

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV080921\
 Data File : VV021761.D
 Acq On : 09 Aug 2021 13:28
 Operator : SY/MD
 Sample : M3287-13ME
 Misc : 4.83g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BGB12ME

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: VV021761.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	108	rVB	103999	148528	9.71%	1.242%
2	1.558	156	161	178	rBV	47849	66691	4.36%	0.558%
3	2.085	315	325	336	rBV	241014	352889	23.06%	2.951%
4	2.725	521	524	525	rBV	688	349	0.02%	0.003%
5	2.863	565	567	570	rBV3	383	196	0.01%	0.002%
6	2.931	585	588	591	rBV	499	284	0.02%	0.002%
7	3.008	609	612	615	rBV3	632	542	0.04%	0.005%
8	3.069	629	631	633	rBV	271	119	0.01%	0.001%
9	3.101	638	641	643	rBV	244	158	0.01%	0.001%
10	3.185	664	667	668	rBV	280	147	0.01%	0.001%
11	3.208	672	674	677	rVV3	342	202	0.01%	0.002%
12	3.236	681	683	686	rVB3	305	134	0.01%	0.001%
13	3.253	686	688	692	rBV2	346	183	0.01%	0.002%
14	3.278	692	696	700	rBV2	282	248	0.02%	0.002%
15	3.304	700	704	705	rBV	202	96	0.01%	0.001%
16	3.314	705	707	709	rVB	153	60	0.00%	0.001%
17	3.339	713	715	718	rBV	193	99	0.01%	0.001%
18	3.359	718	721	725	rBV	220	156	0.01%	0.001%
19	3.420	738	740	743	rBV	231	170	0.01%	0.001%
20	3.458	749	752	755	rBV	335	190	0.01%	0.002%
21	3.564	780	785	788	rBV2	301	307	0.02%	0.003%
22	3.619	800	802	804	rVB2	186	74	0.00%	0.001%
23	3.635	804	807	810	rBV2	239	199	0.01%	0.002%
24	3.661	812	815	817	rBV	270	157	0.01%	0.001%
25	3.732	834	837	838	rBV3	541	290	0.02%	0.002%
26	3.896	877	888	930	rBV	72838	319385	20.87%	2.671%
27	4.346	1013	1028	1063	rBV	223475	596888	39.01%	4.992%
28	4.606	1107	1109	1112	rBV2	383	197	0.01%	0.002%
29	4.815	1170	1174	1176	rBV2	375	193	0.01%	0.002%
30	4.863	1187	1189	1191	rBV	146	68	0.00%	0.001%
31	4.896	1193	1199	1201	rBV5	439	463	0.03%	0.004%
32	4.925	1207	1208	1210	rBV	242	91	0.01%	0.001%
33	5.043	1228	1245	1284	rBV2	597150	1530198	100.00%	12.797%
34	5.545	1399	1401	1404	rBV	285	136	0.01%	0.001%
35	5.564	1405	1407	1409	rBV	311	133	0.01%	0.001%
36	5.616	1409	1423	1460	rBV	470790	1026931	67.11%	8.588%

