

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050421\
 Data File : VV021263.D
 Acq On : 04 May 2021 11:58
 Operator : SY/MD
 Sample : M2249-04
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BG7J3

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: VV021263.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.108	16	21	33	rVB	99021	94519	4.13%	0.495%
2	1.217	51	55	62	rBV6	17331	15145	0.66%	0.079%
3	1.307	75	83	96	rVB	246445	268749	11.75%	1.409%
4	1.571	158	165	174	rBV	199346	221941	9.71%	1.163%
5	2.108	324	332	348	rVB	500802	710883	31.09%	3.726%
6	2.359	407	410	412	rBV3	1426	897	0.04%	0.005%
7	2.413	424	427	429	rBV4	1220	912	0.04%	0.005%
8	2.674	504	508	510	rBV5	1225	770	0.03%	0.004%
9	2.831	554	557	558	rBV2	1752	909	0.04%	0.005%
10	2.953	590	595	599	rBV4	4246	4963	0.22%	0.026%
11	3.047	616	624	631	rBV7	5854	8839	0.39%	0.046%
12	3.214	670	676	679	rBV7	1929	2136	0.09%	0.011%
13	3.394	727	732	735	rBV4	1314	1152	0.05%	0.006%
14	3.471	753	756	760	rVB5	1376	898	0.04%	0.005%
15	3.497	760	764	766	rBV5	1313	1013	0.04%	0.005%
16	3.616	798	801	805	rBV5	939	997	0.04%	0.005%
17	3.680	817	821	823	rBV4	1661	1135	0.05%	0.006%
18	3.706	826	829	831	rBV3	1279	859	0.04%	0.005%
19	3.748	838	842	843	rBV3	2370	1440	0.06%	0.008%
20	3.902	879	890	909	rBV2	115061	353452	15.46%	1.853%
21	4.288	1007	1010	1012	rBV3	1316	854	0.04%	0.004%
22	4.352	1015	1030	1054	rVV2	429307	1051959	46.00%	5.514%
23	4.458	1060	1063	1067	rBV5	2464	1904	0.08%	0.010%
24	4.805	1167	1171	1173	rBV3	1304	900	0.04%	0.005%
25	4.879	1192	1194	1200	rVB6	1177	980	0.04%	0.005%
26	5.050	1231	1247	1275	rBV3	884892	2286826	100.00%	11.986%
27	5.349	1337	1340	1344	rBV5	1458	1119	0.05%	0.006%
28	5.371	1344	1347	1349	rBV5	2036	1409	0.06%	0.007%
29	5.622	1412	1425	1449	rBV	870570	1752006	76.61%	9.183%
30	6.027	1546	1551	1553	rBV6	1556	1647	0.07%	0.009%
31	6.076	1553	1566	1585	rVV2	491689	1010983	44.21%	5.299%
32	6.268	1622	1626	1628	rBV5	2218	1953	0.09%	0.010%
33	6.494	1692	1696	1698	rBV3	1888	1365	0.06%	0.007%
34	6.571	1718	1720	1725	rVB3	2177	1469	0.06%	0.008%
35	6.912	1823	1826	1831	rBV6	1181	1196	0.05%	0.006%
36	6.950	1834	1838	1839	rBV4	1137	791	0.03%	0.004%

