

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072021\
 Data File : VV021686.D
 Acq On : 20 Jul 2021 10:42
 Operator : SY/MD
 Sample : VV0720MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VBLK218

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\SFAMVLM071921WMA.M
 Title : VOC Analysis

Signal : TIC: VV021686.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	95	rVB	243225	245366	14.17%	1.874%
2	1.564	156	163	177	rVB	192945	212744	12.29%	1.625%
3	2.105	322	331	357	rVB	391216	584500	33.75%	4.464%
4	2.506	449	456	468	rVB2	10663	18167	1.05%	0.139%
5	2.551	468	470	472	rBV2	324	147	0.01%	0.001%
6	2.661	501	504	507	rBV4	618	357	0.02%	0.003%
7	2.741	527	529	530	rBV	367	156	0.01%	0.001%
8	2.902	577	579	581	rBV	273	103	0.01%	0.001%
9	2.931	585	588	590	rBV	354	208	0.01%	0.002%
10	3.059	626	628	629	rBV	356	177	0.01%	0.001%
11	3.114	644	645	647	rBV	302	134	0.01%	0.001%
12	3.259	687	690	695	rVB2	319	211	0.01%	0.002%
13	3.281	695	697	699	rBV	299	139	0.01%	0.001%
14	3.320	705	709	712	rBV	211	171	0.01%	0.001%
15	3.365	720	723	729	rVB	324	242	0.01%	0.002%
16	3.394	730	732	735	rVV2	200	153	0.01%	0.001%
17	3.423	739	741	746	rBV2	363	175	0.01%	0.001%
18	3.487	759	761	764	rBB2	266	97	0.01%	0.001%
19	3.613	798	800	802	rBV2	180	68	0.00%	0.001%
20	3.661	811	815	817	rBV2	502	377	0.02%	0.003%
21	3.709	828	830	831	rBV	305	95	0.01%	0.001%
22	3.744	837	841	844	rBV2	321	264	0.02%	0.002%
23	3.831	865	868	870	rBV	289	151	0.01%	0.001%
24	3.873	871	881	923	rBV	137277	381696	22.04%	2.915%
25	4.346	1012	1028	1062	rBV	268781	669158	38.64%	5.111%
26	4.715	1142	1143	1148	rVB2	435	233	0.01%	0.002%
27	4.818	1174	1175	1184	rVB3	514	561	0.03%	0.004%
28	4.870	1184	1191	1194	rBV3	654	554	0.03%	0.004%
29	4.960	1215	1219	1221	rBV	238	181	0.01%	0.001%
30	5.043	1227	1245	1278	rBV2	669818	1731672	100.00%	13.225%
31	5.394	1352	1354	1356	rBV2	726	340	0.02%	0.003%
32	5.452	1371	1372	1374	rBV	223	73	0.00%	0.001%
33	5.465	1374	1376	1378	rBV3	475	215	0.01%	0.002%
34	5.506	1387	1389	1391	rVB3	385	110	0.01%	0.001%
35	5.516	1391	1392	1393	rBV3	319	73	0.00%	0.001%
36	5.616	1410	1423	1458	rBV	497973	1005783	58.08%	7.682%

