

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV080221\
 Data File : VV021716.D
 Acq On : 02 Aug 2021 13:43
 Operator : SY/MD
 Sample : VV0802MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VBLK223

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\SFAMVLM080221WMA.M

Title : VOC Analysis

Signal : TIC: VV021716.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	97	rVB	203208	203059	12.73%	1.673%
2	1.558	154	161	176	rVB	160501	191490	12.00%	1.577%
3	2.105	321	331	353	rVB	344537	509398	31.93%	4.196%
4	2.507	447	456	467	rBV4	5733	9320	0.58%	0.077%
5	2.600	483	485	486	rBV	375	172	0.01%	0.001%
6	2.761	531	535	542	rVB4	910	1021	0.06%	0.008%
7	2.796	542	546	549	rBV2	288	287	0.02%	0.002%
8	2.880	570	572	575	rVB	610	241	0.02%	0.002%
9	2.973	597	601	604	rBV2	394	305	0.02%	0.003%
10	3.092	635	638	640	rBV2	476	264	0.02%	0.002%
11	3.172	661	663	668	rBV2	299	283	0.02%	0.002%
12	3.224	677	679	682	rBV2	285	164	0.01%	0.001%
13	3.240	682	684	688	rBV2	409	266	0.02%	0.002%
14	3.262	688	691	694	rVB	279	155	0.01%	0.001%
15	3.285	694	698	700	rBV	209	142	0.01%	0.001%
16	3.317	703	708	709	rBV	365	244	0.02%	0.002%
17	3.532	773	775	779	rVB2	316	162	0.01%	0.001%
18	3.555	779	782	783	rBV	266	124	0.01%	0.001%
19	3.574	786	788	792	rVV	375	154	0.01%	0.001%
20	3.597	792	795	799	rVB2	273	193	0.01%	0.002%
21	3.632	802	806	809	rVB2	303	193	0.01%	0.002%
22	3.687	819	823	825	rVB	342	220	0.01%	0.002%
23	3.706	825	829	831	rBV2	124	114	0.01%	0.001%
24	3.728	832	836	837	rVV2	393	236	0.01%	0.002%
25	3.786	851	854	857	rBV	310	197	0.01%	0.002%
26	3.870	870	880	914	rBV	143166	372076	23.32%	3.065%
27	4.346	1013	1028	1056	rBV	249844	620156	38.87%	5.109%
28	4.600	1105	1107	1109	rBV4	320	153	0.01%	0.001%
29	4.645	1119	1121	1123	rBV	290	155	0.01%	0.001%
30	4.683	1130	1133	1138	rVB3	515	438	0.03%	0.004%
31	4.709	1138	1141	1142	rBV	244	137	0.01%	0.001%
32	4.741	1149	1151	1153	rBV	274	135	0.01%	0.001%
33	4.767	1154	1159	1160	rBV3	361	236	0.01%	0.002%
34	4.822	1171	1176	1183	rVB2	388	510	0.03%	0.004%
35	4.860	1183	1188	1189	rBV	244	148	0.01%	0.001%
36	4.934	1206	1211	1215	rBV4	577	474	0.03%	0.004%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM080221WMA.M
 Title : VOC Analysis

