

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050321\
 Data File : VV021252.D
 Acq On : 03 May 2021 17:49
 Operator : SY/MD
 Sample : M2177-10ME
 Misc : 2.97g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BG576ME

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\SFAMVLM050321WMA.M
 Title : VOC Analysis

Signal : TIC: VV021252.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.211	49	53	58	rBV3	4919	6064	0.16%	0.022%
2	1.307	76	83	106	rBV	243710	366780	9.64%	1.328%
3	1.458	127	130	134	rBV5	4679	3505	0.09%	0.013%
4	1.568	158	164	176	rBV	164391	244369	6.42%	0.885%
5	2.089	317	326	340	rVB	965410	1387815	36.47%	5.026%
6	2.310	392	395	400	rVB6	2745	2207	0.06%	0.008%
7	2.352	405	408	412	rVB5	2717	1826	0.05%	0.007%
8	2.433	429	433	440	rVV8	3353	5192	0.14%	0.019%
9	2.494	447	452	454	rBV5	5446	4672	0.12%	0.017%
10	2.619	477	491	500	rBV8	6895	16911	0.44%	0.061%
11	2.671	505	507	510	rBV4	2015	1301	0.03%	0.005%
12	2.751	529	532	537	rBV4	1324	1382	0.04%	0.005%
13	2.854	562	564	570	rBV7	1281	1355	0.04%	0.005%
14	3.002	606	610	611	rBV3	1564	1073	0.03%	0.004%
15	3.150	654	656	660	rBV3	1583	1084	0.03%	0.004%
16	3.220	675	678	681	rBV3	1750	1379	0.04%	0.005%
17	3.481	756	759	762	rBV4	1320	1058	0.03%	0.004%
18	3.548	775	780	785	rVB6	1541	1319	0.03%	0.005%
19	3.574	785	788	793	rBV4	1262	1261	0.03%	0.005%
20	3.696	824	826	830	rBV4	1863	1157	0.03%	0.004%
21	3.908	881	892	927	rBV2	120418	525587	13.81%	1.903%
22	4.349	1012	1029	1054	rBV	638599	1613223	42.40%	5.842%
23	4.529	1082	1085	1089	rVB5	1862	1220	0.03%	0.004%
24	4.587	1097	1103	1105	rBV4	1126	1382	0.04%	0.005%
25	4.706	1136	1140	1143	rBV7	1653	1399	0.04%	0.005%
26	4.777	1158	1162	1164	rBV4	1654	1468	0.04%	0.005%
27	4.815	1171	1174	1176	rBV4	1972	1178	0.03%	0.004%
28	4.944	1208	1214	1219	rVB5	1885	2582	0.07%	0.009%
29	5.043	1225	1245	1273	rBV3	1516003	3804859	100.00%	13.780%
30	5.310	1324	1328	1331	rBV7	1296	1112	0.03%	0.004%
31	5.336	1331	1336	1339	rBV6	3161	3240	0.09%	0.012%
32	5.404	1354	1357	1359	rVB3	2221	1165	0.03%	0.004%
33	5.461	1373	1375	1380	rVB5	2478	1915	0.05%	0.007%
34	5.500	1385	1387	1391	rVB4	2130	1191	0.03%	0.004%
35	5.523	1391	1394	1398	rBV6	1454	1206	0.03%	0.004%
36	5.616	1411	1423	1447	rBV	747939	1542382	40.54%	5.586%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050321WMA.M
 Title : VOC Analysis

