

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082621\
 Data File : VV021956.D
 Acq On : 26 Aug 2021 10:35
 Operator : SY/MD
 Sample : VV0826MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VBLK239

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: VV021956.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.304	76	82	100	rVB	163253	166977	12.00%	1.525%
2	1.564	156	163	174	rVB	144989	163416	11.74%	1.492%
3	2.104	322	331	346	rBV	280276	408949	29.38%	3.734%
4	2.510	449	457	470	rVB4	4197	7146	0.51%	0.065%
5	2.593	480	483	485	rBV	251	185	0.01%	0.002%
6	2.625	491	493	497	rBV	412	233	0.02%	0.002%
7	2.741	527	529	531	rBV2	236	132	0.01%	0.001%
8	2.760	531	535	538	rVV2	625	416	0.03%	0.004%
9	2.969	598	600	602	rBV	311	152	0.01%	0.001%
10	3.320	706	709	711	rBV	338	198	0.01%	0.002%
11	3.387	727	730	735	rVB2	267	197	0.01%	0.002%
12	3.510	766	768	771	rVB2	284	140	0.01%	0.001%
13	3.548	778	780	788	rVB2	320	202	0.01%	0.002%
14	3.606	795	798	800	rBV2	225	158	0.01%	0.001%
15	3.699	822	827	831	rBV3	277	290	0.02%	0.003%
16	3.760	843	846	852	rVB3	361	266	0.02%	0.002%
17	3.799	852	858	860	rBV	252	138	0.01%	0.001%
18	3.828	865	867	870	rVB	307	123	0.01%	0.001%
19	3.876	872	882	920	rBV	122901	321744	23.11%	2.938%
20	4.352	1013	1030	1064	rBV2	211681	545729	39.20%	4.983%
21	4.622	1111	1114	1115	rBV2	404	192	0.01%	0.002%
22	4.847	1181	1184	1185	rBV2	313	155	0.01%	0.001%
23	4.863	1187	1189	1196	rVB2	460	314	0.02%	0.003%
24	4.918	1203	1206	1207	rBV2	489	241	0.02%	0.002%
25	4.953	1212	1217	1219	rBV2	268	222	0.02%	0.002%
26	5.050	1229	1247	1279	rBV2	541767	1392047	100.00%	12.710%
27	5.436	1365	1367	1369	rVB	395	156	0.01%	0.001%
28	5.448	1369	1371	1373	rBV	442	215	0.02%	0.002%
29	5.497	1380	1386	1387	rBV3	470	449	0.03%	0.004%
30	5.535	1396	1398	1400	rVB3	397	128	0.01%	0.001%
31	5.619	1412	1424	1450	rBV	434180	875346	62.88%	7.992%
32	5.908	1503	1514	1539	rBV2	41157	86742	6.23%	0.792%
33	6.072	1550	1565	1595	rBV	307507	625125	44.91%	5.708%
34	6.371	1654	1658	1662	rVV3	451	451	0.03%	0.004%
35	6.413	1667	1671	1675	rVB3	588	468	0.03%	0.004%
36	6.452	1680	1683	1686	rVB2	376	194	0.01%	0.002%

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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