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

37	6.992	1840	1851	1875	rBV2	301305	565053	24.71%	2.962%
38	7.320	1941	1953	1971	rBV	1095189	1887157	82.52%	9.891%
39	7.625	2038	2048	2073	rBV	229083	401409	17.55%	2.104%
40	7.834	2110	2113	2115	rBV3	1104	712	0.03%	0.004%
41	7.908	2133	2136	2138	rBV4	1249	793	0.03%	0.004%
42	7.931	2140	2143	2145	rBV3	2100	1290	0.06%	0.007%
43	7.982	2155	2159	2171	rVB9	8676	13229	0.58%	0.069%
44	8.095	2184	2194	2221	rBV	479401	937548	41.00%	4.914%
45	8.419	2292	2295	2297	rBV5	1382	985	0.04%	0.005%
46	8.767	2399	2403	2404	rBV4	1150	776	0.03%	0.004%
47	8.857	2418	2431	2457	rBV	1330700	2146774	93.88%	11.252%
48	9.011	2476	2479	2481	rBV3	1812	1223	0.05%	0.006%
49	9.130	2514	2516	2520	rBV4	1424	768	0.03%	0.004%
50	9.307	2568	2571	2577	rBV5	1159	895	0.04%	0.005%
51	9.333	2577	2579	2582	rBV3	1571	1076	0.05%	0.006%
52	9.384	2590	2595	2597	rBV5	956	793	0.03%	0.004%
53	9.407	2599	2602	2605	rBV4	1602	1311	0.06%	0.007%
54	9.471	2620	2622	2626	rVB5	1060	751	0.03%	0.004%
55	9.616	2665	2667	2673	rVB4	2080	1316	0.06%	0.007%
56	9.686	2684	2689	2692	rBV5	1511	1176	0.05%	0.006%
57	9.812	2724	2728	2730	rBV3	1000	769	0.03%	0.004%
58	9.944	2765	2769	2772	rVB4	2846	2108	0.09%	0.011%
59	10.053	2800	2803	2809	rVB6	2672	2428	0.11%	0.013%
60	10.079	2809	2811	2815	rBV6	1441	1220	0.05%	0.006%
61	10.223	2844	2856	2877	rBV	716860	1135619	49.66%	5.952%
62	10.307	2880	2882	2885	rBV3	2477	1340	0.06%	0.007%
63	10.329	2885	2889	2891	rBV5	2531	1810	0.08%	0.009%
64	10.390	2900	2908	2912	rBV8	5894	8240	0.36%	0.043%
65	10.490	2935	2939	2943	rBV5	2100	1884	0.08%	0.010%
66	10.583	2963	2968	2972	rVV6	2045	1999	0.09%	0.010%
67	10.741	3013	3017	3019	rBV4	1714	1096	0.05%	0.006%
68	10.821	3040	3042	3044	rBV2	1662	905	0.04%	0.005%
69	10.931	3068	3076	3081	rVB8	4538	6180	0.27%	0.032%
70	10.979	3088	3091	3093	rBV2	1277	719	0.03%	0.004%
71	11.046	3105	3112	3114	rVB5	1654	1746	0.08%	0.009%
72	11.069	3114	3119	3121	rBV3	1359	920	0.04%	0.005%
73	11.127	3134	3137	3139	rBV2	1198	738	0.03%	0.004%
74	11.152	3142	3145	3151	rVB7	2940	3230	0.14%	0.017%
75	11.255	3165	3177	3193	rBV	1366341	2124557	92.90%	11.136%
76	11.509	3253	3256	3259	rBV4	2108	1163	0.05%	0.006%

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 Title : VOC Analysis

77	11.632	3282	3294	3313	rBV	1252309	1974214	86.33%	10.348%
78	11.776	3337	3339	3343	rBV5	1754	1013	0.04%	0.005%
79	11.853	3360	3363	3368	rVB5	1984	1655	0.07%	0.009%
80	12.066	3425	3429	3432	rBV6	1986	1647	0.07%	0.009%
81	12.088	3433	3436	3443	rVB6	2236	2547	0.11%	0.013%
82	12.429	3540	3542	3545	rBV3	1588	958	0.04%	0.005%
83	12.445	3545	3547	3551	rVB4	1508	917	0.04%	0.005%
84	12.609	3595	3598	3599	rBV2	2057	1078	0.05%	0.006%
85	12.744	3637	3640	3642	rBV4	2605	1329	0.06%	0.007%
86	12.882	3678	3683	3685	rBV5	1953	1677	0.07%	0.009%
87	12.969	3706	3710	3715	rBV5	2237	2623	0.11%	0.014%
88	13.040	3729	3732	3734	rBV3	1079	784	0.03%	0.004%
89	13.066	3738	3740	3743	rBV	1321	779	0.03%	0.004%
90	13.107	3749	3753	3758	rBV8	1382	1722	0.08%	0.009%
91	13.297	3809	3812	3817	rVV6	1575	1522	0.07%	0.008%
92	13.361	3830	3832	3835	rVB3	2282	1024	0.04%	0.005%
93	13.381	3835	3838	3839	rBV2	1368	765	0.03%	0.004%
94	13.670	3925	3928	3930	rBV3	2234	1162	0.05%	0.006%
95	13.722	3941	3944	3945	rBV2	1575	885	0.04%	0.005%
96	13.818	3970	3974	3976	rBV4	1590	1004	0.04%	0.005%
97	14.242	4102	4106	4108	rBV4	1387	1455	0.06%	0.008%
98	14.474	4175	4178	4182	rBV4	2650	2036	0.09%	0.011%
99	14.548	4197	4201	4202	rBV3	2472	1452	0.06%	0.008%
100	15.551	4510	4513	4515	rBV3	3124	1909	0.08%	0.010%

