

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082321\
 Data File : VV021933.D
 Acq On : 23 Aug 2021 16:11
 Operator : SY/MD
 Sample : M3486-03ME
 Misc : 6.91g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AW9ME

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: VV021933.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	109	rVB	133882	184243	13.57%	1.674%
2	2.076	312	322	334	rBV	276697	397301	29.26%	3.609%
3	2.741	519	529	541	rVB7	2494	4296	0.32%	0.039%
4	2.822	551	554	555	rBV	362	225	0.02%	0.002%
5	3.014	603	614	618	rBV5	1862	2718	0.20%	0.025%
6	3.175	661	664	667	rVB	371	244	0.02%	0.002%
7	3.220	675	678	681	rVB	372	210	0.02%	0.002%
8	3.330	710	712	715	rVB	412	222	0.02%	0.002%
9	3.471	752	756	759	rBV2	330	268	0.02%	0.002%
10	3.571	782	787	792	rBV2	366	432	0.03%	0.004%
11	3.658	811	814	817	rVB3	302	209	0.02%	0.002%
12	3.677	817	820	826	rVB3	344	347	0.03%	0.003%
13	3.738	828	839	853	rVB5	1194	2810	0.21%	0.026%
14	3.793	853	856	860	rBV2	250	206	0.02%	0.002%
15	3.886	875	885	918	rBV	65690	248482	18.30%	2.257%
16	4.339	1011	1026	1063	rVB	192060	519092	38.23%	4.716%
17	4.542	1086	1089	1093	rVB3	716	524	0.04%	0.005%
18	4.564	1093	1096	1097	rBV	426	258	0.02%	0.002%
19	4.741	1147	1151	1155	rBV3	761	629	0.05%	0.006%
20	4.760	1155	1157	1158	rBV2	600	230	0.02%	0.002%
21	4.899	1190	1200	1203	rBV5	754	1109	0.08%	0.010%
22	4.976	1221	1224	1226	rBV2	359	234	0.02%	0.002%
23	5.034	1226	1242	1279	rBV2	539235	1357798	100.00%	12.335%
24	5.275	1315	1317	1320	rVB2	773	416	0.03%	0.004%
25	5.304	1320	1326	1327	rBV3	1921	1346	0.10%	0.012%
26	5.526	1393	1395	1397	rVB2	651	343	0.03%	0.003%
27	5.609	1408	1421	1462	rBV	431719	921179	67.84%	8.369%
28	5.857	1496	1498	1500	rVB	581	262	0.02%	0.002%
29	5.899	1500	1511	1528	rBV2	22884	51146	3.77%	0.465%
30	6.066	1550	1563	1595	rVB	279797	622536	45.85%	5.655%
31	6.317	1638	1641	1643	rBV2	399	301	0.02%	0.003%
32	6.352	1649	1652	1657	rVB3	513	392	0.03%	0.004%
33	6.439	1676	1679	1680	rBV2	439	240	0.02%	0.002%
34	6.635	1728	1740	1743	rBV6	1567	2756	0.20%	0.025%
35	6.719	1761	1766	1769	rBV4	647	545	0.04%	0.005%
36	6.841	1799	1804	1807	rBV2	229	241	0.02%	0.002%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

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Filtering: 5

Sampling : 1

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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

