

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\V090121\
 Data File : VV022065.D
 Acq On : 01 Sep 2021 14:24
 Operator : SY/MD
 Sample : M3579-13MEDL 5X
 Misc : 6.76g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 GB6B5MEDL

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\SFAMVLM082721WMA.M
 Title : VOC Analysis

Signal : TIC: VV022065.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	75	82	100	rBV	181512	194398	15.39%	1.750%
2	1.539	149	155	175	rVB	136516	162064	12.83%	1.459%
3	2.098	319	329	344	rBV	314341	461142	36.51%	4.151%
4	2.378	414	416	421	rVB2	518	333	0.03%	0.003%
5	2.410	421	426	429	rBV2	727	569	0.05%	0.005%
6	2.432	429	433	436	rBV3	733	759	0.06%	0.007%
7	2.503	445	455	467	rVB3	9127	14699	1.16%	0.132%
8	2.616	478	490	507	rBV	11073	24588	1.95%	0.221%
9	2.966	596	599	603	rBV2	352	355	0.03%	0.003%
10	3.050	623	625	627	rBV	252	124	0.01%	0.001%
11	3.088	634	637	638	rBV	234	111	0.01%	0.001%
12	3.149	652	656	658	rBV	355	231	0.02%	0.002%
13	3.355	718	720	724	rVB	238	130	0.01%	0.001%
14	3.397	730	733	737	rVB2	399	279	0.02%	0.003%
15	3.503	763	766	768	rBV2	286	207	0.02%	0.002%
16	3.590	790	793	796	rVB	268	163	0.01%	0.001%
17	3.638	806	808	809	rBV	271	89	0.01%	0.001%
18	3.776	847	851	852	rVB3	246	118	0.01%	0.001%
19	3.876	872	882	921	rBV	105245	296126	23.44%	2.666%
20	4.346	1013	1028	1058	rBV	195470	490161	38.81%	4.412%
21	4.870	1187	1191	1193	rBV	350	236	0.02%	0.002%
22	4.956	1215	1218	1219	rBV	215	118	0.01%	0.001%
23	5.043	1227	1245	1274	rBV2	502455	1263071	100.00%	11.370%
24	5.436	1365	1367	1371	rVB2	259	119	0.01%	0.001%
25	5.522	1392	1394	1396	rVB2	421	150	0.01%	0.001%
26	5.571	1405	1409	1410	rBV	380	222	0.02%	0.002%
27	5.616	1411	1423	1457	rVV	414017	832486	65.91%	7.494%
28	5.911	1502	1515	1533	rBV7	19120	45237	3.58%	0.407%
29	6.069	1550	1564	1588	rBV	272006	560974	44.41%	5.050%
30	6.278	1625	1629	1632	rBV4	498	350	0.03%	0.003%
31	6.329	1639	1645	1647	rBV3	521	556	0.04%	0.005%
32	6.394	1662	1665	1669	rBV	418	386	0.03%	0.003%
33	6.429	1673	1676	1679	rVB2	399	267	0.02%	0.002%
34	6.587	1722	1725	1729	rVB3	461	361	0.03%	0.003%
35	6.632	1735	1739	1740	rBV3	281	190	0.02%	0.002%
36	6.657	1745	1747	1749	rBV2	240	152	0.01%	0.001%