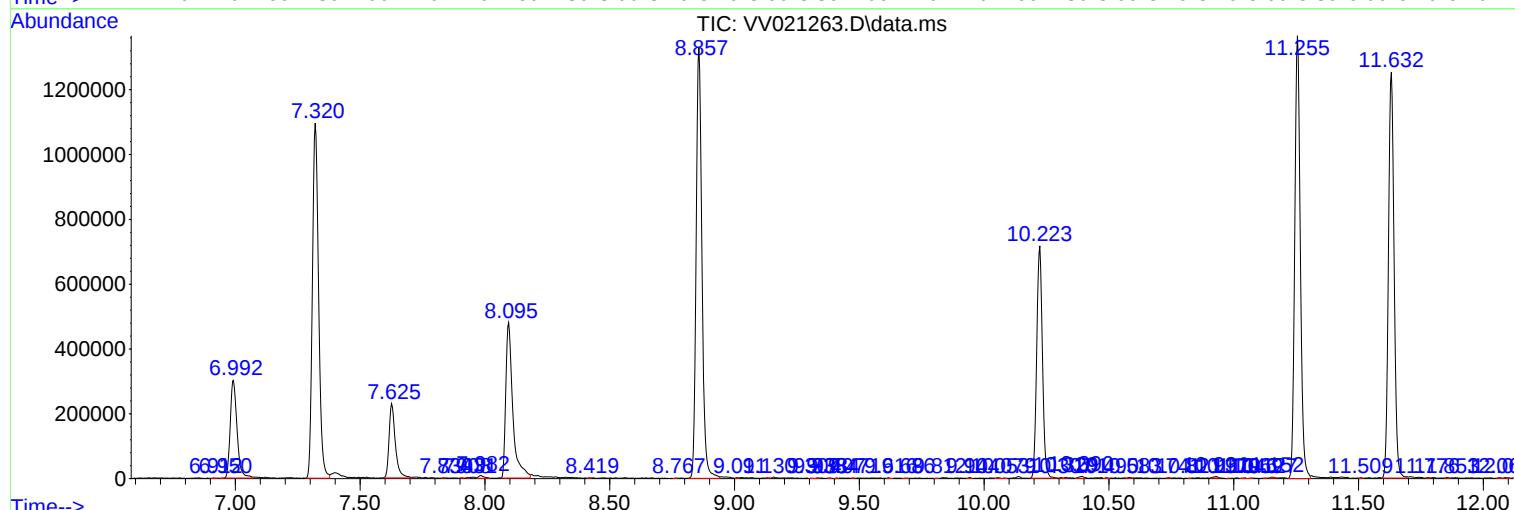
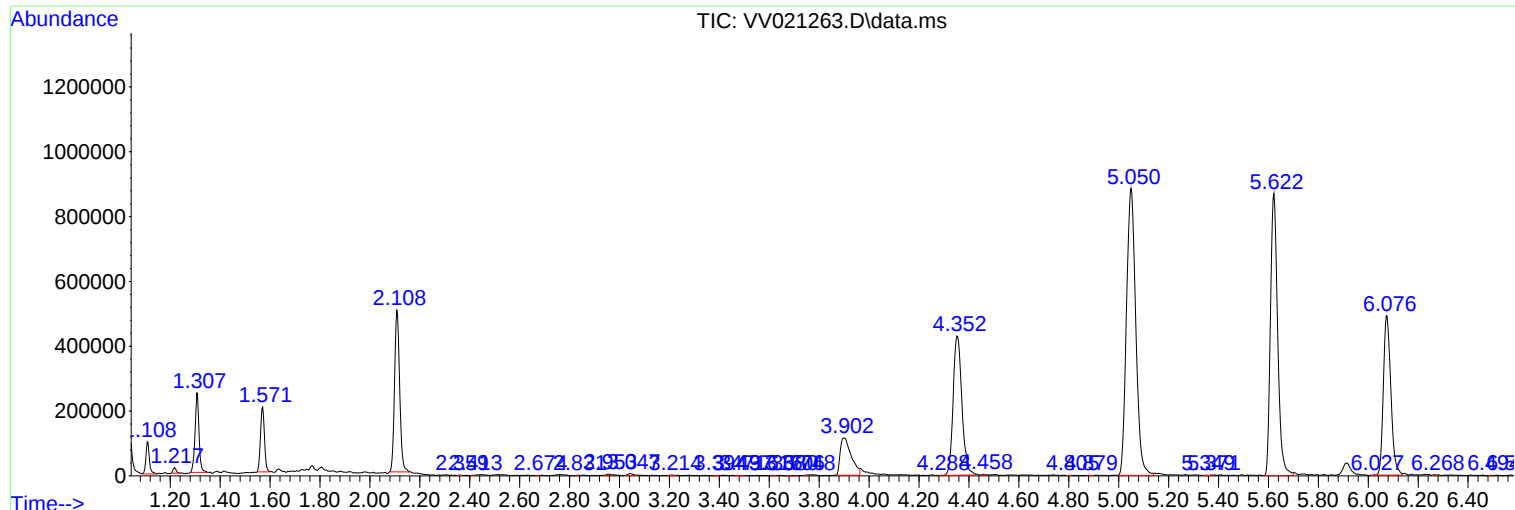
Sum of corrected areas: 19078833