37	6.487	1692	1694	1698	rBV	199	156	0.01%	0.001%
38	6.558	1713	1716	1722	rBV4	384	333	0.02%	0.003%
39	6.616	1731	1734	1737	rBV2	319	190	0.01%	0.002%
40	6.667	1748	1750	1752	rBV2	572	288	0.02%	0.003%
41	6.722	1765	1767	1770	rVB2	278	193	0.01%	0.002%
42	6.773	1781	1783	1785	rBV2	273	115	0.01%	0.001%
43	6.853	1805	1808	1811	rBV	254	200	0.01%	0.002%
44	6.931	1827	1832	1834	rBV2	196	175	0.01%	0.002%
45	6.947	1834	1837	1839	rBV2	266	183	0.01%	0.002%
46	6.989	1839	1850	1872	rBV	175368	322554	23.17%	2.945%
47	7.201	1913	1916	1918	rBV2	462	319	0.02%	0.003%
48	7.320	1939	1953	1971	rBV	667320	1171359	84.15%	10.695%
49	7.625	2038	2048	2074	rBV	120431	213487	15.34%	1.949%
50	7.911	2135	2137	2141	rVB2	329	213	0.02%	0.002%
51	7.976	2155	2157	2161	rBV2	503	306	0.02%	0.003%
52	8.021	2169	2171	2173	rBV	216	125	0.01%	0.001%
53	8.046	2177	2179	2182	rBV2	184	144	0.01%	0.001%
54	8.091	2182	2193	2230	rBV2	340232	681432	48.95%	6.222%
55	8.387	2283	2285	2286	rBV	481	161	0.01%	0.001%
56	8.516	2321	2325	2327	rBV3	335	249	0.02%	0.002%
57	8.529	2327	2329	2332	rBV2	236	180	0.01%	0.002%
58	8.587	2345	2347	2348	rBV	247	132	0.01%	0.001%
59	8.805	2411	2415	2418	rBV3	292	260	0.02%	0.002%
60	8.853	2418	2430	2455	rBV	645595	1067706	76.70%	9.748%
61	9.066	2493	2496	2498	rBV2	284	199	0.01%	0.002%
62	9.088	2500	2503	2505	rBV2	452	222	0.02%	0.002%
63	9.117	2510	2512	2514	rVB3	375	165	0.01%	0.002%
64	9.136	2515	2518	2520	rBV4	646	416	0.03%	0.004%
65	9.194	2531	2536	2540	rBV2	560	455	0.03%	0.004%
66	9.332	2575	2579	2581	rBV	336	207	0.01%	0.002%
67	9.432	2606	2610	2612	rBV2	258	166	0.01%	0.002%
68	9.509	2632	2634	2639	rVB3	529	344	0.02%	0.003%
69	9.558	2645	2649	2651	rBV3	443	388	0.03%	0.004%
70	9.625	2667	2670	2674	rVB2	339	276	0.02%	0.003%
71	9.654	2674	2679	2681	rBV2	253	206	0.01%	0.002%
72	9.686	2684	2689	2692	rVV2	290	227	0.02%	0.002%
73	9.705	2694	2695	2698	rVB	360	145	0.01%	0.001%
74	9.750	2705	2709	2713	rBV2	206	163	0.01%	0.001%
75	9.857	2740	2742	2748	rVB3	304	262	0.02%	0.002%
76	9.940	2765	2768	2771	rVB	305	188	0.01%	0.002%

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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

77	9.998	2783	2786	2790	rVV2	346	286	0.02%	0.003%
78	10.027	2793	2795	2797	rVV2	295	146	0.01%	0.001%
79	10.056	2801	2804	2807	rBV2	232	198	0.01%	0.002%
80	10.130	2820	2827	2840	rVB3	3349	5919	0.43%	0.054%
81	10.175	2840	2841	2843	rBV	297	158	0.01%	0.001%
82	10.220	2843	2855	2875	rBV	393187	632711	45.45%	5.777%
83	10.419	2913	2917	2918	rBV2	280	140	0.01%	0.001%
84	10.496	2939	2941	2943	rBV2	254	117	0.01%	0.001%
85	10.750	3018	3020	3024	rBV	359	186	0.01%	0.002%
86	10.795	3032	3034	3035	rBV	288	121	0.01%	0.001%
87	10.869	3054	3057	3059	rBV2	472	281	0.02%	0.003%
88	11.069	3117	3119	3124	rVB2	230	143	0.01%	0.001%
89	11.149	3139	3144	3149	rBV5	1224	1409	0.10%	0.013%
90	11.252	3164	3176	3197	rBV	714426	1114731	80.08%	10.178%
91	11.532	3260	3263	3264	rBV2	356	195	0.01%	0.002%
92	11.625	3280	3292	3323	rBV	708642	1127000	80.96%	10.290%
93	12.094	3434	3438	3441	rBV3	634	542	0.04%	0.005%
94	12.217	3473	3476	3479	rVB3	450	256	0.02%	0.002%
95	12.403	3531	3534	3537	rVB	343	204	0.01%	0.002%
96	12.490	3559	3561	3565	rBV	304	148	0.01%	0.001%
97	12.593	3591	3593	3594	rBV	349	128	0.01%	0.001%
98	12.654	3608	3612	3619	rBV3	593	758	0.05%	0.007%
99	12.940	3699	3701	3704	rVB2	374	171	0.01%	0.002%
100	13.522	3874	3882	3890	rBV3	2275	3019	0.22%	0.028%