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 Title : VOC Analysis

37	6.728	1766	1769	1770	rBV	147	93	0.01%	0.001%
38	6.802	1790	1792	1793	rBV	284	123	0.01%	0.001%
39	6.873	1812	1814	1817	rVB2	276	119	0.01%	0.001%
40	6.898	1817	1822	1824	rBV2	197	152	0.01%	0.001%
41	6.911	1824	1826	1830	rBV2	142	97	0.01%	0.001%
42	6.934	1830	1833	1836	rVB2	334	214	0.02%	0.002%
43	6.989	1837	1850	1870	rBV	145103	267689	21.19%	2.410%
44	7.316	1940	1952	1970	rBV	602285	1036515	82.06%	9.330%
45	7.622	2038	2047	2071	rBV	98789	170066	13.46%	1.531%
46	7.818	2105	2108	2112	rVB3	555	323	0.03%	0.003%
47	7.841	2112	2115	2119	rBV	264	232	0.02%	0.002%
48	7.931	2141	2143	2144	rBV	246	100	0.01%	0.001%
49	7.976	2144	2157	2179	rVV	619292	1041382	82.45%	9.374%
50	8.091	2183	2193	2228	rVV	327309	609417	48.25%	5.486%
51	8.615	2354	2356	2360	rVB2	397	196	0.02%	0.002%
52	8.673	2372	2374	2376	rBV2	311	133	0.01%	0.001%
53	8.709	2382	2385	2387	rBV2	331	171	0.01%	0.002%
54	8.763	2396	2402	2414	rVB3	390	696	0.06%	0.006%
55	8.853	2418	2430	2450	rBV	613576	986339	78.09%	8.879%
56	9.008	2475	2478	2479	rBV2	536	317	0.03%	0.003%
57	9.053	2489	2492	2494	rBV2	306	203	0.02%	0.002%
58	9.233	2546	2548	2551	rVB2	255	124	0.01%	0.001%
59	9.255	2552	2555	2557	rBV3	433	239	0.02%	0.002%
60	9.310	2570	2572	2573	rVB	265	86	0.01%	0.001%
61	9.326	2573	2577	2579	rBV	352	191	0.02%	0.002%
62	9.355	2583	2586	2590	rVV3	396	342	0.03%	0.003%
63	9.390	2594	2597	2603	rVB	6676	4012	0.32%	0.036%
64	9.458	2616	2618	2623	rVB3	467	356	0.03%	0.003%
65	9.484	2624	2626	2630	rVB2	252	128	0.01%	0.001%
66	9.506	2630	2633	2636	rBV2	232	192	0.02%	0.002%
67	9.558	2647	2649	2651	rBV	386	205	0.02%	0.002%
68	9.586	2656	2658	2661	rBV	290	132	0.01%	0.001%
69	9.606	2661	2664	2666	rBV	266	121	0.01%	0.001%
70	9.914	2758	2760	2763	rBV	212	158	0.01%	0.001%
71	10.133	2819	2828	2839	rVB4	2997	5262	0.42%	0.047%
72	10.220	2842	2855	2875	rBV	381905	603724	47.80%	5.435%
73	10.467	2929	2932	2938	rVB3	425	401	0.03%	0.004%
74	10.580	2961	2967	2973	rBV4	1365	1770	0.14%	0.016%
75	10.648	2986	2988	2990	rBV2	369	181	0.01%	0.002%
76	10.664	2990	2993	2997	rVB3	508	385	0.03%	0.003%

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Title : VOC Analysis

77	10.770	3021	3026	3027	rBV2	266	221	0.02%	0.002%
78	10.795	3032	3034	3037	rBV2	324	227	0.02%	0.002%
79	10.879	3058	3060	3062	rBV	467	173	0.01%	0.002%
80	10.966	3085	3087	3092	rVB3	446	224	0.02%	0.002%
81	11.030	3103	3107	3109	rBV2	437	366	0.03%	0.003%
82	11.043	3109	3111	3113	rVB2	485	232	0.02%	0.002%
83	11.078	3120	3122	3125	rVB	275	102	0.01%	0.001%
84	11.152	3137	3145	3153	rBV5	1453	2384	0.19%	0.021%
85	11.197	3158	3159	3164	rVB3	478	211	0.02%	0.002%
86	11.252	3164	3176	3193	rBV	638714	995403	78.81%	8.960%
87	11.503	3251	3254	3257	rBV2	483	446	0.04%	0.004%
88	11.532	3258	3263	3271	rVB5	2160	3148	0.25%	0.028%
89	11.628	3280	3293	3311	rBV	614170	974612	77.16%	8.773%
90	11.889	3373	3374	3376	rBV	473	193	0.02%	0.002%
91	12.213	3472	3475	3477	rVB2	412	183	0.01%	0.002%
92	12.255	3484	3488	3491	rVB3	262	218	0.02%	0.002%
93	12.548	3575	3579	3581	rBV	304	194	0.02%	0.002%
94	12.596	3588	3594	3595	rBV3	860	625	0.05%	0.006%
95	12.644	3607	3609	3611	rBV2	363	160	0.01%	0.001%
96	13.509	3868	3878	3897	rBV	21232	37764	2.99%	0.340%
97	13.731	3943	3947	3949	rBV3	392	335	0.03%	0.003%
98	13.901	3997	4000	4002	rBV2	535	249	0.02%	0.002%
99	14.544	4197	4200	4201	rBV2	509	255	0.02%	0.002%
100	14.824	4279	4287	4296	rBV3	4204	7020	0.56%	0.063%