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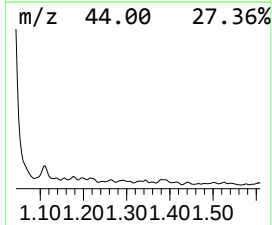
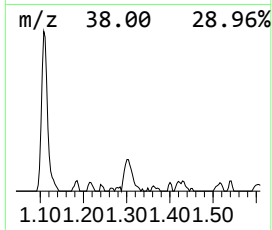
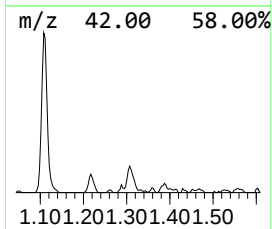
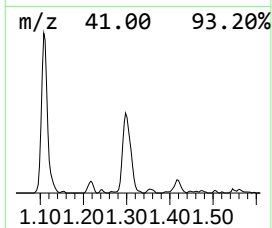
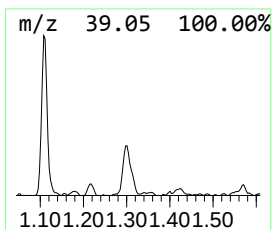
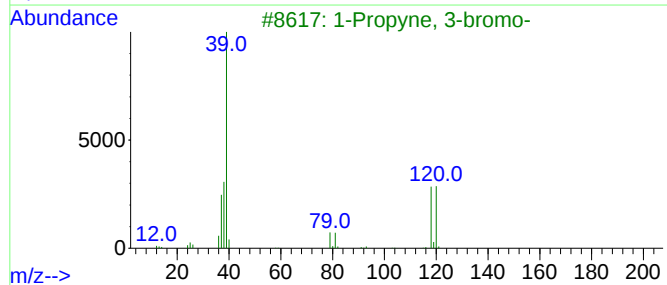
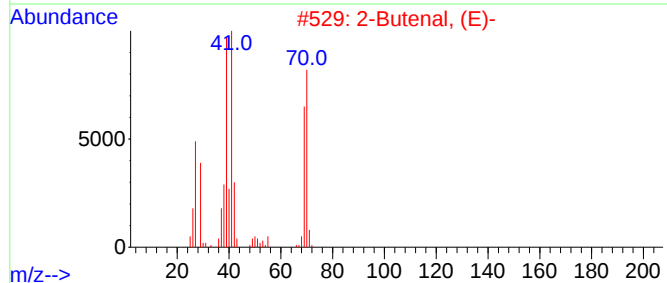
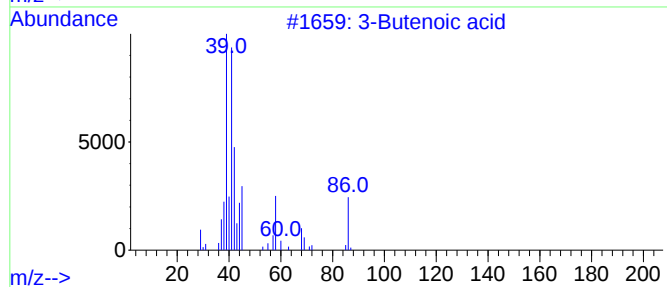
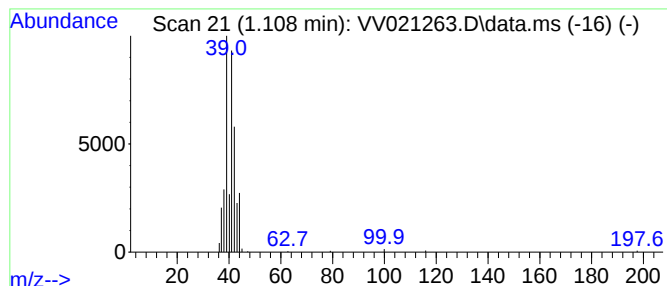
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050321WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 3-Butenoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.108	2.70 ug/L	94519	1,4-Difluorobenzene	5.622

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Butenoic acid	86	C4H6O2	000625-38-7	83
2			2-Butenal, (E)-	70	C4H6O	000123-73-9	78
3			1-Propyne, 3-bromo-	118	C3H3Br	000106-96-7	56
4			Dimethylketene	70	C4H6O	000598-26-5	43
5			Propene	42	C3H6	000115-07-1	40



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Butenoic acid	1.108	2.7	ug/L	94519	1	5.622	1752010	50.0