

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011222\
 Data File : VV024330.D
 Acq On : 12 Jan 2022 14:48
 Operator : SY/MD
 Sample : N1074-21ME
 Misc : 6.22g/5.0mL/100ul/5.0mL/MSVOA_V/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BGLM4ME

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\SFAMVLM123121WMA.M
 Title : VOC Analysis

Signal : TIC: VV024330.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.310	77	84	100	rVB	80394	84033	11.32%	1.254%
2	1.571	158	165	177	rVB	79193	88437	11.91%	1.320%
3	2.108	322	332	361	rVB	145807	228059	30.71%	3.404%
4	2.211	361	364	368	rVB2	294	206	0.03%	0.003%
5	2.301	389	392	393	rBV	279	161	0.02%	0.002%
6	2.436	430	434	438	rVB2	279	282	0.04%	0.004%
7	2.513	451	458	463	rVB3	1105	1210	0.16%	0.018%
8	2.580	474	479	484	rBB	150	230	0.03%	0.003%
9	2.616	484	490	494	rBV2	669	814	0.11%	0.012%
10	2.670	504	507	510	rVB	316	203	0.03%	0.003%
11	2.687	510	512	516	rBV	165	159	0.02%	0.002%
12	2.761	532	535	538	rBB2	325	199	0.03%	0.003%
13	2.799	545	547	552	rBV2	286	260	0.04%	0.004%
14	2.966	593	599	601	rBB	219	187	0.03%	0.003%
15	3.005	609	611	616	rBB	227	187	0.03%	0.003%
16	3.037	616	621	625	rBV	191	268	0.04%	0.004%
17	3.108	640	643	646	rBB	256	168	0.02%	0.003%
18	3.799	854	858	862	rBB	136	163	0.02%	0.002%
19	3.879	872	883	921	rBV	71024	221868	29.87%	3.312%
20	4.243	994	996	1000	rBV	409	331	0.04%	0.005%
21	4.342	1010	1027	1051	rBV3	146117	357753	48.17%	5.340%
22	4.510	1076	1079	1085	rVB2	529	450	0.06%	0.007%
23	4.555	1090	1093	1095	rBV2	259	164	0.02%	0.002%
24	4.577	1098	1100	1103	rVB	348	182	0.02%	0.003%
25	4.600	1103	1107	1110	rBB2	267	237	0.03%	0.004%
26	4.915	1199	1205	1208	rBB2	221	208	0.03%	0.003%
27	4.963	1215	1220	1223	rBV	313	379	0.05%	0.006%
28	5.040	1227	1244	1275	rBV3	278329	742178	99.93%	11.078%
29	5.297	1321	1324	1326	rVB2	276	176	0.02%	0.003%
30	5.333	1333	1335	1339	rVV	214	147	0.02%	0.002%
31	5.407	1355	1358	1361	rBV2	280	213	0.03%	0.003%
32	5.481	1378	1381	1384	rVB2	293	175	0.02%	0.003%
33	5.516	1389	1392	1394	rBV2	529	323	0.04%	0.005%
34	5.609	1409	1421	1448	rBV	301492	609521	82.07%	9.098%
35	5.799	1477	1480	1485	rVB	456	367	0.05%	0.005%
36	5.828	1485	1489	1492	rBV2	446	311	0.04%	0.005%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
 Title : VOC Analysis

