

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082021\
 Data File : VV021910.D
 Acq On : 20 Aug 2021 13:23
 Operator : SY/MD
 Sample : M3458-01ME
 Misc : 6.50g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AB3ME

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: VV021910.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	104	rBV	114423	158137	11.54%	1.489%
2	2.073	312	321	334	rBV	265425	375664	27.42%	3.538%
3	2.490	445	451	469	rVB2	11983	21576	1.57%	0.203%
4	2.597	482	484	488	rBV3	504	359	0.03%	0.003%
5	2.770	536	538	542	rVB2	525	292	0.02%	0.003%
6	2.857	562	565	568	rBV	302	211	0.02%	0.002%
7	2.889	572	575	579	rBV2	346	298	0.02%	0.003%
8	2.912	579	582	585	rBV3	371	239	0.02%	0.002%
9	2.960	594	597	599	rBV2	390	231	0.02%	0.002%
10	3.150	650	656	658	rBV	297	249	0.02%	0.002%
11	3.166	658	661	668	rVB3	450	470	0.03%	0.004%
12	3.208	668	674	677	rBV3	365	329	0.02%	0.003%
13	3.259	686	690	694	rBV	431	436	0.03%	0.004%
14	3.343	714	716	723	rVB2	405	264	0.02%	0.002%
15	3.449	742	749	754	rBV2	306	372	0.03%	0.004%
16	3.526	770	773	775	rBV3	328	207	0.02%	0.002%
17	3.580	788	790	794	rBV	296	190	0.01%	0.002%
18	3.642	804	809	812	rBV2	438	299	0.02%	0.003%
19	3.815	861	863	868	rVB2	272	186	0.01%	0.002%
20	3.892	877	887	920	rBV2	75900	279324	20.39%	2.630%
21	4.346	1009	1028	1056	rBV	202756	534967	39.04%	5.038%
22	4.600	1104	1107	1109	rBV2	476	346	0.03%	0.003%
23	4.802	1164	1170	1172	rBV2	270	284	0.02%	0.003%
24	4.818	1172	1175	1180	rVV4	382	398	0.03%	0.004%
25	4.857	1184	1187	1190	rBV3	482	395	0.03%	0.004%
26	4.924	1204	1208	1210	rBV2	564	455	0.03%	0.004%
27	5.040	1227	1244	1285	rBV2	551844	1370155	100.00%	12.903%
28	5.613	1409	1422	1457	rVV	418447	891939	65.10%	8.399%
29	5.902	1500	1512	1532	rBV	27552	62561	4.57%	0.589%
30	6.069	1551	1564	1592	rBV	282034	613779	44.80%	5.780%
31	6.317	1636	1641	1644	rBV3	337	227	0.02%	0.002%
32	6.342	1647	1649	1651	rBV	378	242	0.02%	0.002%
33	6.381	1659	1661	1663	rBV	293	191	0.01%	0.002%
34	6.410	1667	1670	1671	rBV2	524	315	0.02%	0.003%
35	6.481	1689	1692	1694	rBV	376	200	0.01%	0.002%
36	6.638	1737	1741	1742	rBV2	682	508	0.04%	0.005%

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Integrator: RTE

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 Title : VOC Analysis

37	6.728	1766	1769	1772	rVB3	725	470	0.03%	0.004%
38	6.802	1789	1792	1796	rVV3	383	393	0.03%	0.004%
39	6.892	1818	1820	1823	rBV2	356	189	0.01%	0.002%
40	6.912	1823	1826	1831	rBV3	262	281	0.02%	0.003%

41	6.989	1837	1850	1875	rBV	152160	301951	22.04%	2.843%
42	7.207	1916	1918	1919	rBV2	488	223	0.02%	0.002%
43	7.262	1932	1935	1938	rBV3	544	401	0.03%	0.004%
44	7.317	1940	1952	1971	rBV	625577	1124739	82.09%	10.592%
45	7.625	2038	2048	2075	rBV2	101871	199526	14.56%	1.879%

46	7.770	2090	2093	2095	rBV	467	312	0.02%	0.003%
47	7.786	2095	2098	2101	rVV4	785	480	0.04%	0.005%
48	7.876	2121	2126	2128	rBV2	410	383	0.03%	0.004%
49	7.934	2143	2144	2147	rBV2	354	198	0.01%	0.002%
50	8.066	2183	2185	2186	rBV	492	182	0.01%	0.002%

