

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV083121\
 Data File : VV022038.D
 Acq On : 31 Aug 2021 13:43
 Operator : SY/MD
 Sample : M3579-12MEDL 10X
 Misc : 6.52g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 GB6B4MEDL

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: VV022038.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	98	rVB	106698	112051	10.86%	1.228%
2	1.539	150	155	166	rVB	95669	113712	11.02%	1.246%
3	2.098	319	329	347	rBV	203865	303720	29.45%	3.327%
4	2.622	479	492	502	rVV2	5082	10985	1.06%	0.120%
5	2.732	523	526	532	rBV4	420	496	0.05%	0.005%
6	2.757	532	534	536	rBV	413	216	0.02%	0.002%
7	3.008	608	612	615	rVB2	279	171	0.02%	0.002%
8	3.027	615	618	621	rBV2	388	268	0.03%	0.003%
9	3.449	746	749	753	rBV2	372	209	0.02%	0.002%
10	3.571	782	787	789	rBV	245	164	0.02%	0.002%
11	3.799	855	858	861	rBV2	544	301	0.03%	0.003%
12	3.818	861	864	867	rBV2	237	155	0.02%	0.002%
13	3.876	872	882	919	rBV	95731	269085	26.09%	2.948%
14	4.233	991	993	995	rBV	350	154	0.01%	0.002%
15	4.349	1012	1029	1066	rBV	153251	409935	39.74%	4.491%
16	4.529	1081	1085	1087	rBV	495	347	0.03%	0.004%
17	4.596	1103	1106	1110	rVB3	571	309	0.03%	0.003%
18	4.770	1157	1160	1163	rBV	360	250	0.02%	0.003%
19	4.854	1183	1186	1188	rBV4	407	227	0.02%	0.002%
20	4.873	1190	1192	1196	rVB2	383	198	0.02%	0.002%