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 BGB12ME

Integration Parameters: LSCINT.P

Integrator: RTE

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Filtering: 5

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Peak Location: TOP

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Peak separation: 5

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

37	5.902	1500	1512	1533	rBV2	45965	103136	6.74%	0.863%
38	6.069	1552	1564	1599	rVB	317216	711906	46.52%	5.954%
39	6.349	1647	1651	1653	rBV3	514	467	0.03%	0.004%
40	6.420	1672	1673	1677	rVB	420	165	0.01%	0.001%
41	6.439	1677	1679	1682	rBV2	403	258	0.02%	0.002%
42	6.519	1700	1704	1706	rBV2	470	364	0.02%	0.003%
43	6.641	1729	1742	1748	rBV9	2439	5294	0.35%	0.044%
44	6.770	1779	1782	1788	rBV5	636	566	0.04%	0.005%
45	6.796	1788	1790	1794	rVV3	625	449	0.03%	0.004%
46	6.818	1794	1797	1800	rVB	433	234	0.02%	0.002%
47	6.831	1800	1801	1805	rBV	422	226	0.01%	0.002%
48	6.876	1813	1815	1822	rBV2	391	390	0.03%	0.003%
49	6.908	1822	1825	1826	rBV	721	385	0.03%	0.003%
50	6.989	1838	1850	1883	rBV	180232	373065	24.38%	3.120%
51	7.317	1940	1952	1971	rBV	705163	1255492	82.05%	10.499%
52	7.625	2036	2048	2078	rBV	119731	251034	16.41%	2.099%
53	7.831	2111	2112	2117	rBV2	399	338	0.02%	0.003%
54	7.854	2117	2119	2120	rBV2	312	83	0.01%	0.001%
55	7.892	2128	2131	2135	rBV3	393	278	0.02%	0.002%
56	7.924	2139	2141	2143	rVB2	216	103	0.01%	0.001%
57	7.947	2143	2148	2149	rBV2	341	275	0.02%	0.002%
58	7.979	2153	2158	2163	rVB3	576	533	0.03%	0.004%
59	8.024	2170	2172	2174	rVB	276	92	0.01%	0.001%
60	8.043	2174	2178	2180	rBV2	351	283	0.02%	0.002%
61	8.117	2183	2201	2238	rBV2	261592	816941	53.39%	6.832%
62	8.596	2347	2350	2353	rBV2	338	231	0.02%	0.002%
63	8.619	2356	2357	2362	rVB3	523	309	0.02%	0.003%
64	8.641	2362	2364	2367	rBV3	312	155	0.01%	0.001%
65	8.706	2382	2384	2387	rVB	182	86	0.01%	0.001%
66	8.738	2390	2394	2396	rBV	277	250	0.02%	0.002%
67	8.857	2419	2431	2455	rBV	689984	1248922	81.62%	10.444%
68	9.146	2514	2521	2535	rBV5	3867	7263	0.47%	0.061%
69	9.262	2555	2557	2559	rBV	251	150	0.01%	0.001%
70	9.313	2571	2573	2578	rBV	289	161	0.01%	0.001%
71	9.403	2600	2601	2604	rVB2	342	119	0.01%	0.001%
72	9.452	2614	2616	2619	rBV	298	191	0.01%	0.002%
73	9.477	2619	2624	2626	rBV2	647	625	0.04%	0.005%
74	9.558	2641	2649	2659	rVB6	3173	4841	0.32%	0.040%
75	9.667	2680	2683	2686	rBV3	740	580	0.04%	0.005%
76	9.738	2704	2705	2707	rBV3	413	147	0.01%	0.001%

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 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BGB12ME

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

77	9.760	2707	2712	2717	rVV5	1117	1373	0.09%	0.011%
78	9.854	2732	2741	2742	rBV4	1061	1095	0.07%	0.009%
79	9.908	2750	2758	2767	rBV2	8861	13384	0.87%	0.112%
80	10.021	2790	2793	2798	rBV4	691	624	0.04%	0.005%
81	10.223	2845	2856	2873	rVB	394119	680068	44.44%	5.687%
82	10.458	2925	2929	2934	rBV5	1823	1804	0.12%	0.015%
83	10.751	3010	3020	3022	rBV6	1145	1477	0.10%	0.012%
84	10.879	3055	3060	3062	rBV2	1270	1218	0.08%	0.010%
85	11.030	3103	3107	3110	rBV	916	870	0.06%	0.007%
86	11.149	3136	3144	3153	rBV6	2776	5160	0.34%	0.043%
87	11.255	3165	3177	3198	rBV	782867	1224988	80.05%	10.244%
88	11.567	3271	3274	3278	rBV4	881	895	0.06%	0.007%
89	11.628	3281	3293	3318	rVB	722930	1172179	76.60%	9.803%
90	11.908	3378	3380	3384	rBV	507	422	0.03%	0.004%
91	12.017	3411	3414	3419	rBV2	513	523	0.03%	0.004%
92	12.091	3432	3437	3438	rBV3	745	651	0.04%	0.005%
93	12.175	3461	3463	3465	rBV2	456	188	0.01%	0.002%
94	12.226	3477	3479	3480	rBV2	170	57	0.00%	0.000%
95	12.252	3484	3487	3489	rBV2	920	601	0.04%	0.005%
96	12.468	3552	3554	3555	rBV	413	140	0.01%	0.001%
97	12.886	3677	3684	3692	rBV6	2511	3479	0.23%	0.029%
98	13.513	3872	3879	3890	rVB3	7785	12102	0.79%	0.101%
99	13.641	3916	3919	3924	rVB4	1048	865	0.06%	0.007%