51	8.108	2186	2198	2233	rVV2	268494	632488	46.16%	5.956%
52	8.368	2277	2279	2281	rBV	618	206	0.02%	0.002%
53	8.432	2297	2299	2302	rBV4	310	187	0.01%	0.002%
54	8.516	2322	2325	2332	rVB4	781	652	0.05%	0.006%
55	8.551	2332	2336	2337	rBV2	428	258	0.02%	0.002%

56	8.616	2355	2356	2360	rBV2	443	297	0.02%	0.003%
57	8.670	2369	2373	2374	rBV3	462	242	0.02%	0.002%
58	8.699	2381	2382	2385	rBV2	361	244	0.02%	0.002%
59	8.857	2418	2431	2456	rBV	611393	1080664	78.87%	10.176%
60	9.072	2496	2498	2500	rVB2	507	209	0.02%	0.002%

61	9.101	2503	2507	2508	rBV	412	201	0.01%	0.002%
62	9.146	2515	2521	2526	rBV5	1506	1843	0.13%	0.017%
63	9.284	2562	2564	2569	rVB	474	228	0.02%	0.002%
64	9.310	2569	2572	2575	rBV2	278	195	0.01%	0.002%
65	9.333	2575	2579	2582	rVB3	384	309	0.02%	0.003%

66	9.484	2623	2626	2628	rVV2	350	190	0.01%	0.002%
67	9.548	2644	2646	2648	rBV	552	305	0.02%	0.003%
68	9.683	2685	2688	2689	rVV2	336	185	0.01%	0.002%
69	9.712	2692	2697	2698	rBV2	425	350	0.03%	0.003%
70	9.786	2716	2720	2721	rBV2	419	203	0.01%	0.002%

71	9.805	2724	2726	2728	rVB	391	210	0.02%	0.002%
72	9.876	2745	2748	2751	rBV3	446	315	0.02%	0.003%
73	9.905	2755	2757	2761	rVB3	263	183	0.01%	0.002%
74	9.931	2761	2765	2767	rBV	265	228	0.02%	0.002%
75	10.024	2791	2794	2797	rBV2	403	215	0.02%	0.002%

76	10.127	2814	2826	2838	rVB6	3654	6385	0.47%	0.060%
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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M

Title : VOC Analysis

77	10.223	2844	2856	2881	rBV	426316	699683	51.07%	6.589%
78	10.490	2937	2939	2943	rVB4	678	411	0.03%	0.004%
79	10.551	2956	2958	2960	rBV2	460	247	0.02%	0.002%
80	10.815	3037	3040	3042	rBV2	352	295	0.02%	0.003%
81	10.876	3057	3059	3064	rBV4	517	576	0.04%	0.005%
82	10.921	3067	3073	3086	rVB7	3533	6292	0.46%	0.059%
83	11.027	3102	3106	3109	rBV3	749	682	0.05%	0.006%
84	11.143	3136	3142	3152	rBV4	1873	2870	0.21%	0.027%
85	11.252	3164	3176	3200	rBV	712069	1108185	80.88%	10.436%
86	11.628	3281	3293	3313	rBV	705211	1112091	81.17%	10.472%
87	11.853	3354	3363	3364	rBV5	1171	1354	0.10%	0.013%
88	12.252	3479	3487	3489	rBV3	1159	1297	0.09%	0.012%
89	12.304	3501	3503	3507	rBV3	365	249	0.02%	0.002%
90	12.519	3568	3570	3574	rVB2	541	238	0.02%	0.002%
91	12.706	3626	3628	3632	rVV	424	290	0.02%	0.003%
92	12.796	3651	3656	3658	rBV2	569	403	0.03%	0.004%
93	12.886	3681	3684	3685	rBV2	781	479	0.03%	0.005%
94	13.226	3787	3790	3795	rBV2	382	287	0.02%	0.003%
95	13.419	3847	3850	3852	rBV3	435	251	0.02%	0.002%
96	13.480	3867	3869	3871	rBV2	475	212	0.02%	0.002%
97	13.516	3871	3880	3892	rBV3	2905	5547	0.40%	0.052%
98	13.587	3897	3902	3904	rBV2	396	399	0.03%	0.004%
99	14.336	4133	4135	4137	rBV	387	187	0.01%	0.002%
100	14.397	4148	4154	4161	rVB5	3076	3677	0.27%	0.035%