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 Title : VOC Analysis

37	5.905	1501	1513	1528	rBV2	31475	66647	3.85%	0.509%
38	6.069	1549	1564	1591	rBV	376426	771466	44.55%	5.892%
39	6.304	1635	1637	1639	rVB	415	153	0.01%	0.001%
40	6.362	1654	1655	1658	rVB3	336	153	0.01%	0.001%
41	6.381	1658	1661	1662	rBV2	366	206	0.01%	0.002%
42	6.391	1662	1664	1668	rVB	497	260	0.02%	0.002%
43	6.407	1668	1669	1670	rBV	197	70	0.00%	0.001%
44	6.442	1677	1680	1685	rVB2	449	298	0.02%	0.002%
45	6.506	1694	1700	1703	rBV2	771	843	0.05%	0.006%
46	6.638	1733	1741	1745	rBV5	1327	2078	0.12%	0.016%
47	6.741	1771	1773	1774	rBV	294	127	0.01%	0.001%
48	6.789	1784	1788	1792	rBV2	394	362	0.02%	0.003%
49	6.815	1795	1796	1802	rVB2	262	171	0.01%	0.001%
50	6.940	1833	1835	1837	rBV	179	68	0.00%	0.001%
51	6.985	1837	1849	1870	rBV	228997	413406	23.87%	3.157%
52	7.317	1940	1952	1969	rBV	819139	1431259	82.65%	10.931%
53	7.622	2036	2047	2072	rBV	154565	270644	15.63%	2.067%
54	7.895	2130	2132	2133	rBV	354	154	0.01%	0.001%
55	7.927	2140	2142	2144	rVB2	271	91	0.01%	0.001%
56	7.956	2149	2151	2153	rBV2	343	169	0.01%	0.001%
57	8.034	2170	2175	2180	rVB5	694	758	0.04%	0.006%
58	8.088	2180	2192	2232	rBV	419257	833183	48.11%	6.363%
59	8.526	2326	2328	2329	rBV	264	105	0.01%	0.001%
60	8.680	2373	2376	2378	rBV2	438	262	0.02%	0.002%
61	8.709	2382	2385	2387	rBV	268	201	0.01%	0.002%
62	8.796	2409	2412	2414	rBV2	335	159	0.01%	0.001%
63	8.812	2415	2417	2418	rBV	332	131	0.01%	0.001%
64	8.853	2418	2430	2456	rBV	716507	1188029	68.61%	9.073%
65	9.021	2478	2482	2488	rVB5	1597	1662	0.10%	0.013%
66	9.149	2515	2522	2533	rVV8	2292	3815	0.22%	0.029%
67	9.194	2534	2536	2541	rVB2	529	327	0.02%	0.002%
68	9.236	2547	2549	2552	rBV2	355	195	0.01%	0.001%
69	9.300	2567	2569	2573	rVB2	333	193	0.01%	0.001%
70	9.326	2573	2577	2580	rBV	339	313	0.02%	0.002%
71	9.429	2607	2609	2614	rVB2	383	245	0.01%	0.002%
72	9.458	2614	2618	2622	rBV2	264	243	0.01%	0.002%
73	9.484	2624	2626	2629	rVV2	140	38	0.00%	0.000%
74	9.635	2671	2673	2677	rVB2	259	127	0.01%	0.001%
75	9.760	2709	2712	2714	rBV	203	148	0.01%	0.001%
76	9.805	2722	2726	2727	rBV2	259	162	0.01%	0.001%

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 Title : VOC Analysis

77	9.850	2738	2740	2745	rVB	517	293	0.02%	0.002%
78	9.870	2745	2746	2747	rBV	126	29	0.00%	0.000%
79	9.937	2761	2767	2777	rVB6	1699	2103	0.12%	0.016%
80	10.050	2801	2802	2806	rVB3	333	174	0.01%	0.001%
81	10.130	2818	2827	2841	rVB2	5349	9326	0.54%	0.071%
82	10.217	2842	2854	2879	rBV	481971	756967	43.71%	5.781%
83	10.667	2987	2994	2997	rVB3	1008	1124	0.06%	0.009%
84	10.879	3058	3060	3062	rBV2	481	212	0.01%	0.002%
85	10.921	3063	3073	3086	rVB5	6660	11225	0.65%	0.086%
86	11.040	3103	3110	3112	rBV4	1063	1313	0.08%	0.010%
87	11.146	3135	3143	3151	rBV5	2537	4084	0.24%	0.031%
88	11.249	3164	3175	3195	rBV	748883	1170272	67.58%	8.938%
89	11.480	3245	3247	3250	rVB2	888	412	0.02%	0.003%
90	11.496	3250	3252	3254	rBV	448	139	0.01%	0.001%
91	11.551	3263	3269	3270	rBV4	510	479	0.03%	0.004%
92	11.625	3279	3292	3315	rBV	779100	1256529	72.56%	9.597%
93	11.773	3335	3338	3339	rBV2	967	525	0.03%	0.004%
94	11.837	3355	3358	3359	rBV2	944	462	0.03%	0.004%
95	12.291	3497	3499	3500	rBV	441	203	0.01%	0.002%
96	12.329	3507	3511	3515	rBV2	515	418	0.02%	0.003%
97	12.654	3605	3612	3620	rBV4	2987	5120	0.30%	0.039%
98	13.271	3797	3804	3814	rVB4	4390	6847	0.40%	0.052%
99	13.512	3871	3879	3888	rBV3	9045	13891	0.80%	0.106%
100	13.750	3947	3953	3964	rVB4	5413	7654	0.44%	0.058%