37	5.902	1496	1512	1527	rBV5	17158	36505	4.92%	0.545%
38	6.002	1540	1543	1545	rVV2	353	251	0.03%	0.004%
39	6.063	1549	1562	1589	rBV2	178839	366739	49.38%	5.474%
40	6.239	1616	1617	1621	rVB2	349	148	0.02%	0.002%
41	6.268	1625	1626	1632	rVB	457	288	0.04%	0.004%
42	6.330	1643	1645	1647	rBV	350	194	0.03%	0.003%
43	6.420	1669	1673	1674	rBV	171	143	0.02%	0.002%
44	6.458	1682	1685	1690	rBB	253	211	0.03%	0.003%
45	6.484	1690	1693	1696	rBV2	251	233	0.03%	0.003%
46	6.516	1701	1703	1707	rVB	462	253	0.03%	0.004%
47	6.577	1719	1722	1727	rBV2	314	326	0.04%	0.005%
48	6.635	1736	1740	1747	rVB4	536	747	0.10%	0.011%
49	6.667	1748	1750	1752	rBV4	323	167	0.02%	0.002%
50	6.748	1770	1775	1776	rBV	273	255	0.03%	0.004%
51	6.786	1781	1787	1791	rBB	152	172	0.02%	0.003%
52	6.809	1792	1794	1799	rBB	154	152	0.02%	0.002%
53	6.883	1814	1817	1820	rBV	226	198	0.03%	0.003%
54	6.902	1820	1823	1824	rVB	348	166	0.02%	0.002%
55	6.982	1837	1848	1877	rBV	98357	179889	24.22%	2.685%
56	7.104	1883	1886	1892	rBV3	455	385	0.05%	0.006%
57	7.178	1906	1909	1911	rBV2	391	224	0.03%	0.003%
58	7.310	1939	1950	1969	rBV	296174	512973	69.07%	7.657%
59	7.497	2005	2008	2009	rBV	245	148	0.02%	0.002%
60	7.619	2035	2046	2070	rVV	71083	125219	16.86%	1.869%
61	7.796	2099	2101	2103	rVV	280	146	0.02%	0.002%
62	7.863	2120	2122	2124	rVB	347	151	0.02%	0.002%
63	7.940	2141	2146	2153	rVB3	803	1014	0.14%	0.015%
64	8.085	2180	2191	2205	rBV	252892	454440	61.19%	6.783%
65	8.426	2289	2297	2302	rBV3	1252	1824	0.25%	0.027%
66	8.509	2321	2323	2327	rBV2	343	142	0.02%	0.002%
67	8.564	2338	2340	2345	rVB2	457	453	0.06%	0.007%
68	8.593	2345	2349	2351	rBV2	282	252	0.03%	0.004%
69	8.847	2414	2428	2447	rBV	462693	742661	100.00%	11.085%
70	9.198	2533	2537	2539	rVV	195	145	0.02%	0.002%
71	9.423	2601	2607	2609	rBV2	257	308	0.04%	0.005%
72	9.593	2656	2660	2664	rBV	163	214	0.03%	0.003%
73	9.612	2664	2666	2671	rVB2	256	256	0.03%	0.004%
74	9.754	2707	2710	2717	rVB2	235	180	0.02%	0.003%
75	9.780	2717	2718	2722	rBV2	242	148	0.02%	0.002%
76	10.107	2817	2820	2822	rBV	265	158	0.02%	0.002%

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Peak Location: TOP

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77	10.127	2824	2826	2832	rVB3	440	297	0.04%	0.004%
78	10.214	2841	2853	2870	rBV	316647	495831	66.76%	7.401%
79	10.313	2882	2884	2886	rVB2	371	185	0.02%	0.003%
80	10.329	2886	2889	2892	rBV	290	231	0.03%	0.003%
81	10.378	2899	2904	2909	rBV2	649	760	0.10%	0.011%
82	10.490	2937	2939	2944	rVB	248	153	0.02%	0.002%
83	10.580	2964	2967	2972	rBV2	342	250	0.03%	0.004%
84	10.644	2982	2987	2988	rBV	196	190	0.03%	0.003%
85	10.918	3065	3072	3079	rBV3	892	1243	0.17%	0.019%
86	11.246	3162	3174	3198	rBV	464088	716923	96.53%	10.701%
87	11.384	3215	3217	3219	rBV2	355	154	0.02%	0.002%
88	11.416	3226	3227	3229	rBV2	396	143	0.02%	0.002%
89	11.622	3279	3291	3313	rBV	452938	712649	95.96%	10.637%
90	11.799	3344	3346	3350	rVB	419	289	0.04%	0.004%
91	11.889	3370	3374	3377	rVB2	358	248	0.03%	0.004%
92	11.992	3402	3406	3407	rBV	186	154	0.02%	0.002%
93	12.085	3432	3435	3440	rBV	226	143	0.02%	0.002%
94	12.111	3440	3443	3448	rBV	229	175	0.02%	0.003%
95	12.580	3587	3589	3593	rVB	333	188	0.03%	0.003%
96	12.683	3617	3621	3624	rBV2	239	155	0.02%	0.002%
97	13.082	3740	3745	3747	rBV	178	161	0.02%	0.002%
98	13.442	3854	3857	3859	rBV	398	204	0.03%	0.003%
99	13.988	4025	4027	4030	rVB2	302	153	0.02%	0.002%
100	14.422	4160	4162	4164	rBV	350	167	0.02%	0.002%