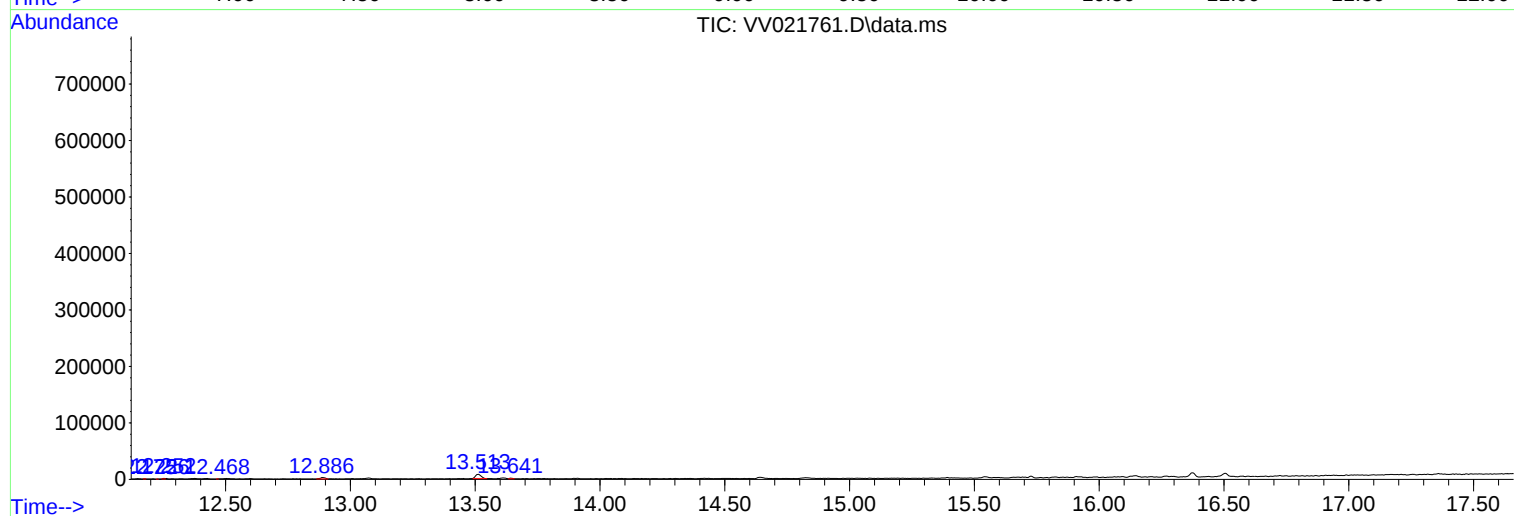
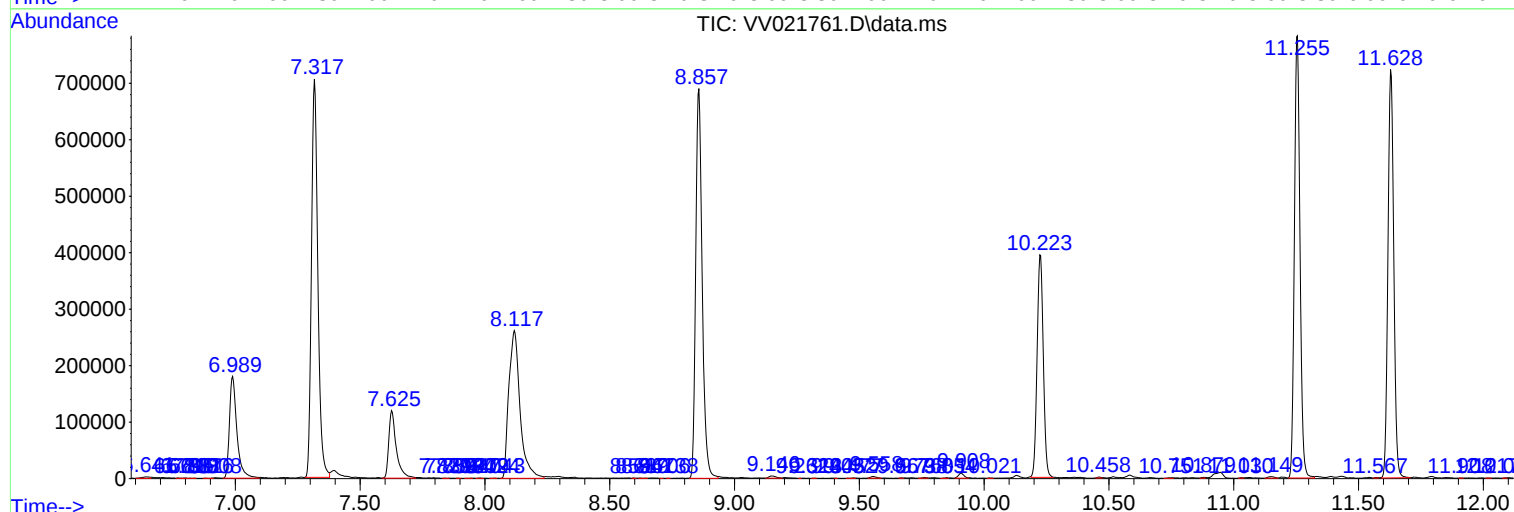
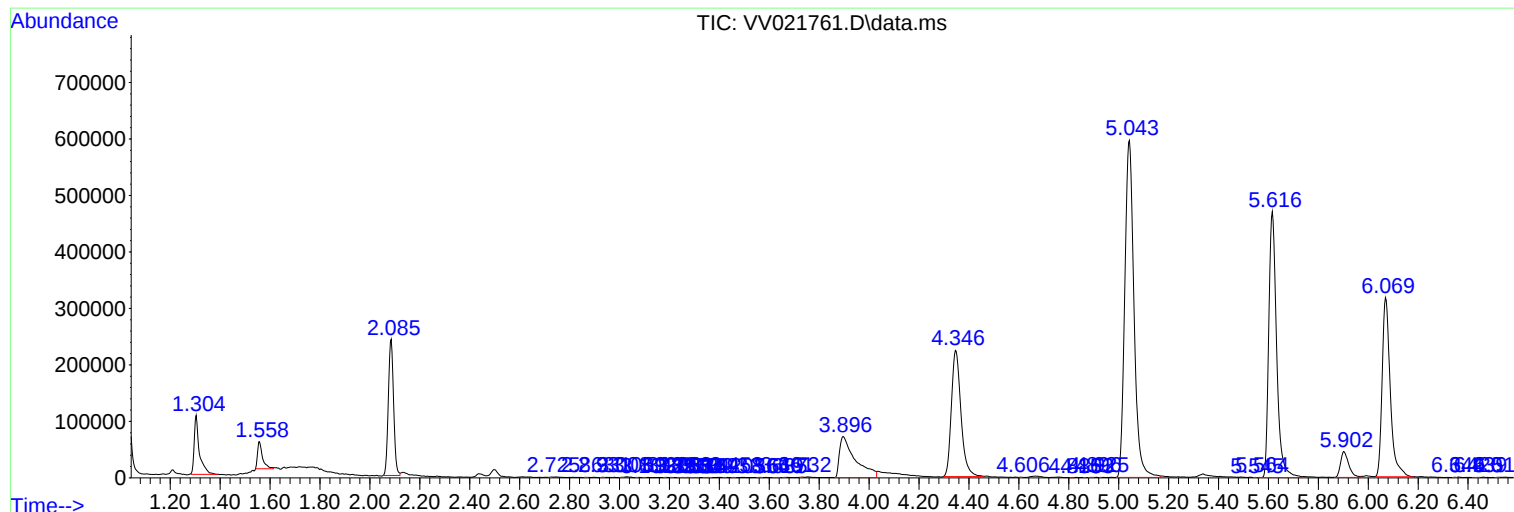
Sum of corrected areas: 11957701