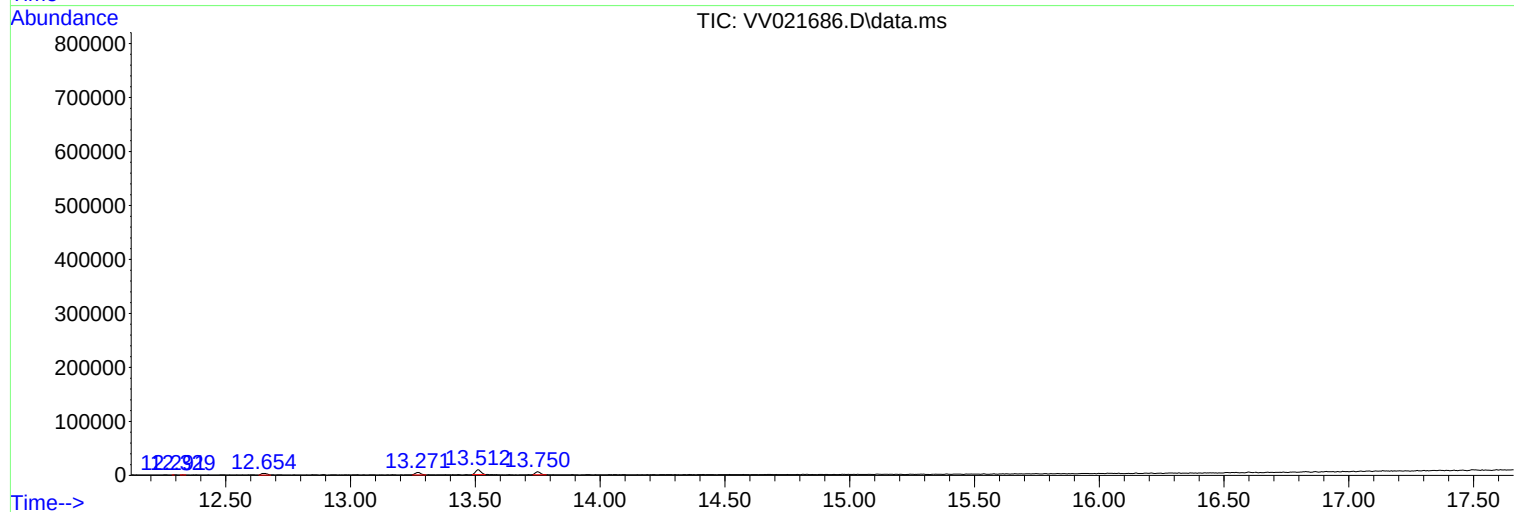
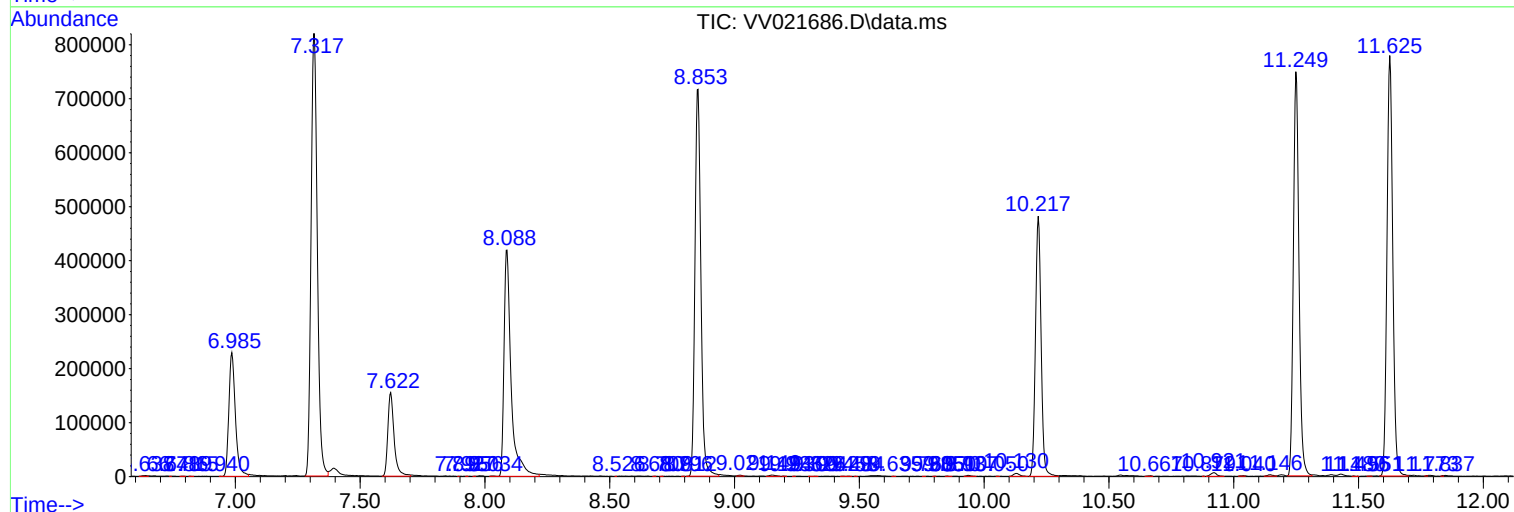