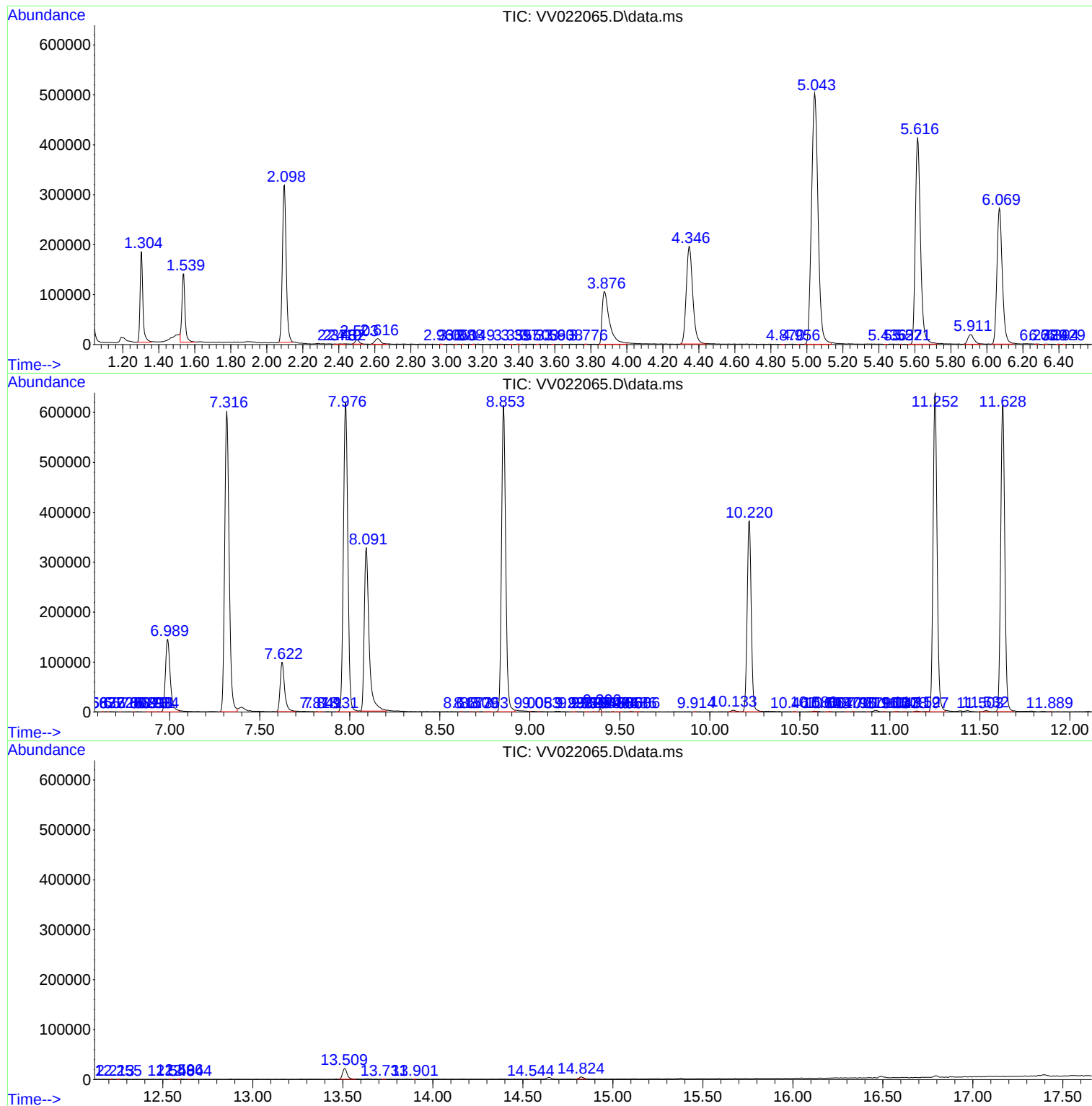
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082721WMA.M
Quant Title : VOC Analysis