37	5.047	1228	1246	1272	rBV2	622605	1595600	100.00%	13.144%
38	5.391	1352	1353	1355	rBV	471	213	0.01%	0.002%
39	5.497	1383	1386	1391	rVB4	576	333	0.02%	0.003%
40	5.526	1391	1395	1401	rVB4	379	470	0.03%	0.004%
41	5.616	1409	1423	1459	rBV	458855	929579	58.26%	7.658%
42	5.841	1490	1493	1496	rBV2	572	385	0.02%	0.003%
43	5.905	1501	1513	1537	rVV2	41828	89116	5.59%	0.734%
44	6.069	1551	1564	1588	rBV	348954	717507	44.97%	5.911%
45	6.375	1654	1659	1664	rBV3	520	574	0.04%	0.005%
46	6.397	1664	1666	1667	rBV	362	145	0.01%	0.001%
47	6.429	1672	1676	1680	rBV2	430	293	0.02%	0.002%
48	6.452	1680	1683	1684	rBV	247	141	0.01%	0.001%
49	6.523	1698	1705	1708	rBV3	567	650	0.04%	0.005%
50	6.539	1708	1710	1711	rBV3	296	115	0.01%	0.001%
51	6.632	1733	1739	1740	rBV2	861	668	0.04%	0.006%
52	6.687	1754	1756	1761	rVB4	831	490	0.03%	0.004%
53	6.728	1764	1769	1771	rVB3	356	287	0.02%	0.002%
54	6.770	1779	1782	1785	rVB2	197	146	0.01%	0.001%
55	6.799	1786	1791	1797	rVB4	520	565	0.04%	0.005%
56	6.892	1818	1820	1821	rBV4	221	108	0.01%	0.001%
57	6.934	1832	1833	1838	rVB	356	196	0.01%	0.002%
58	6.986	1838	1849	1880	rBV	213390	387853	24.31%	3.195%
59	7.317	1940	1952	1970	rBV	766456	1311838	82.22%	10.807%
60	7.622	2037	2047	2071	rBV	143626	251808	15.78%	2.074%
61	7.944	2143	2147	2151	rBV2	497	418	0.03%	0.003%
62	7.986	2158	2160	2162	rBV2	584	289	0.02%	0.002%
63	8.043	2176	2178	2180	rBV	254	135	0.01%	0.001%
64	8.088	2182	2192	2229	rBV2	411860	811438	50.85%	6.684%
65	8.706	2381	2384	2388	rBV3	311	221	0.01%	0.002%
66	8.754	2396	2399	2400	rBV2	268	174	0.01%	0.001%
67	8.854	2418	2430	2474	rBV	677098	1110044	69.57%	9.144%
68	9.021	2479	2482	2488	rVB5	1060	923	0.06%	0.008%
69	9.066	2494	2496	2500	rBV3	286	221	0.01%	0.002%
70	9.121	2511	2513	2516	rVB2	448	210	0.01%	0.002%
71	9.137	2516	2518	2520	rBV3	640	389	0.02%	0.003%
72	9.188	2532	2534	2538	rVB	317	167	0.01%	0.001%
73	9.291	2564	2566	2569	rVB	380	129	0.01%	0.001%
74	9.378	2591	2593	2597	rBV2	243	164	0.01%	0.001%
75	9.494	2627	2629	2632	rVB2	331	161	0.01%	0.001%
76	9.596	2658	2661	2662	rBV	408	218	0.01%	0.002%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM080221WMA.M
 Title : VOC Analysis

77	9.664	2677	2682	2684	rBV	263	259	0.02%	0.002%
78	9.680	2684	2687	2694	rVB4	448	417	0.03%	0.003%
79	9.725	2699	2701	2705	rVB2	400	215	0.01%	0.002%
80	9.757	2705	2711	2718	rBV2	304	391	0.02%	0.003%
81	9.973	2774	2778	2781	rBV	363	312	0.02%	0.003%
82	10.008	2786	2789	2792	rBV2	547	326	0.02%	0.003%
83	10.130	2818	2827	2840	rVB2	4842	7908	0.50%	0.065%
84	10.217	2842	2854	2881	rBV	450404	706923	44.30%	5.823%
85	10.381	2903	2905	2911	rVB4	976	863	0.05%	0.007%
86	10.445	2923	2925	2927	rBV	383	202	0.01%	0.002%
87	10.542	2952	2955	2956	rBV2	565	328	0.02%	0.003%
88	10.751	3017	3020	3022	rBV2	474	278	0.02%	0.002%
89	10.921	3066	3073	3086	rVB5	3905	6220	0.39%	0.051%
90	11.014	3094	3102	3103	rBV	290	364	0.02%	0.003%
91	11.146	3136	3143	3153	rBV4	2047	3072	0.19%	0.025%
92	11.249	3163	3175	3197	rBV	694699	1089428	68.28%	8.974%
93	11.497	3250	3252	3253	rBV	311	100	0.01%	0.001%
94	11.625	3280	3292	3316	rBV	750381	1191952	74.70%	9.819%
95	11.812	3348	3350	3352	rBV	397	232	0.01%	0.002%
96	11.854	3357	3363	3370	rBV5	858	1074	0.07%	0.009%
97	11.905	3376	3379	3385	rBV3	475	416	0.03%	0.003%
98	11.995	3405	3407	3410	rVB2	362	161	0.01%	0.001%
99	12.124	3443	3447	3451	rVB2	415	361	0.02%	0.003%
100	12.413	3535	3537	3539	rBV2	378	134	0.01%	0.001%