21	4.902	1196	1201	1204	rBV2	627	370	0.04%	0.004%
22	4.934	1204	1211	1213	rBV2	304	301	0.03%	0.003%
23	4.947	1213	1215	1219	rBV2	344	249	0.02%	0.003%
24	5.043	1229	1245	1285	rBV2	406280	1031457	100.00%	11.300%
25	5.307	1326	1327	1335	rVB6	435	323	0.03%	0.004%
26	5.497	1384	1386	1389	rVV2	381	196	0.02%	0.002%
27	5.526	1392	1395	1398	rBV2	332	226	0.02%	0.002%
28	5.616	1409	1423	1455	rBV	365679	737297	71.48%	8.077%
29	5.905	1501	1513	1528	rBV4	29591	63198	6.13%	0.692%
30	6.069	1550	1564	1589	rBV	230186	474659	46.02%	5.200%
31	6.262	1622	1624	1630	rVB3	732	518	0.05%	0.006%
32	6.288	1630	1632	1638	rBV4	318	194	0.02%	0.002%
33	6.323	1640	1643	1648	rBV3	249	214	0.02%	0.002%
34	6.381	1659	1661	1665	rVB2	229	165	0.02%	0.002%
35	6.429	1674	1676	1681	rVB3	257	221	0.02%	0.002%
36	6.500	1695	1698	1704	rBV3	530	386	0.04%	0.004%

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

37	6.603	1727	1730	1732	rVB	379	198	0.02%	0.002%
38	6.622	1732	1736	1740	rBV3	533	486	0.05%	0.005%
39	6.648	1740	1744	1748	rVV4	598	551	0.05%	0.006%
40	6.680	1752	1754	1757	rBV	227	169	0.02%	0.002%
41	6.802	1788	1792	1795	rBV2	302	166	0.02%	0.002%
42	6.989	1838	1850	1875	rBV2	122495	224453	21.76%	2.459%
43	7.191	1910	1913	1914	rBV	551	313	0.03%	0.003%
44	7.317	1940	1952	1971	rBV	477939	831467	80.61%	9.109%
45	7.625	2037	2048	2071	rBV	81767	145059	14.06%	1.589%