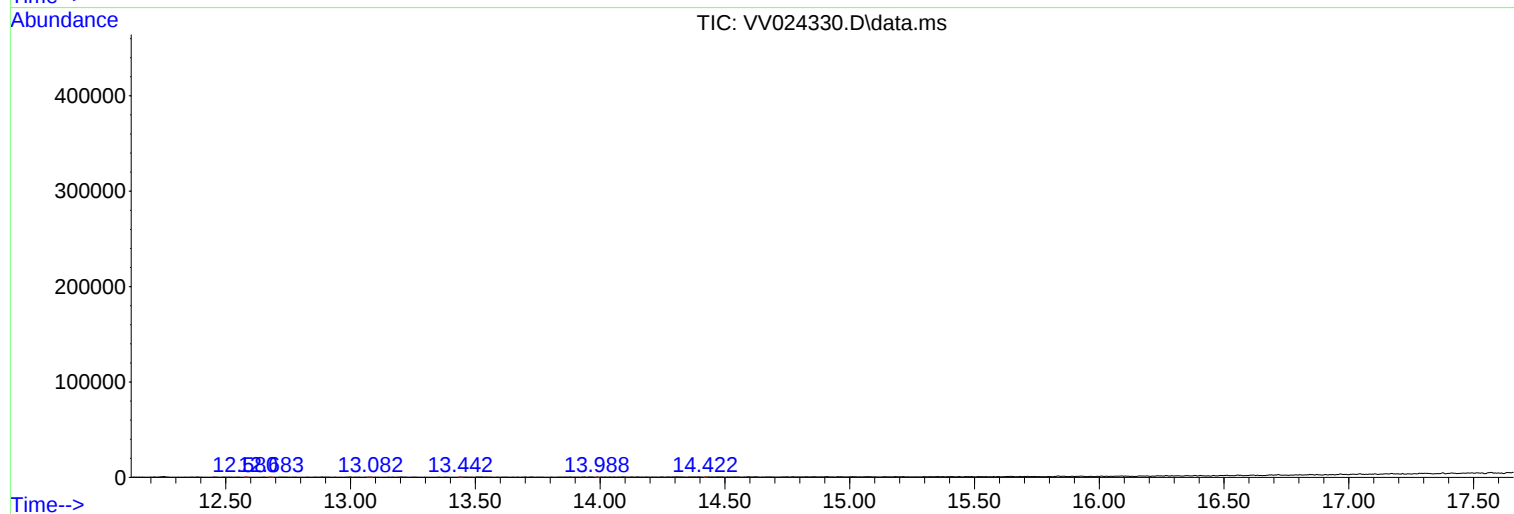
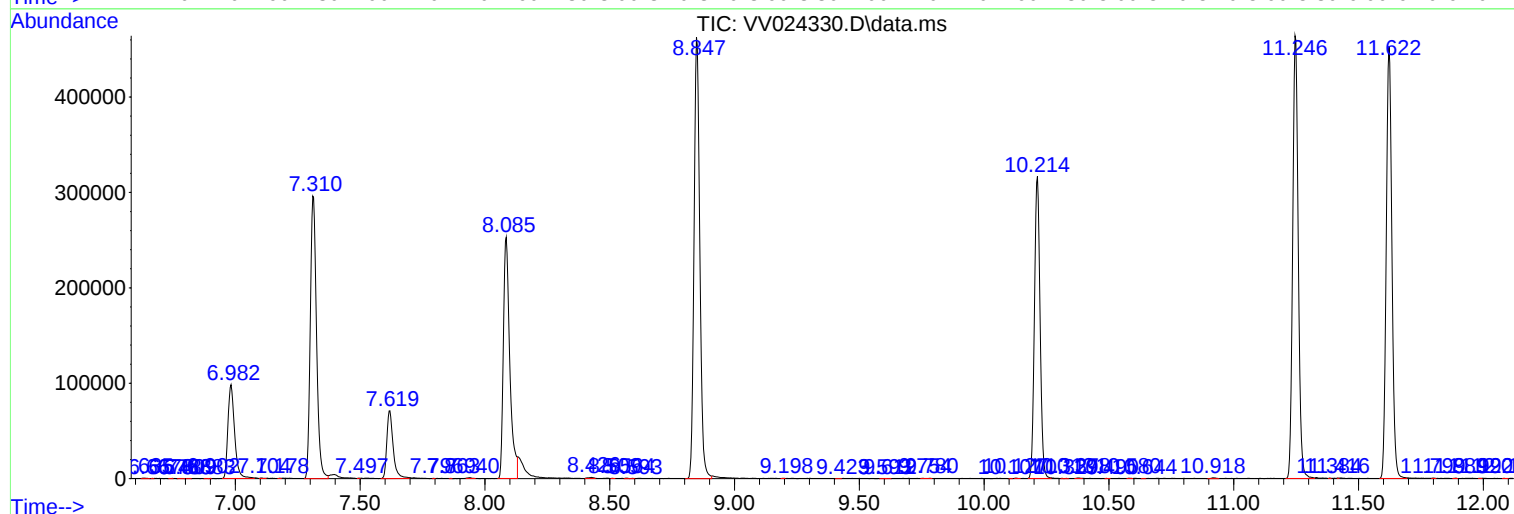