37	6.908	1820	1825	1826	rBV	805	614	0.05%	0.006%
38	6.982	1837	1848	1879	rBV	158928	317589	23.39%	2.885%
39	7.233	1924	1926	1927	rBV	374	192	0.01%	0.002%
40	7.243	1927	1929	1930	rBV2	796	385	0.03%	0.003%
41	7.313	1939	1951	1969	rBV	638180	1151287	84.79%	10.459%
42	7.622	2037	2047	2072	rBV2	105562	210626	15.51%	1.913%
43	7.844	2115	2116	2123	rVB4	589	513	0.04%	0.005%
44	7.966	2152	2154	2156	rBV2	724	412	0.03%	0.004%
45	8.030	2172	2174	2177	rBV2	441	363	0.03%	0.003%
46	8.101	2184	2196	2227	rBV	281106	634497	46.73%	5.764%
47	8.471	2308	2311	2312	rBV3	432	223	0.02%	0.002%
48	8.497	2318	2319	2322	rBV	470	298	0.02%	0.003%
49	8.712	2385	2386	2391	rVB3	494	276	0.02%	0.003%
50	8.780	2405	2407	2410	rBV4	631	437	0.03%	0.004%
51	8.853	2416	2430	2451	rBV	659041	1144317	84.28%	10.396%
52	9.079	2496	2500	2502	rBV3	379	301	0.02%	0.003%
53	9.111	2508	2510	2512	rBV3	513	292	0.02%	0.003%
54	9.252	2552	2554	2557	rVB	414	201	0.01%	0.002%
55	9.291	2562	2566	2569	rBV2	469	341	0.03%	0.003%
56	9.336	2572	2580	2583	rBV3	434	534	0.04%	0.005%
57	9.413	2601	2604	2606	rBV3	489	288	0.02%	0.003%
58	9.551	2640	2647	2654	rBV2	5178	7972	0.59%	0.072%
59	9.667	2678	2683	2684	rBV3	1079	721	0.05%	0.007%
60	9.709	2691	2696	2702	rVB7	1444	1726	0.13%	0.016%
61	9.731	2702	2703	2707	rVB2	395	199	0.01%	0.002%
62	9.751	2707	2709	2714	rVB3	795	477	0.04%	0.004%
63	9.805	2718	2726	2734	rBV5	1055	1866	0.14%	0.017%
64	9.850	2737	2740	2748	rVB3	941	988	0.07%	0.009%
65	9.940	2759	2768	2777	rVV3	2634	3417	0.25%	0.031%
66	10.014	2789	2791	2792	rBV2	379	201	0.01%	0.002%
67	10.046	2799	2801	2805	rBV2	387	273	0.02%	0.002%
68	10.082	2809	2812	2814	rBV	357	185	0.01%	0.002%
69	10.130	2817	2827	2836	rBV3	5626	9308	0.69%	0.085%
70	10.220	2843	2855	2873	rBV	406293	664223	48.92%	6.034%
71	10.432	2916	2921	2922	rBV2	625	516	0.04%	0.005%
72	10.545	2950	2956	2957	rBV4	1869	1658	0.12%	0.015%
73	10.722	3009	3011	3012	rBV4	476	221	0.02%	0.002%
74	10.815	3036	3040	3042	rBV3	392	350	0.03%	0.003%
75	10.879	3054	3060	3063	rBV5	1179	1332	0.10%	0.012%
76	10.921	3066	3073	3087	rVB4	9569	16186	1.19%	0.147%

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 ClientSampleId :
 C0AW9ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Peak Location: TOP

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Peak separation: 5

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

77	11.027	3100	3106	3108	rBV2	1088	954	0.07%	0.009%
78	11.149	3135	3144	3151	rBV8	3253	6032	0.44%	0.055%
79	11.252	3165	3176	3201	rBV	819301	1262489	92.98%	11.469%
80	11.535	3262	3264	3267	rBV	343	219	0.02%	0.002%
81	11.628	3281	3293	3312	rBV	731853	1177199	86.70%	10.694%
82	11.911	3378	3381	3383	rBV2	634	415	0.03%	0.004%
83	12.185	3465	3466	3470	rVB2	564	297	0.02%	0.003%
84	12.246	3482	3485	3486	rBV	552	378	0.03%	0.003%
85	12.329	3509	3511	3516	rBV3	418	314	0.02%	0.003%
86	12.558	3578	3582	3585	rBV3	375	342	0.03%	0.003%
87	12.596	3590	3594	3595	rBV3	759	597	0.04%	0.005%
88	12.654	3604	3612	3622	rVB6	3618	6061	0.45%	0.055%
89	12.847	3670	3672	3674	rBV	378	182	0.01%	0.002%
90	12.889	3680	3685	3695	rVB7	3049	4343	0.32%	0.039%
91	13.098	3747	3750	3751	rBV	501	230	0.02%	0.002%
92	13.220	3786	3788	3791	rVB	412	190	0.01%	0.002%
93	13.268	3794	3803	3812	rVV6	5556	8464	0.62%	0.077%
94	13.326	3818	3821	3828	rBV3	499	436	0.03%	0.004%
95	13.509	3871	3878	3887	rBV3	14887	22670	1.67%	0.206%
96	13.599	3904	3906	3909	rVB2	409	195	0.01%	0.002%
97	13.667	3925	3927	3929	rBV2	416	224	0.02%	0.002%
98	13.747	3946	3952	3962	rVB3	5529	7870	0.58%	0.071%
99	14.525	4191	4194	4197	rVB3	806	423	0.03%	0.004%
100	15.252	4414	4420	4427	rVB8	5193	7559	0.56%	0.069%