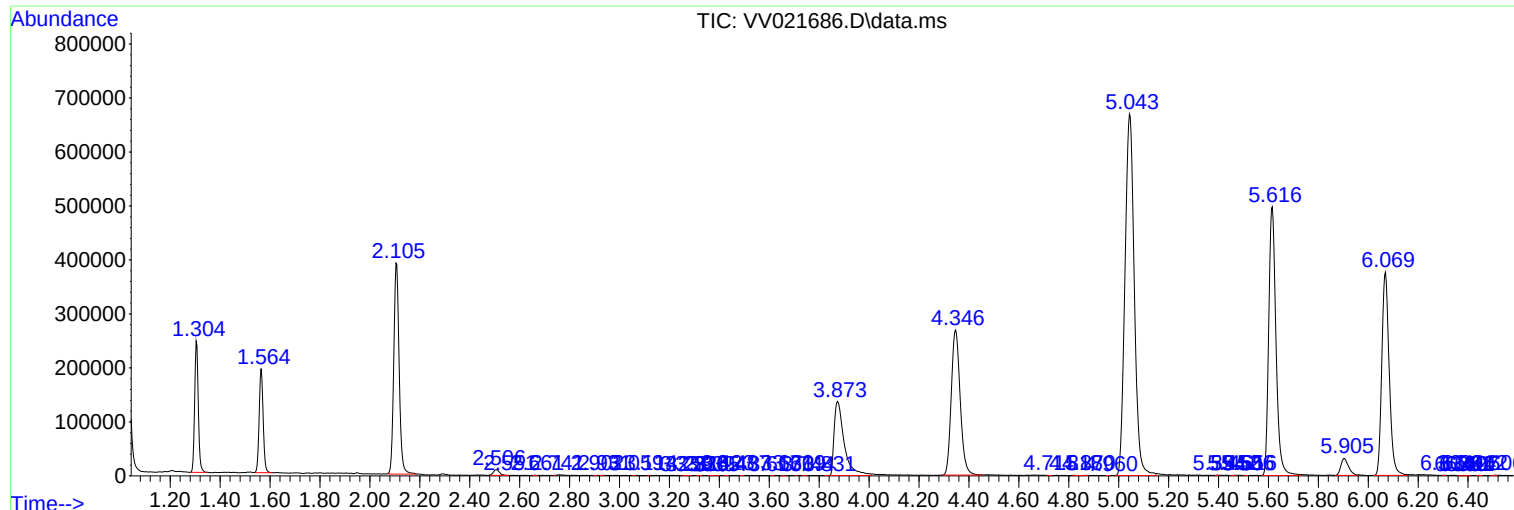
Sum of corrected areas: 13093573