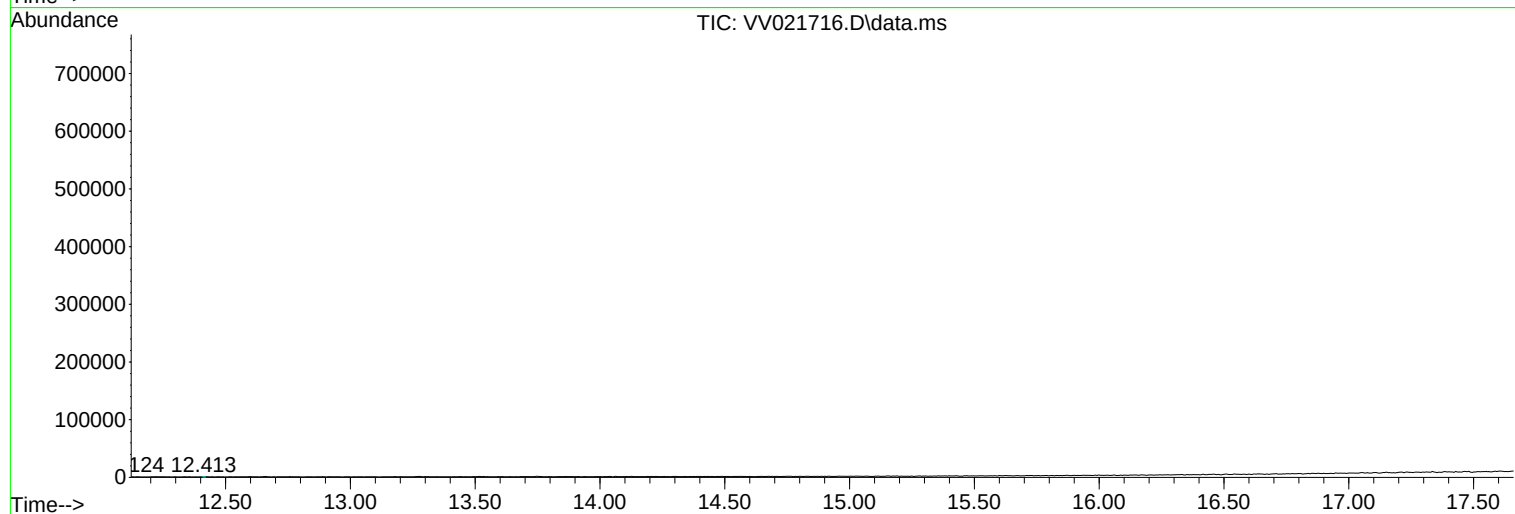
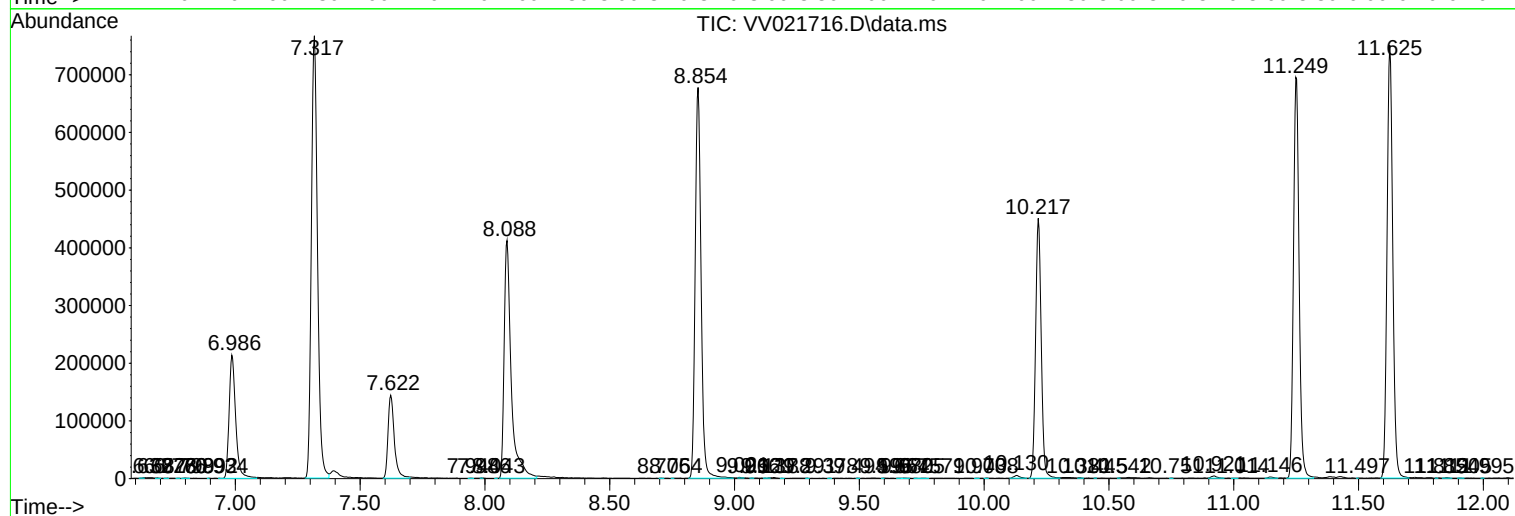