37	5.719	1453	1455	1460	rVB6	2661	2345	0.06%	0.008%
38	5.777	1470	1473	1477	rBV6	1711	1412	0.04%	0.005%
39	5.860	1495	1499	1502	rVV5	1348	1125	0.03%	0.004%
40	5.908	1503	1514	1530	rVV3	59748	126005	3.31%	0.456%
41	6.008	1543	1545	1551	rVB6	2440	1851	0.05%	0.007%
42	6.072	1551	1565	1589	rBV2	769899	1649377	43.35%	5.973%
43	6.198	1599	1604	1606	rVB6	1786	1765	0.05%	0.006%
44	6.214	1606	1609	1614	rVB5	2486	2113	0.06%	0.008%
45	6.252	1617	1621	1625	rVB5	1723	1302	0.03%	0.005%
46	6.320	1637	1642	1644	rVB5	1910	1698	0.04%	0.006%
47	6.336	1644	1647	1651	rVB5	1610	1191	0.03%	0.004%
48	6.436	1675	1678	1683	rBV5	1330	1375	0.04%	0.005%
49	6.580	1719	1723	1727	rBV6	1726	1529	0.04%	0.006%
50	6.603	1727	1730	1732	rVV3	1810	1327	0.03%	0.005%
51	6.616	1732	1734	1737	rVV4	2142	1595	0.04%	0.006%
52	6.641	1737	1742	1744	rVV6	3776	4304	0.11%	0.016%
53	6.667	1748	1750	1755	rVV6	5949	4882	0.13%	0.018%
54	6.703	1759	1761	1764	rVV2	2715	1534	0.04%	0.006%
55	6.735	1767	1771	1774	rVB5	2138	1525	0.04%	0.006%
56	6.764	1778	1780	1781	rVV2	2118	1100	0.03%	0.004%
57	6.773	1781	1783	1786	rVV3	2901	2095	0.06%	0.008%
58	6.793	1786	1789	1794	rVV6	2677	2585	0.07%	0.009%
59	6.822	1796	1798	1803	rVV4	2032	1284	0.03%	0.005%
60	6.854	1803	1808	1811	rVB4	1728	1594	0.04%	0.006%
61	6.989	1837	1850	1876	rBV2	466391	951254	25.00%	3.445%
62	7.182	1908	1910	1914	rVB4	1902	1171	0.03%	0.004%
63	7.204	1914	1917	1919	rBV4	1465	1093	0.03%	0.004%
64	7.259	1927	1934	1940	rBV9	3769	5713	0.15%	0.021%
65	7.320	1940	1953	1971	rBV	1799301	3178974	83.55%	11.513%
66	7.625	2036	2048	2078	rVV2	326818	688837	18.10%	2.495%
67	7.802	2098	2103	2109	rBV8	2516	3779	0.10%	0.014%
68	7.831	2109	2112	2114	rVB4	2002	1357	0.04%	0.005%
69	7.895	2129	2132	2137	rBV5	1517	1561	0.04%	0.006%
70	7.924	2137	2141	2144	rVV5	1743	1328	0.03%	0.005%
71	7.960	2149	2152	2155	rVV5	2937	2183	0.06%	0.008%
72	7.989	2157	2161	2166	rVB7	3191	3589	0.09%	0.013%
73	8.124	2184	2203	2237	rBV3	456247	1593765	41.89%	5.772%
74	8.339	2267	2270	2272	rBV4	2064	1507	0.04%	0.005%
75	8.352	2272	2274	2279	rVB5	1653	1438	0.04%	0.005%
76	8.455	2304	2306	2317	rVB5	3089	3700	0.10%	0.013%

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 Title : VOC Analysis

77	8.584	2342	2346	2347	rBV3	1781	1340	0.04%	0.005%
78	8.860	2420	2432	2459	rBV	1075868	1994078	52.41%	7.222%
79	9.114	2505	2511	2515	rBV7	5574	7489	0.20%	0.027%
80	9.243	2549	2551	2555	rVB3	1939	1187	0.03%	0.004%
81	9.323	2568	2576	2581	rBV9	6932	10563	0.28%	0.038%
82	9.394	2595	2598	2603	rVB5	1513	1366	0.04%	0.005%
83	9.426	2603	2608	2611	rBV7	2084	1767	0.05%	0.006%
84	9.452	2611	2616	2624	rBV7	5715	8395	0.22%	0.030%
85	9.513	2632	2635	2638	rBV3	2151	1282	0.03%	0.005%
86	9.564	2644	2651	2653	rBV7	3803	3618	0.10%	0.013%
87	9.683	2684	2688	2689	rBV2	4551	2935	0.08%	0.011%
88	9.767	2706	2714	2717	rBV10	4039	5629	0.15%	0.020%
89	9.911	2752	2759	2767	rVB10	8213	15828	0.42%	0.057%
90	9.976	2772	2779	2782	rBV7	10418	11951	0.31%	0.043%
91	10.063	2799	2806	2813	rBV7	5017	7364	0.19%	0.027%
92	10.133	2819	2828	2837	rBV3	41609	63352	1.67%	0.229%
93	10.230	2844	2858	2875	rBV	1056687	1860449	48.90%	6.738%
94	10.394	2902	2909	2916	rVB8	24425	35810	0.94%	0.130%
95	10.834	3040	3046	3056	rVB8	15066	22943	0.60%	0.083%
96	11.037	3103	3109	3116	rBV8	22626	35344	0.93%	0.128%
97	11.149	3137	3144	3153	rBV4	62994	96400	2.53%	0.349%
98	11.259	3168	3178	3195	rBV	1336469	2110732	55.47%	7.644%
99	11.635	3283	3295	3313	rBV	2192255	3468796	91.17%	12.563%
100	11.789	3337	3343	3344	rBV3	29654	28471	0.75%	0.103%