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



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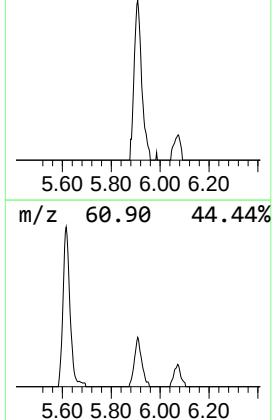
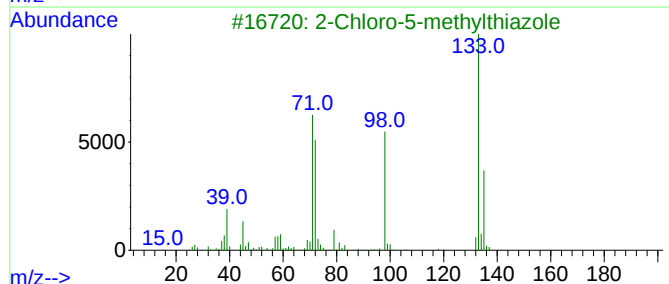
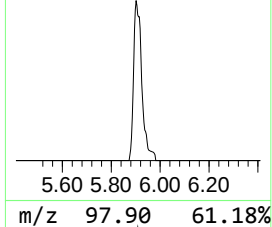
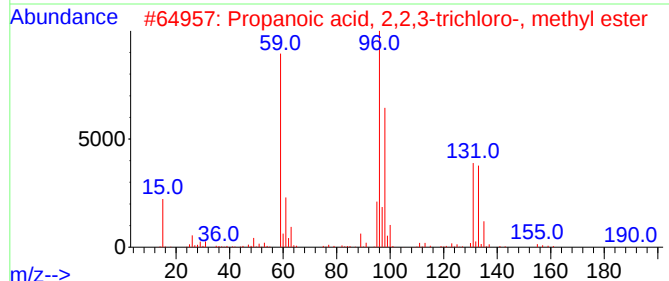
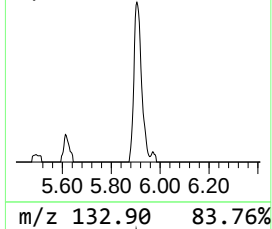
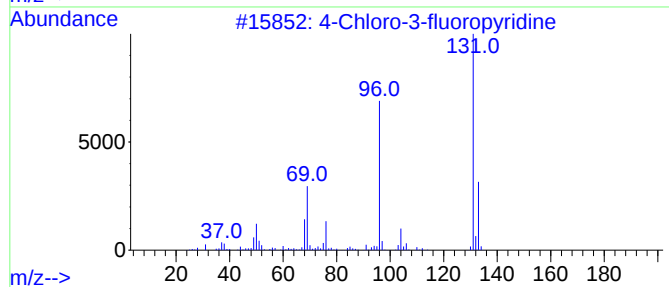
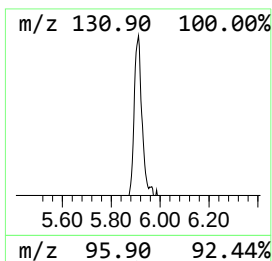
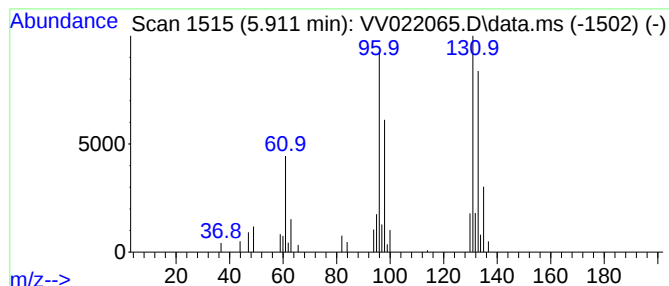
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082721WMA.M
Quant Title : VOC Analysis

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.
5.911	2.72 ug/L	45237	1,4-Difluorobenzene	5.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	32
2			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	25
3			2-Chloro-5-methylthiazole	133	C4H4ClNS	033342-65-3	25
4			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	25
5			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	23



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	5.911	2.7	ug/L	45237	1	5.616	832486	50.0