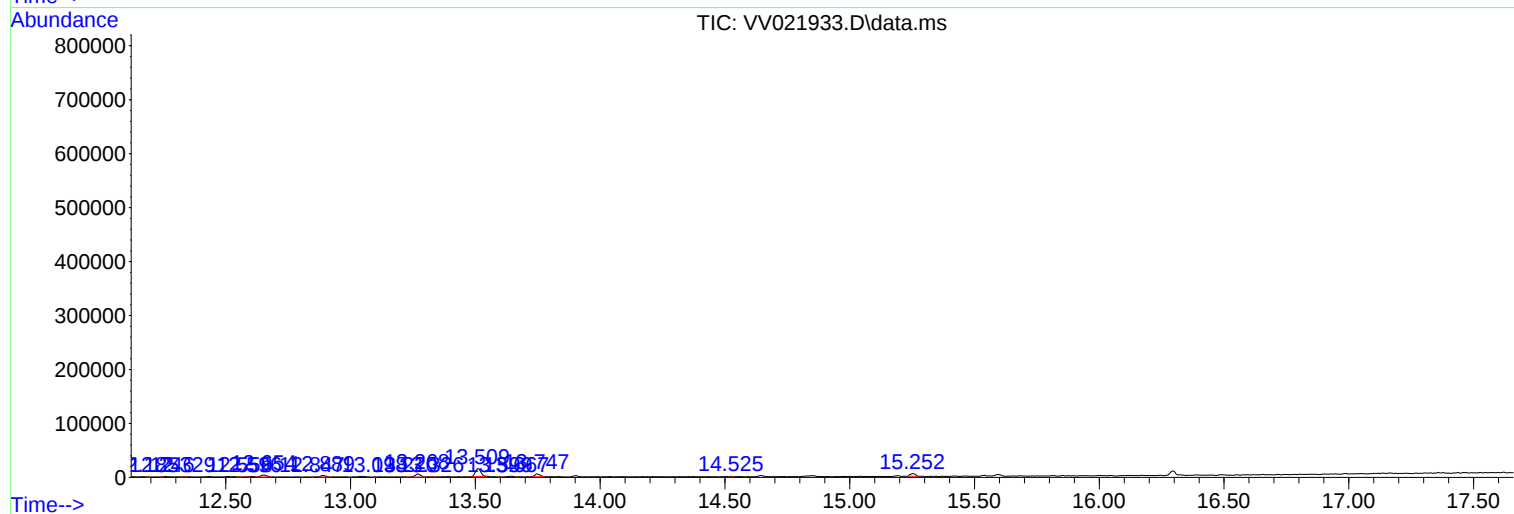
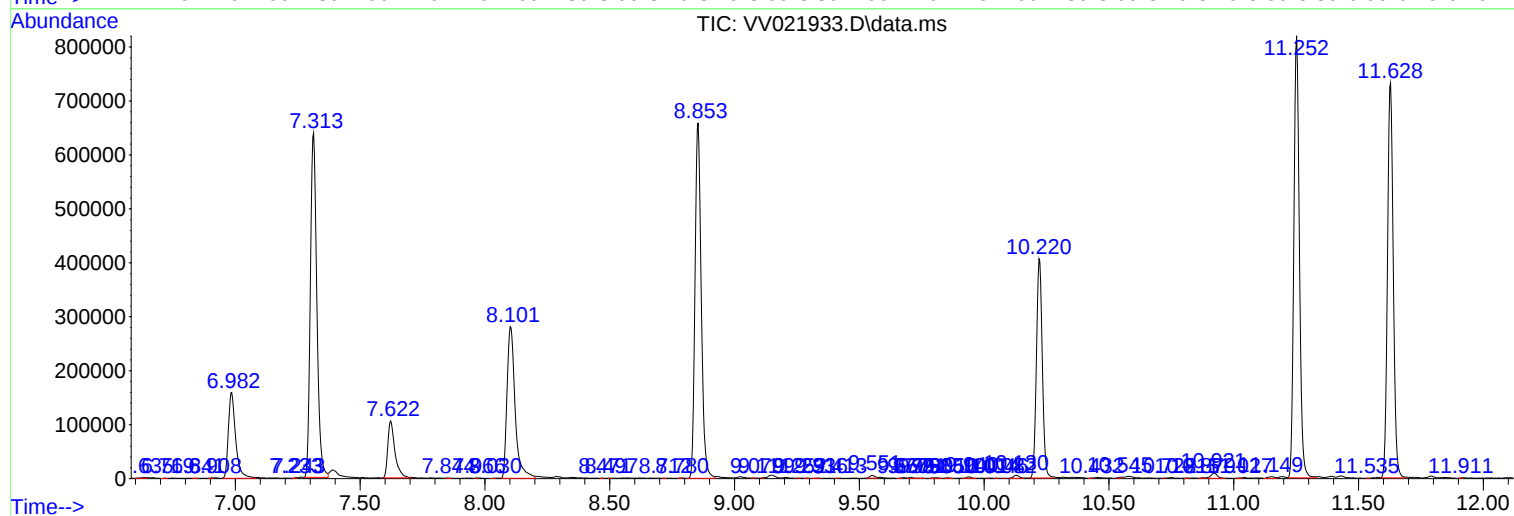
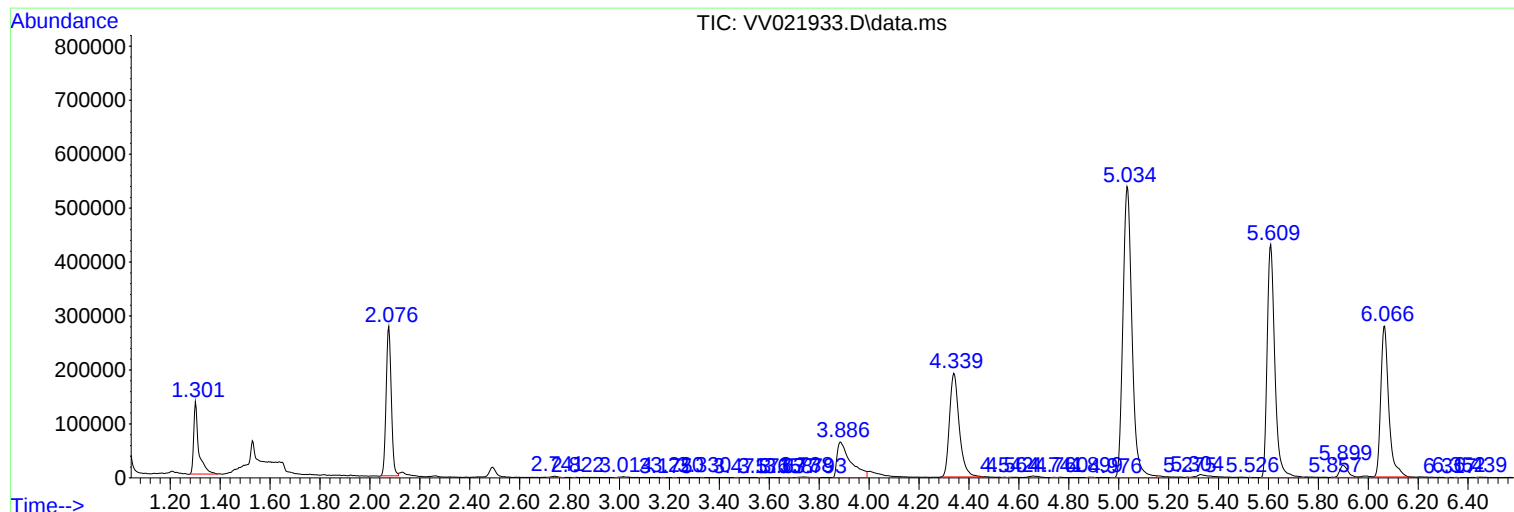
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Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082321\
Data File : VV021933.D
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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AW9ME