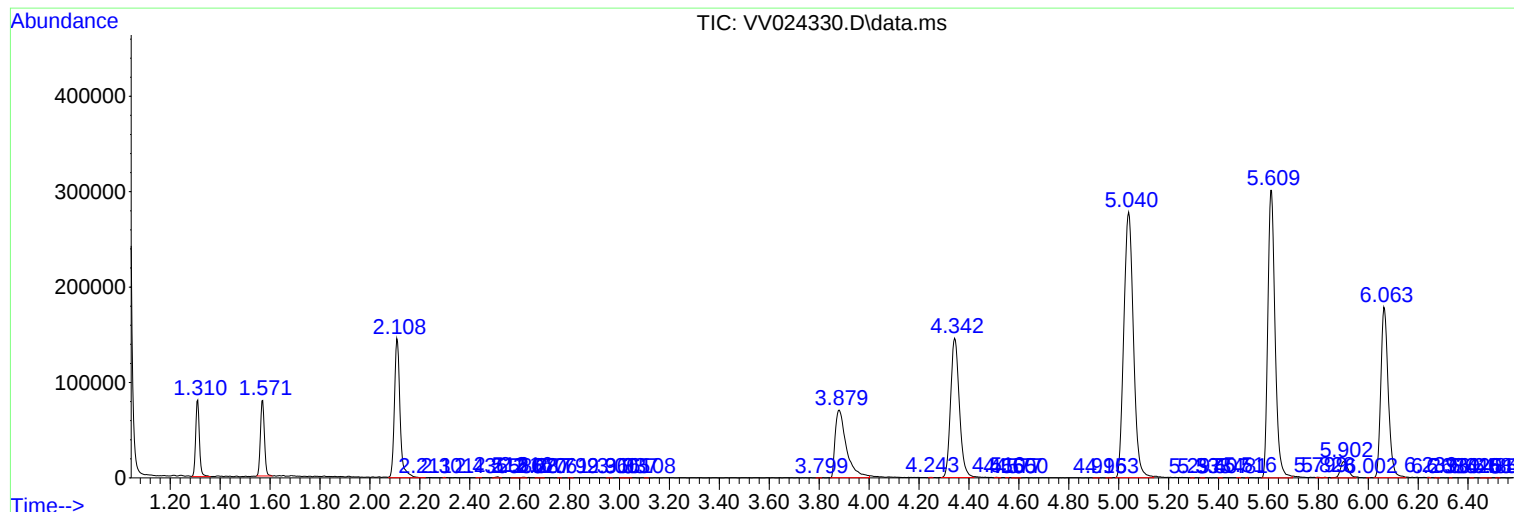
Sum of corrected areas: 6699733