46	7.844	2114	2116	2119	rVB3	504	288	0.03%	0.003%
47	7.866	2119	2123	2125	rBV	541	310	0.03%	0.003%
48	7.886	2127	2129	2133	rVB3	323	221	0.02%	0.002%
49	7.905	2133	2135	2139	rBV2	299	188	0.02%	0.002%
50	7.976	2144	2157	2180	rBV	369924	624302	60.53%	6.839%
51	8.091	2183	2193	2227	rBV2	271905	522221	50.63%	5.721%
52	8.545	2329	2334	2335	rBV3	505	437	0.04%	0.005%
53	8.596	2348	2350	2355	rBV3	518	502	0.05%	0.005%
54	8.667	2369	2372	2376	rVB2	469	302	0.03%	0.003%
55	8.747	2394	2397	2400	rVB2	286	221	0.02%	0.002%
56	8.808	2412	2416	2418	rBV2	388	185	0.02%	0.002%
57	8.854	2418	2430	2453	rBV	552763	907265	87.96%	9.939%
58	9.230	2543	2547	2548	rBV	281	191	0.02%	0.002%
59	9.275	2556	2561	2565	rVB2	338	249	0.02%	0.003%
60	9.307	2567	2571	2574	rVB2	317	211	0.02%	0.002%
61	9.407	2598	2602	2609	rVB2	277	242	0.02%	0.003%
62	9.535	2640	2642	2649	rBV3	653	427	0.04%	0.005%
63	9.583	2655	2657	2663	rVB3	279	243	0.02%	0.003%
64	9.770	2713	2715	2717	rBV	364	206	0.02%	0.002%
65	9.934	2764	2766	2771	rVV2	297	192	0.02%	0.002%
66	9.976	2777	2779	2781	rBV2	301	161	0.02%	0.002%
67	10.130	2819	2827	2832	rBV4	1571	1971	0.19%	0.022%
68	10.217	2841	2854	2869	rBV	321758	506849	49.14%	5.553%
69	10.358	2894	2898	2899	rBV2	240	179	0.02%	0.002%
70	10.435	2918	2922	2928	rBV3	345	368	0.04%	0.004%
71	10.574	2962	2965	2966	rBV2	304	165	0.02%	0.002%