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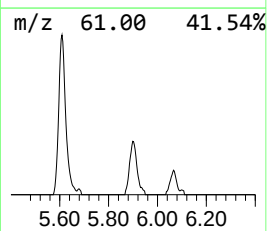
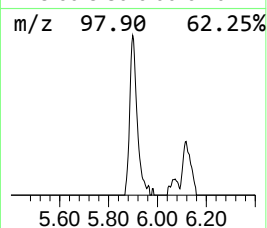
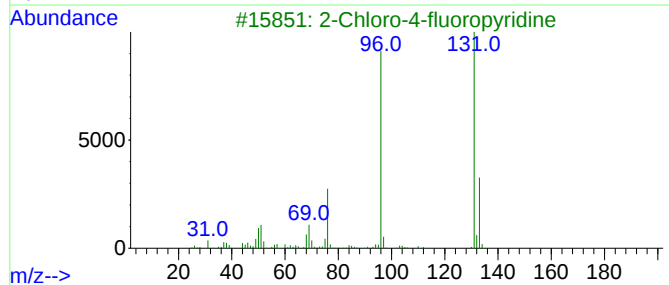
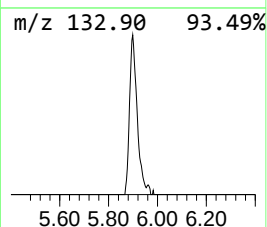
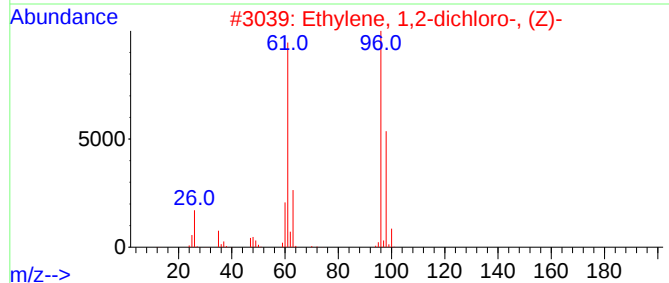
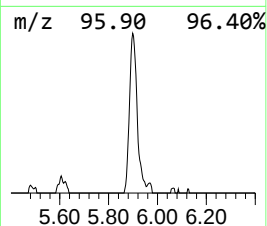
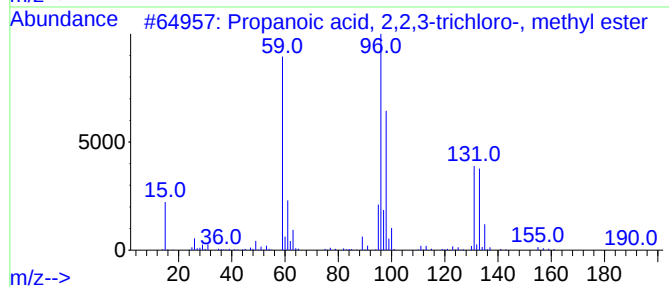
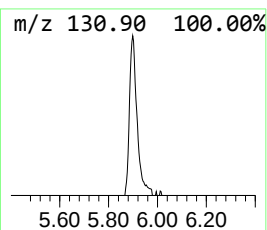
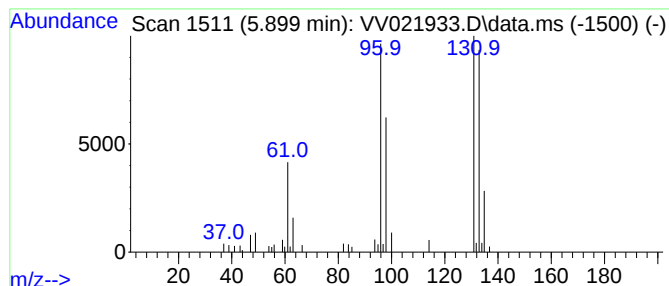
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.899	2.78 ug/L	51146	1,4-Difluorobenzene	5.609

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	56
2			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
3			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	32
4			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	25
5			6-Amino-1,2-dihydro-1,2,4,5-tetr...	131	C2H5N5S	1000435-40-1	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	5.899	2.8	ug/L	51146	1	5.609	921179	50.0