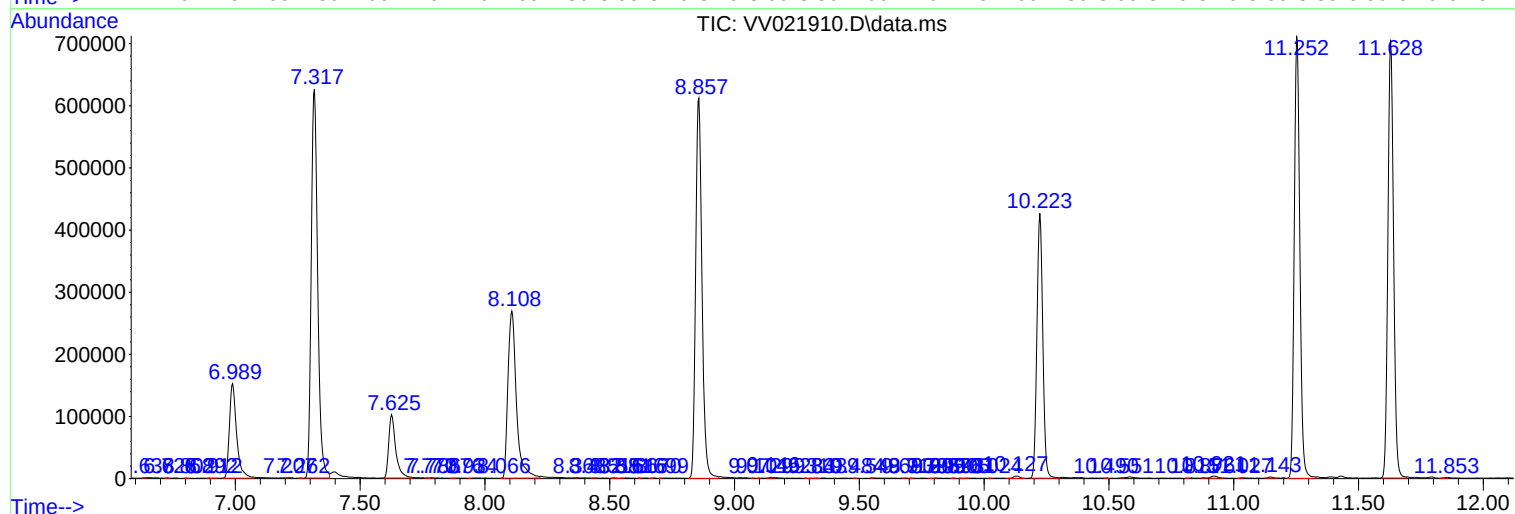
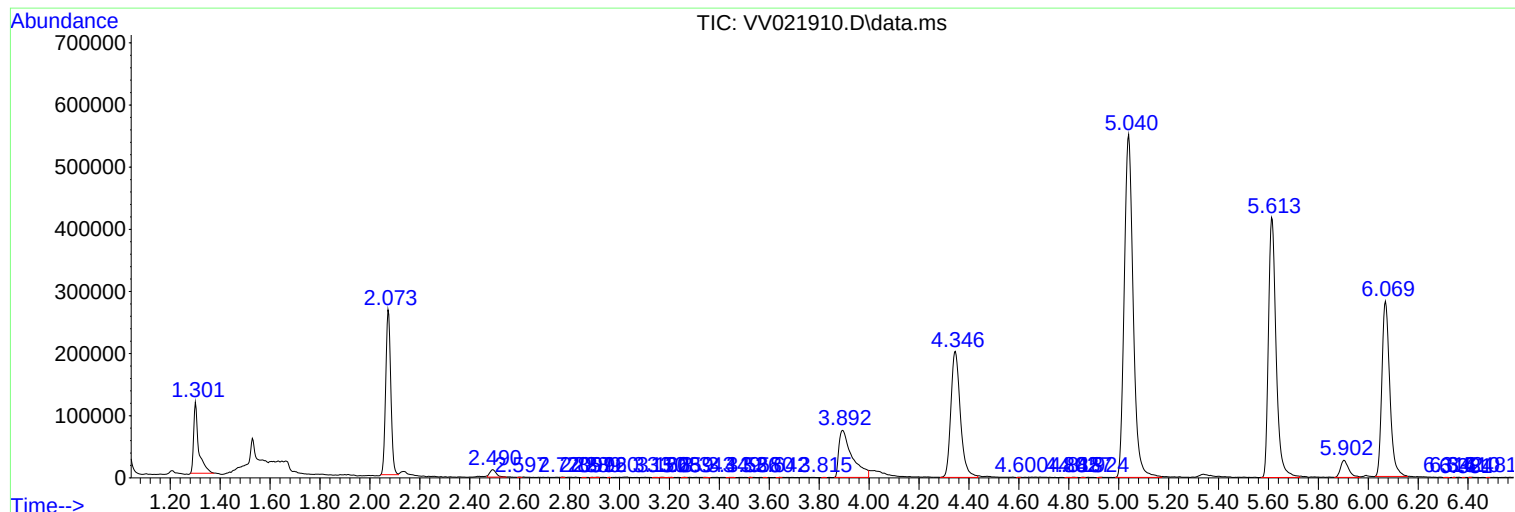
Sum of corrected areas: 10619217