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ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
BGLM4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.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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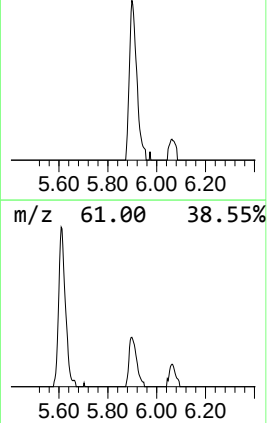
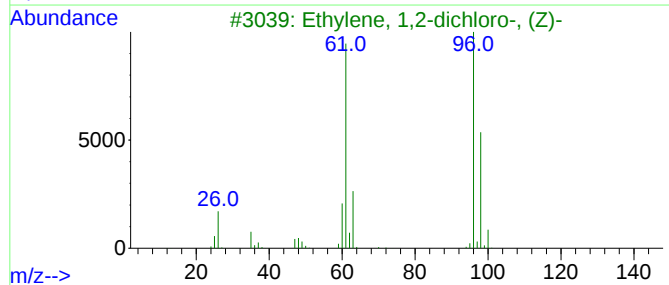
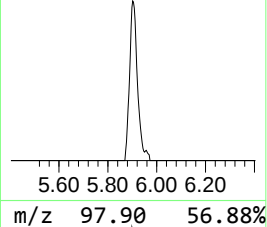
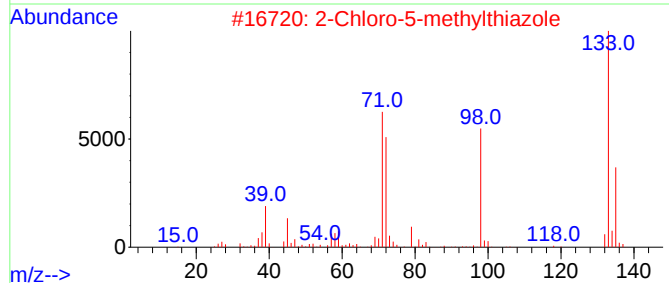
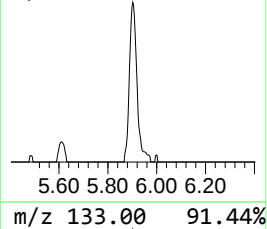
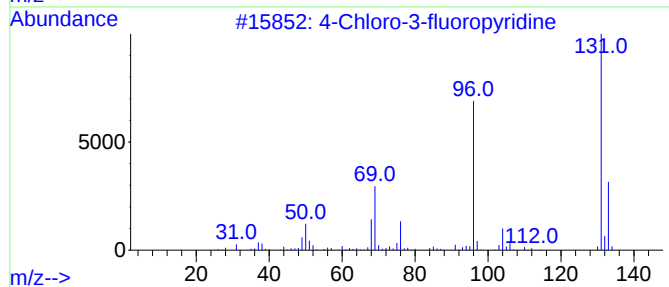
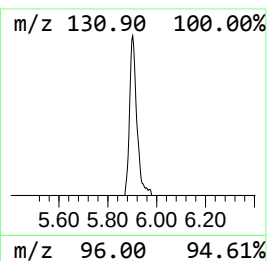
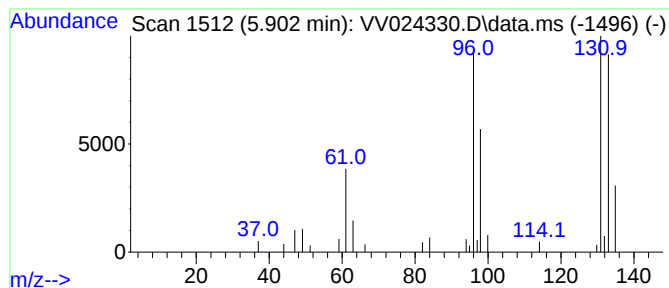
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
Quant Title : VOC Analysis

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	2.99 ug/L	36505	1,4-Difluorobenzene	5.612

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	43
2			2-Chloro-5-methylthiazole	133	C4H4ClNS	033342-65-3	30
3			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	30
4			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	23
5			Heptanoic acid, heptyl ester	228	C14H28O2	000624-09-9	16



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	5.902	3.0	ug/L	36505	1	5.612	609521	50.0