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Instrument :
MSVOA_V
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM071921WMA.M
Quant Title : VOC Analysis

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



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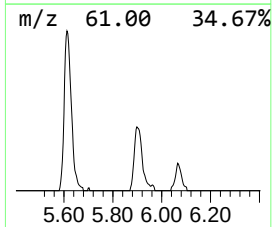
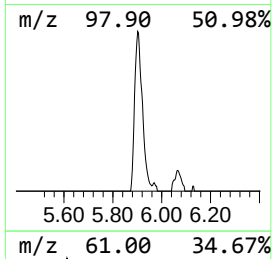
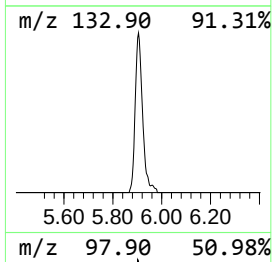
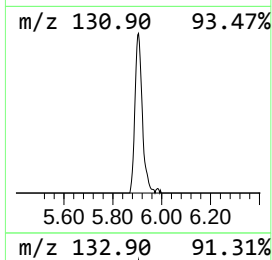
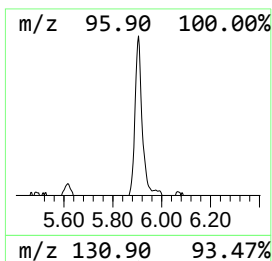
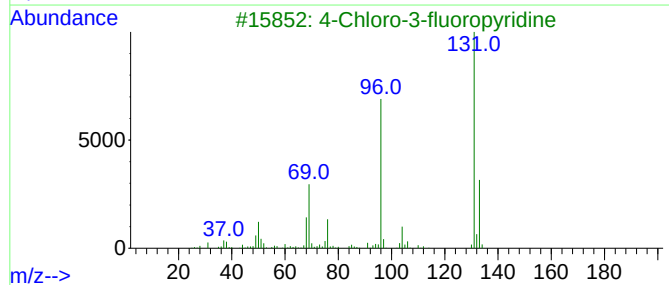
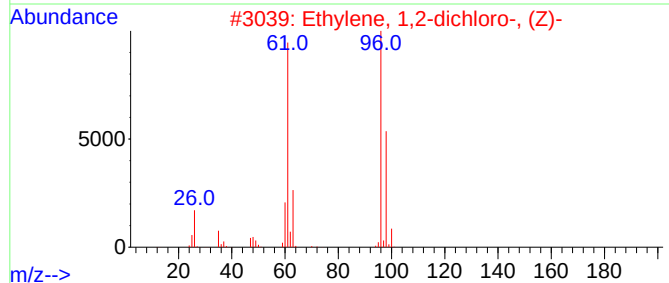
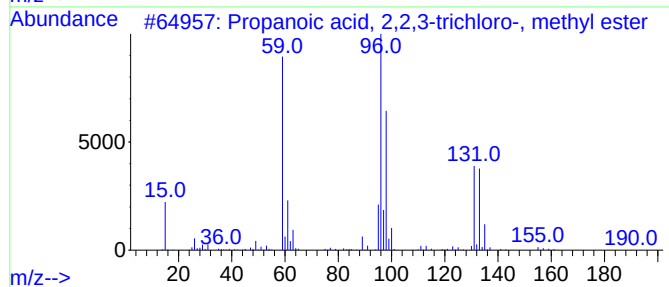
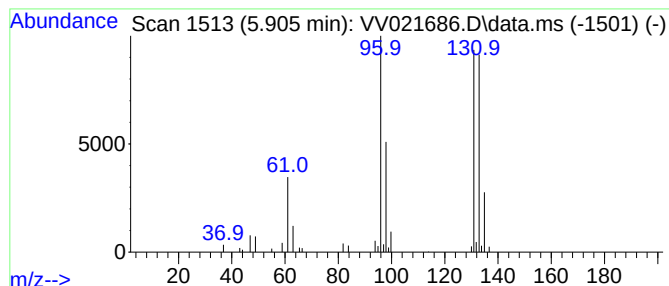
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM071921WMA.M
Quant Title : VOC Analysis

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.
5.905	3.31 ug/L	66647	1,4-Difluorobenzene	5.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	37
2			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	30
3			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	27
4			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	25
5			2-Chloro-5-methylthiazole	133	C4H4ClNS	033342-65-3	16



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	5.905	3.3	ug/L	66647	1	5.616	1005780	50.0