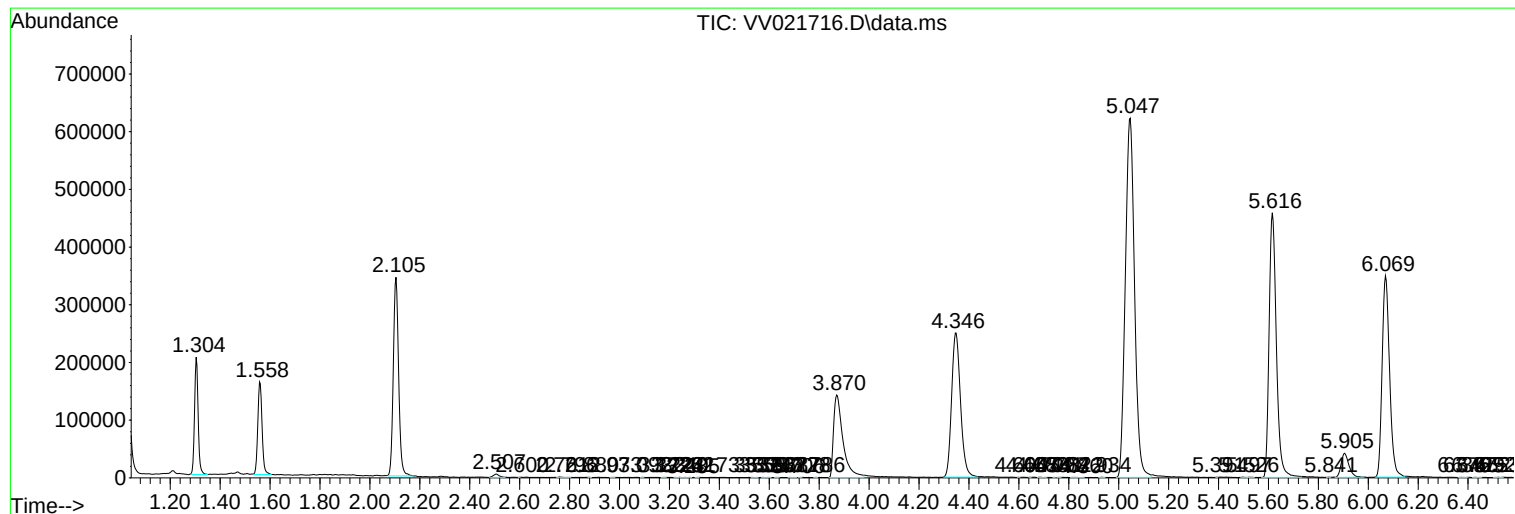
Sum of corrected areas: 12139339