72	10.847	3045	3050	3052	rBV2	453	370	0.04%	0.004%
73	10.895	3063	3065	3067	rBV2	252	152	0.01%	0.002%
74	10.921	3067	3073	3083	rVB7	1644	2844	0.28%	0.031%
75	10.966	3083	3087	3089	rBV2	380	245	0.02%	0.003%
76	11.030	3104	3107	3110	rBV	223	196	0.02%	0.002%

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77	11.252	3164	3176	3196	rBV	614585	955323	92.62%	10.466%
78	11.545	3263	3267	3269	rBV2	575	429	0.04%	0.005%
79	11.574	3274	3276	3280	rBV4	367	260	0.03%	0.003%
80	11.625	3280	3292	3314	rBV	539742	859662	83.34%	9.418%
81	11.876	3368	3370	3373	rBV2	363	234	0.02%	0.003%
82	11.934	3386	3388	3391	rVV	334	161	0.02%	0.002%
83	11.959	3392	3396	3400	rVV3	343	299	0.03%	0.003%
84	11.979	3400	3402	3407	rVV	345	271	0.03%	0.003%
85	12.095	3436	3438	3440	rVB2	435	161	0.02%	0.002%
86	12.117	3443	3445	3448	rVB2	552	249	0.02%	0.003%
87	12.152	3453	3456	3460	rBV3	482	312	0.03%	0.003%
88	12.255	3485	3488	3491	rVB2	510	235	0.02%	0.003%
89	12.329	3508	3511	3515	rVB2	363	228	0.02%	0.002%
90	12.368	3520	3523	3526	rVB	296	161	0.02%	0.002%
91	12.384	3526	3528	3531	rBV	464	334	0.03%	0.004%
92	12.513	3566	3568	3569	rBV	431	160	0.02%	0.002%
93	12.612	3597	3599	3602	rBV	242	152	0.01%	0.002%
94	12.763	3643	3646	3649	rBV2	291	222	0.02%	0.002%
95	12.789	3653	3654	3661	rVV2	368	298	0.03%	0.003%
96	13.072	3739	3742	3747	rBV2	362	253	0.02%	0.003%