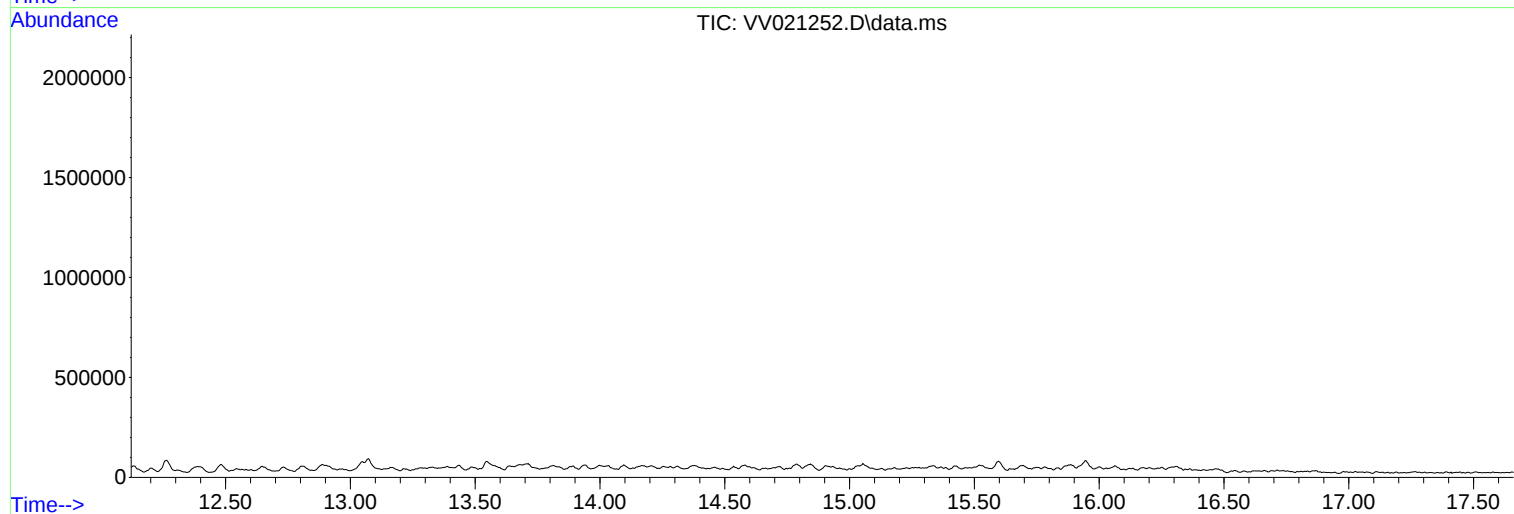
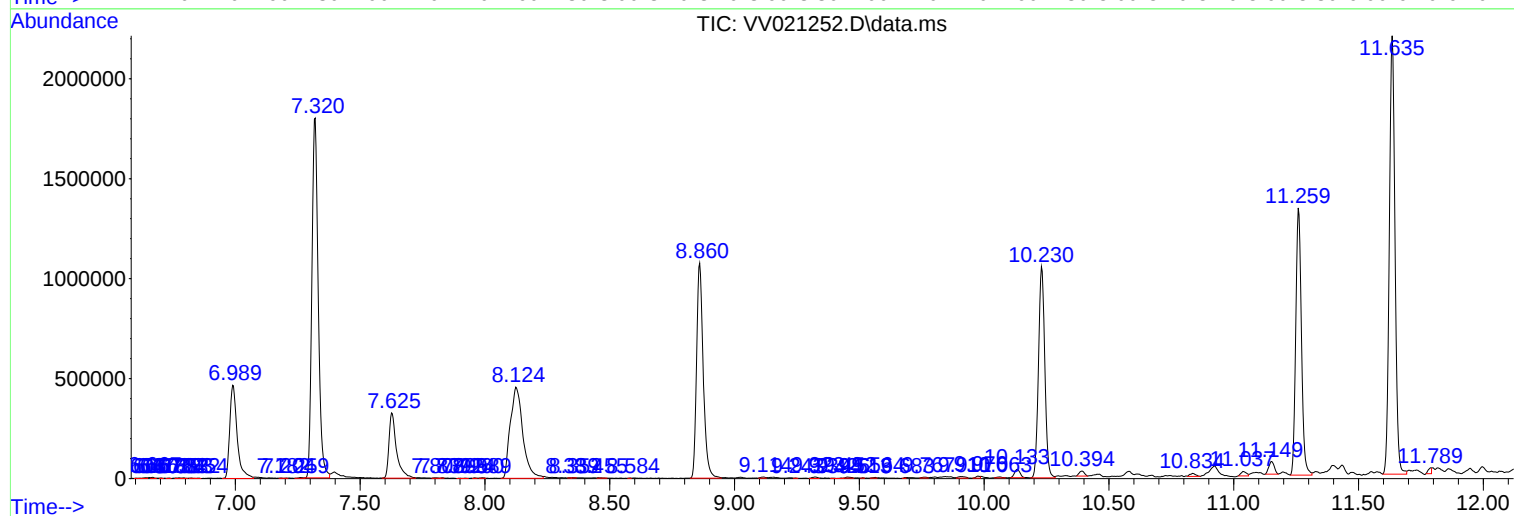