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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VBLK223

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM080221WMA.M
Quant Title : VOC Analysis

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



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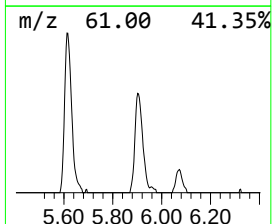
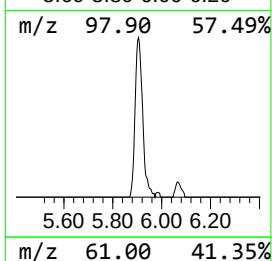
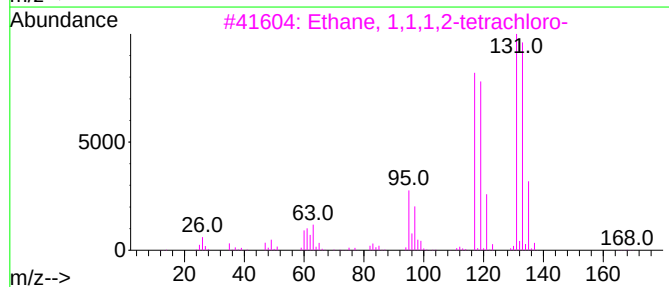
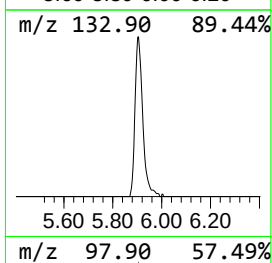
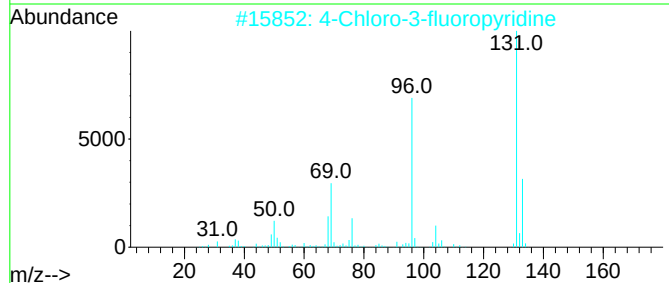
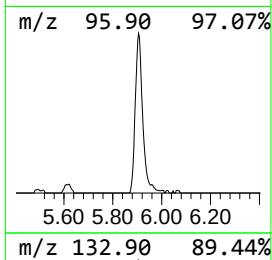
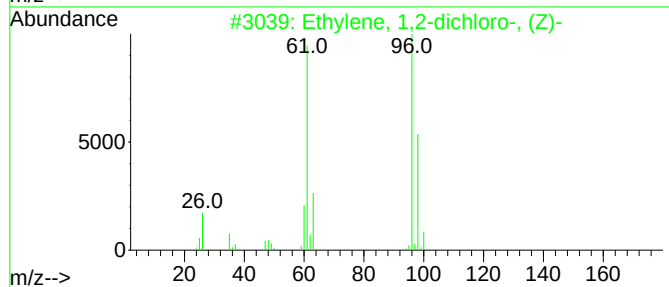
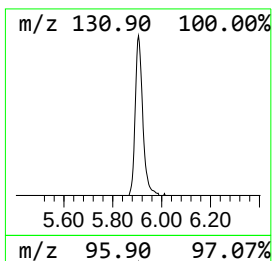
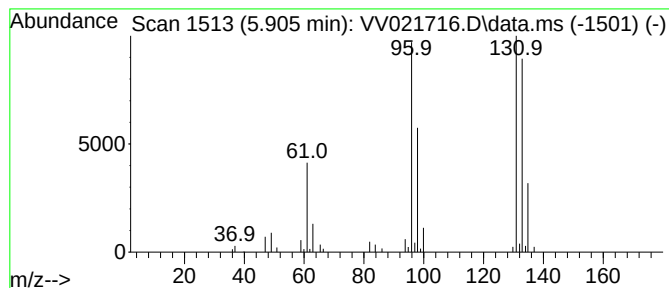
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM080221WMA.M
Quant Title : VOC Analysis

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	4.79 ug/L	89116	1,4-Difluorobenzene	5.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
2			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	38
3			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	25
4			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	25
5			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	5.905	4.8	ug/L	89116	1	5.616	929579	50.0