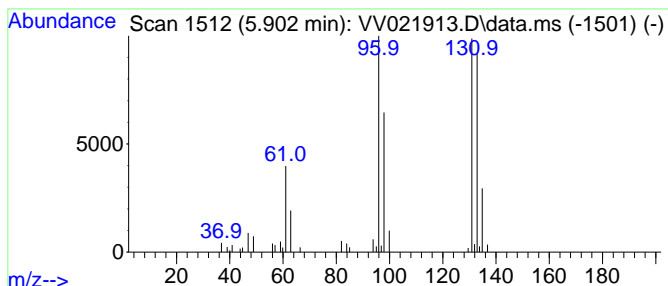
TIC Library : C:\Database\NIST20.L  
 TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.902	3.19 ug/L	60621	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	50
2			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	35
3			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	25
4			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	23
5			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	12



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	5.902	3.2	ug/L	60621	1	5.612	950357	50.0