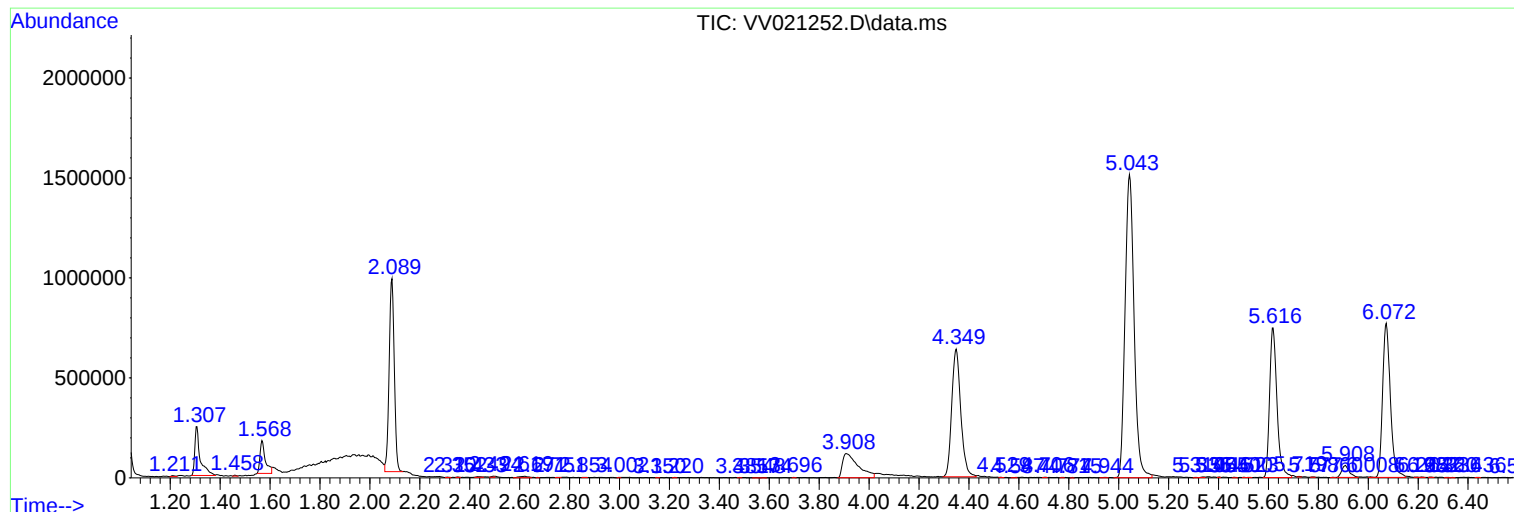
Sum of corrected areas: 27612070