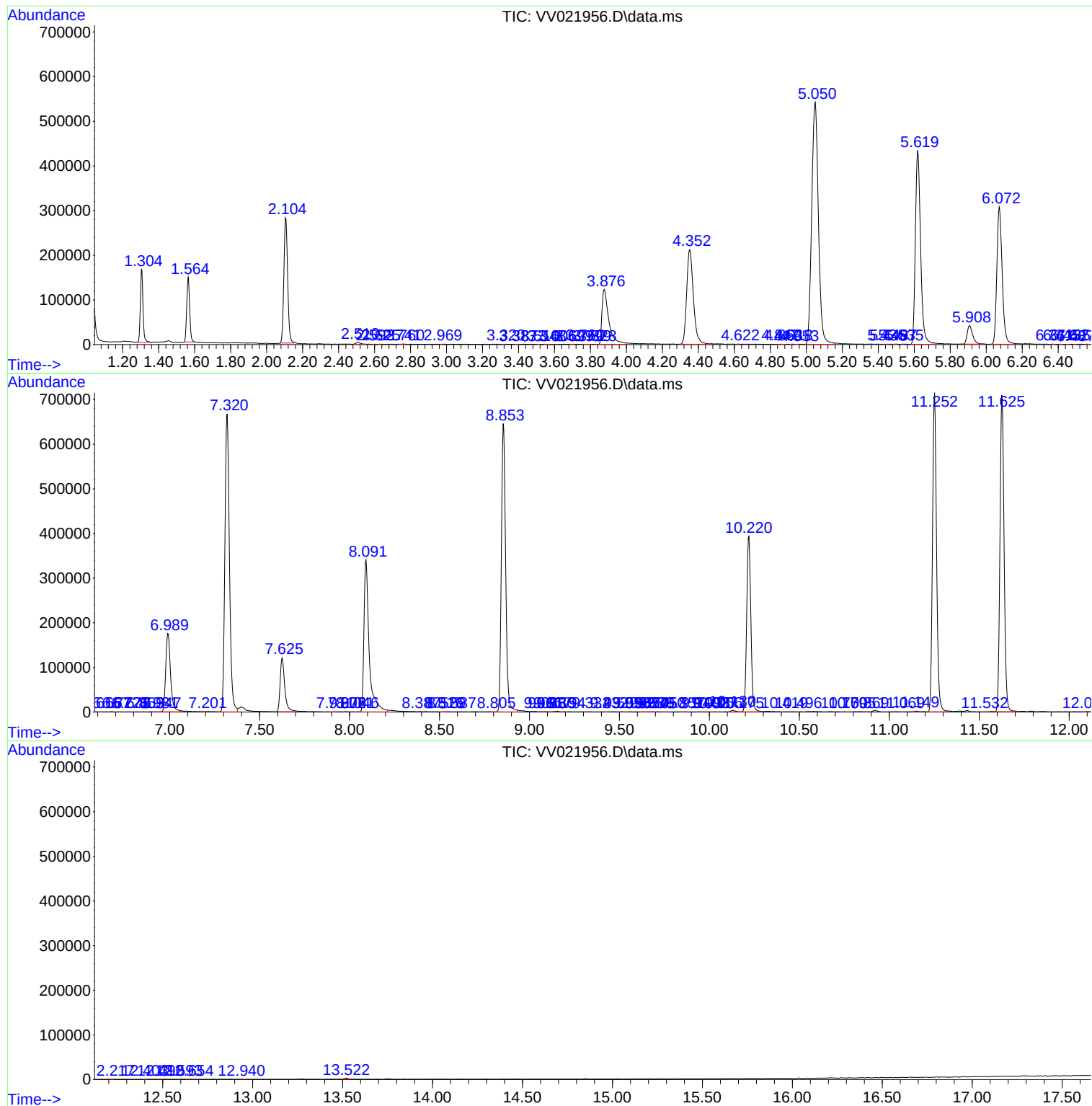
Sum of corrected areas: 10952692

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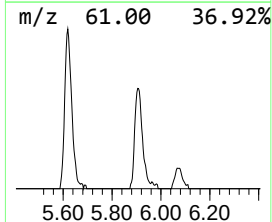
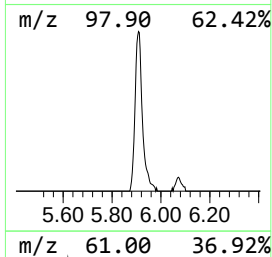
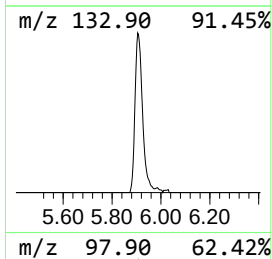
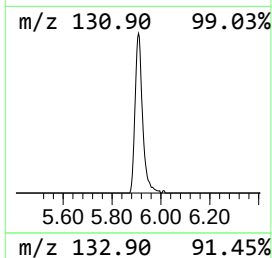
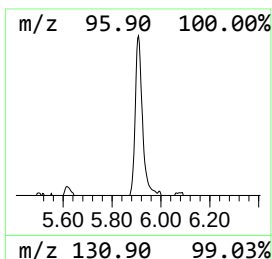
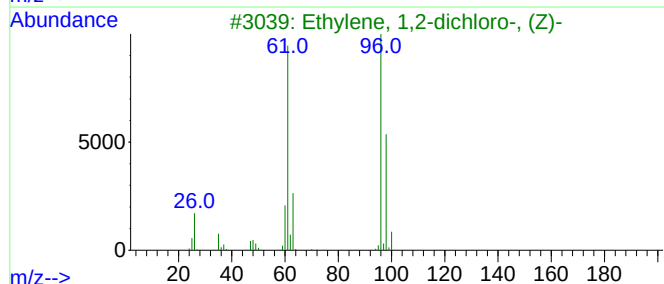
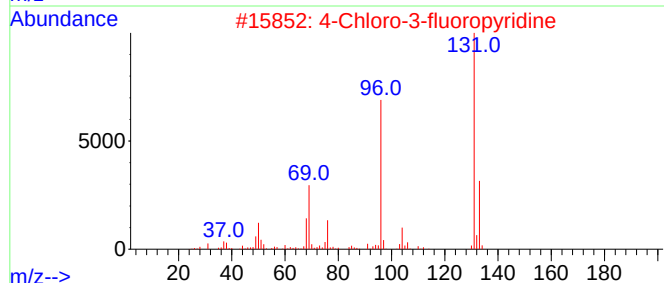
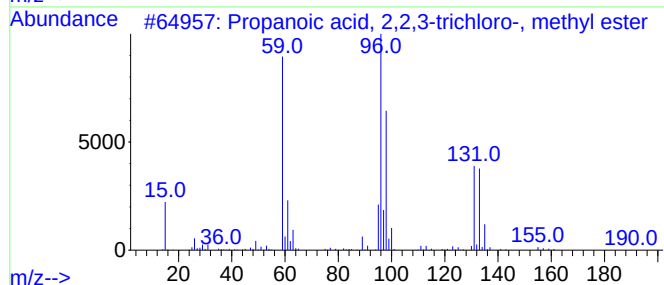
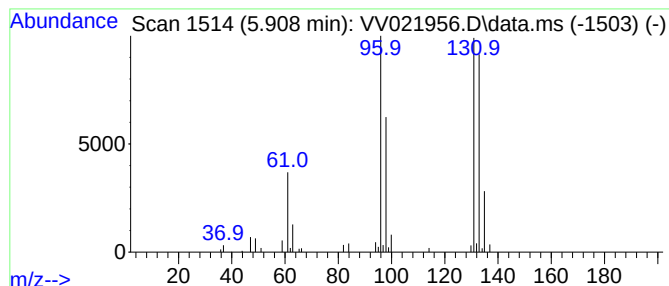
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.908	4.95 ug/L	86742	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	37
2			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	32
3			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	30
4			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	25
5			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	5.908	5.0	ug/L	86742	1	5.619	875346	50.0