97	13.252	3796	3798	3802	rBV2	287	169	0.02%	0.002%
98	13.599	3904	3906	3907	rBV	360	154	0.01%	0.002%
99	14.226	4097	4101	4102	rBV	414	272	0.03%	0.003%
100	14.400	4153	4155	4159	rBV2	574	303	0.03%	0.003%

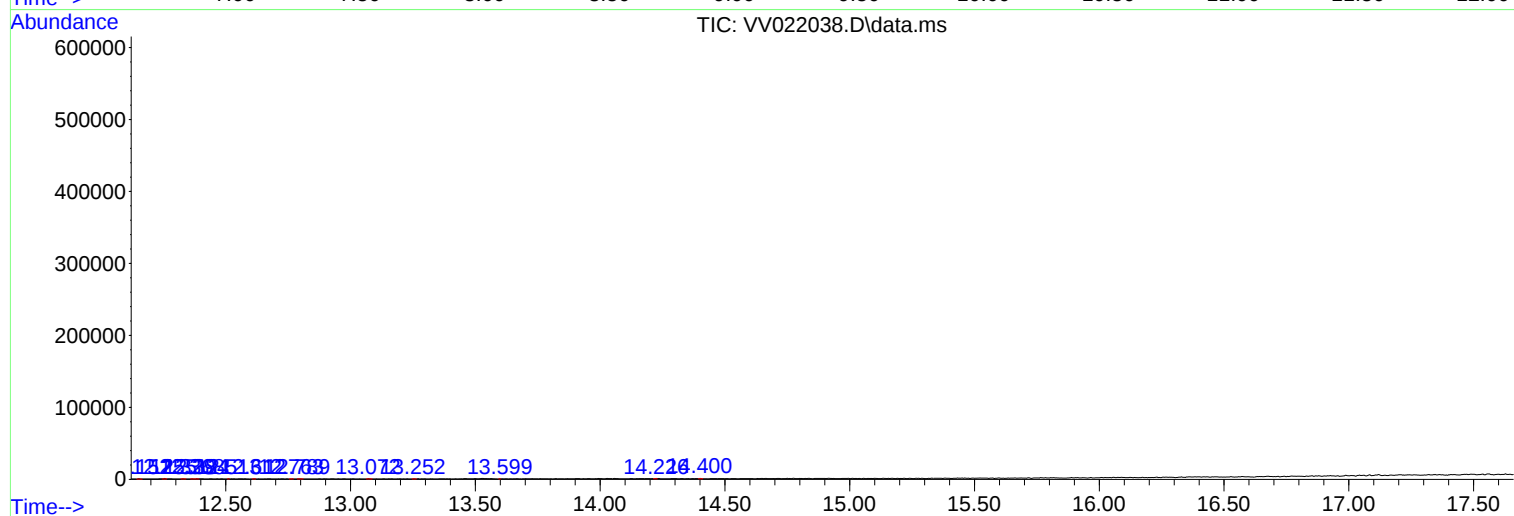
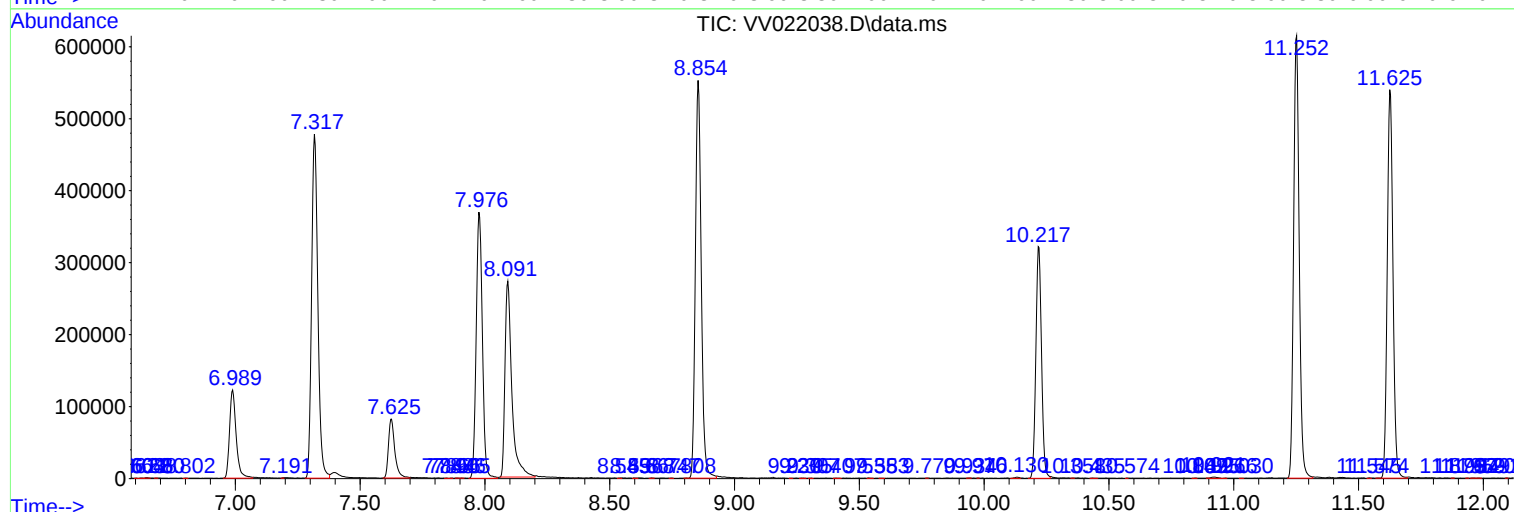
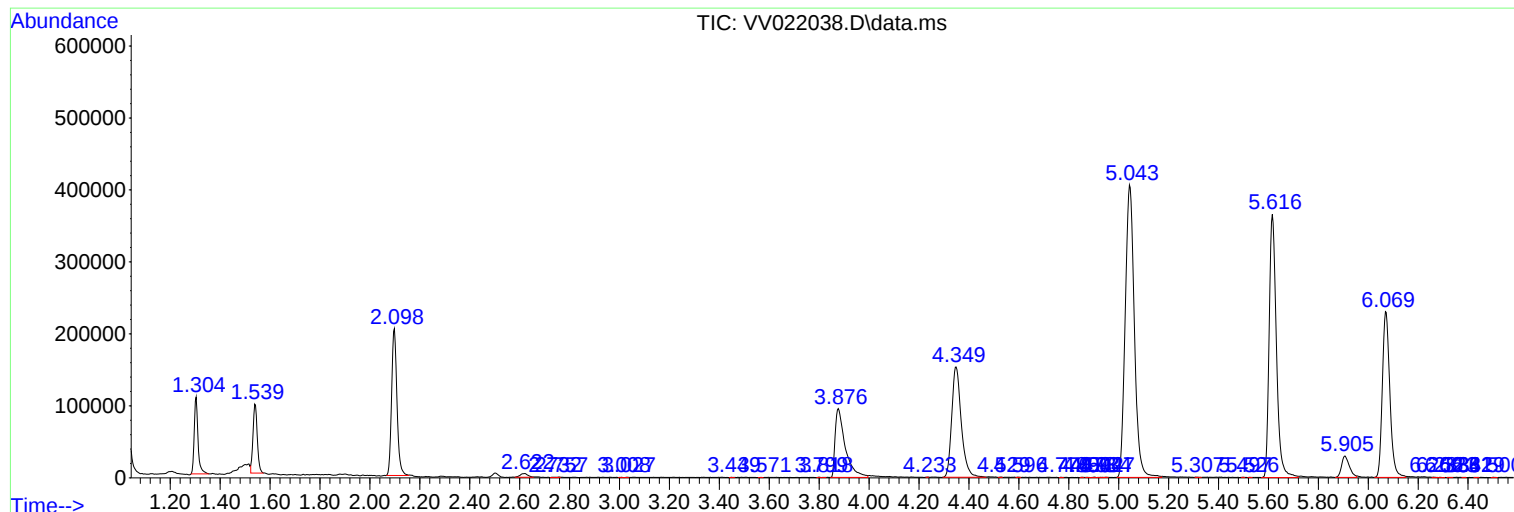
Sum of corrected areas: 9127994

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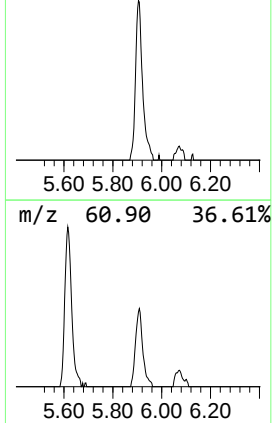
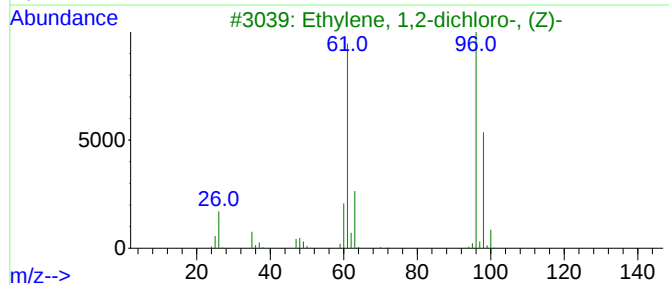
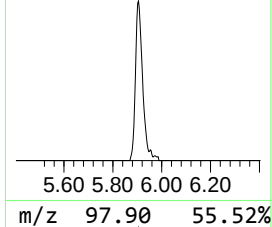
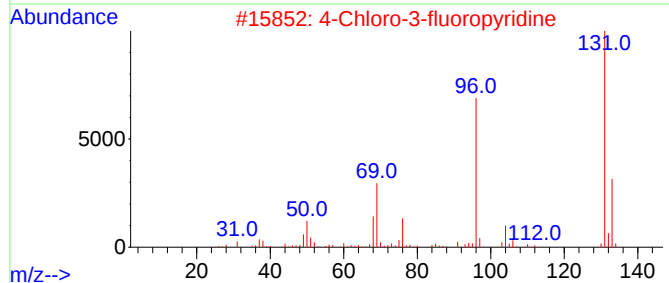
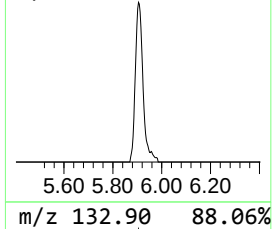
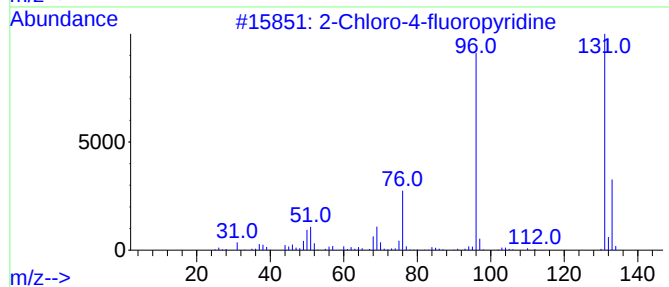
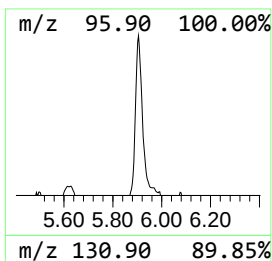
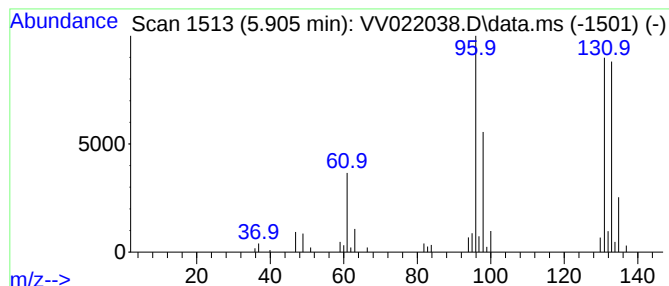
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082721WMA.M
Quant Title : VOC Analysis

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.
5.905	4.29 ug/L	63198	1,4-Difluorobenzene	5.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	32
2			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	27
3			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	27
4			2-Chloro-5-methylthiazole	133	C4H4ClNS	033342-65-3	22
5			Acetylthiosemicarbazide	133	C3H7N3OS	002302-88-7	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	5.905	4.3	ug/L	63198	1	5.616	737297	50.0