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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AB3ME

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 :
MSVOA_V
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C0AB3ME

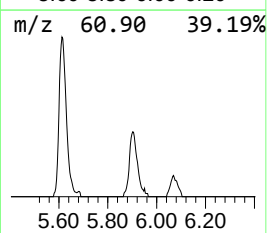
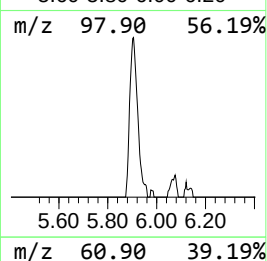
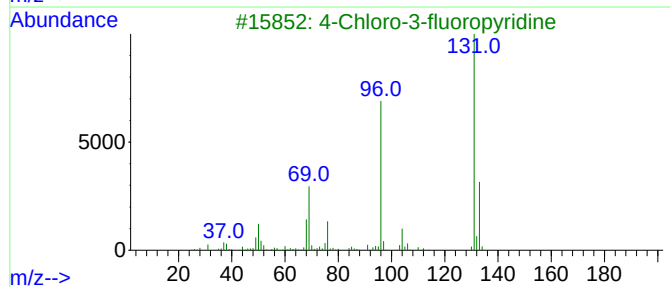
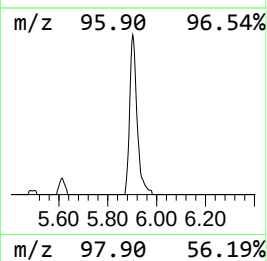
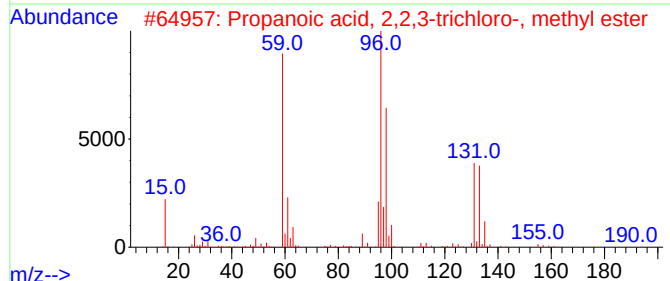
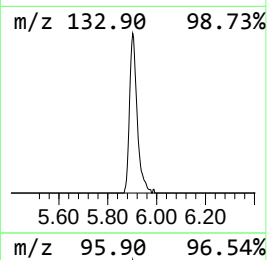
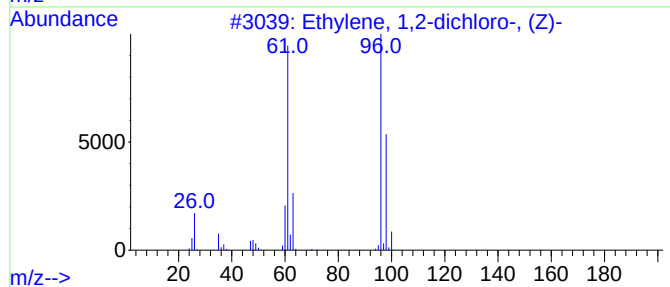
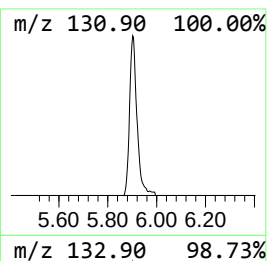
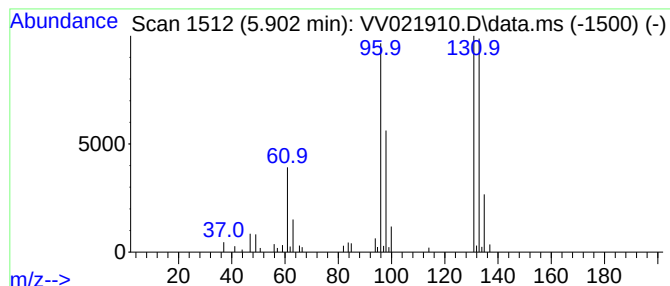
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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.
5.902	3.51 ug/L	62561	1,4-Difluorobenzene	5.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
2			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	36
3			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	32
4			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	25
5			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	23



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	5.902	3.5	ug/L	62561	1	5.613	891939	50.0