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Instrument :
MSVOA_V
ClientSampleId :
BG576ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050321WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Instrument :
MSVOA_V
ClientSampleId :
BG576ME

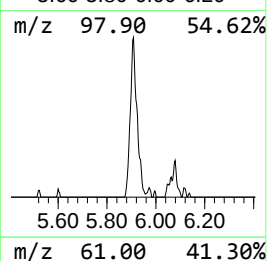
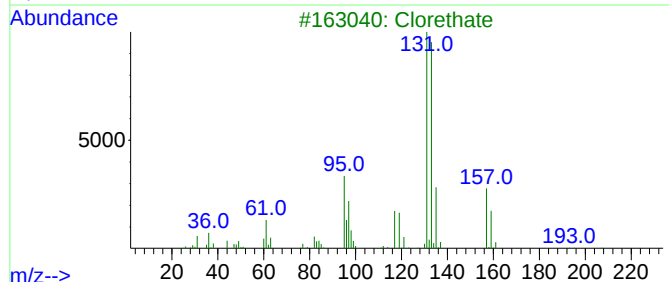
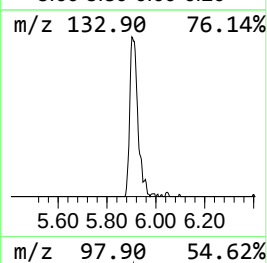
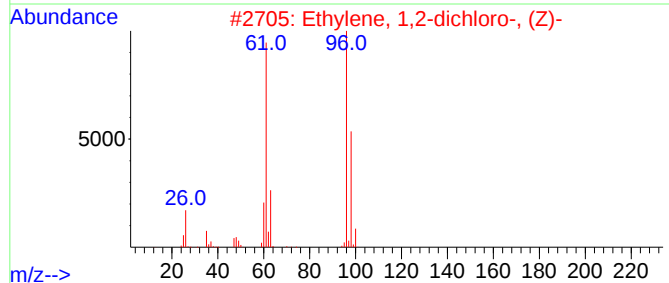
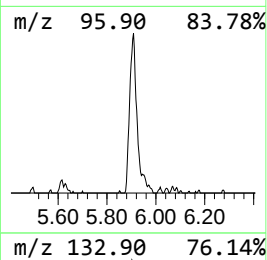
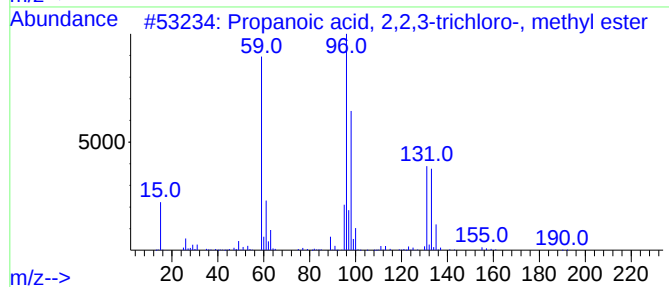
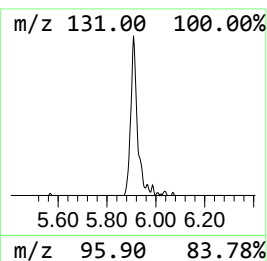
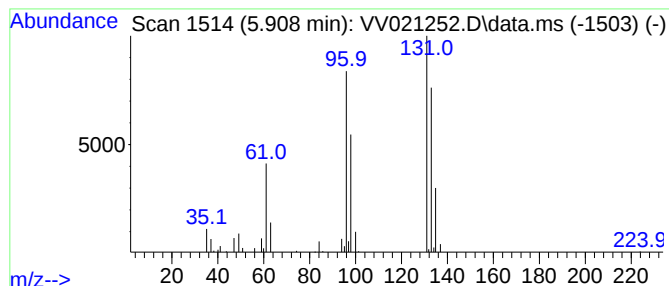
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050321WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propanoic acid, 2,2,3-trich... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.908	4.08 ug/L	126005	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	50
2			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	35
3			Cloethate	322	C5H4Cl6O3	005634-37-7	25
4			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	25
5			Carbamic acid, acetylthio-, O-me...	133	C4H7NO2S	016696-87-0	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	5.908	4.1	ug/L	126005	1	5.616	1542380	50.0