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV080921\
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Operator : SY/MD
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Misc : 4.83g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGB12ME

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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Instrument :
MSVOA_V
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BGB12ME

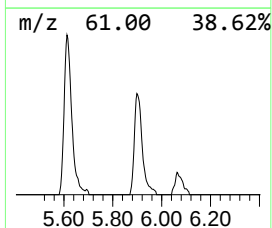
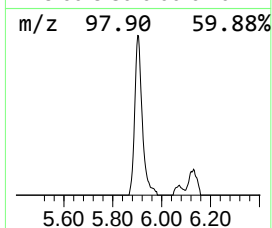
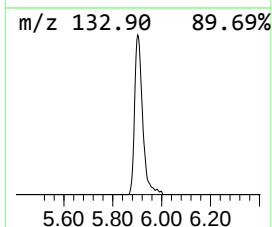
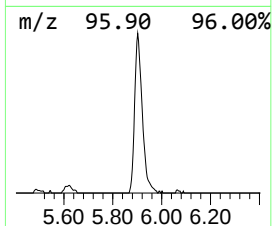
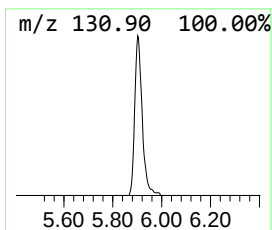
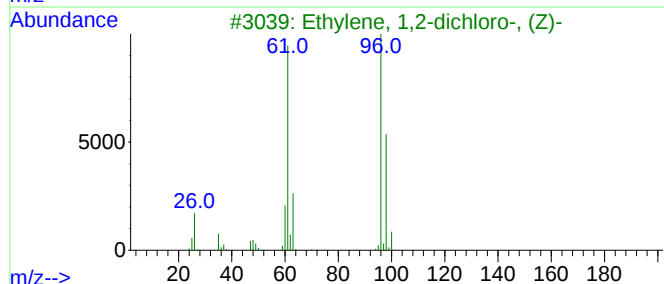
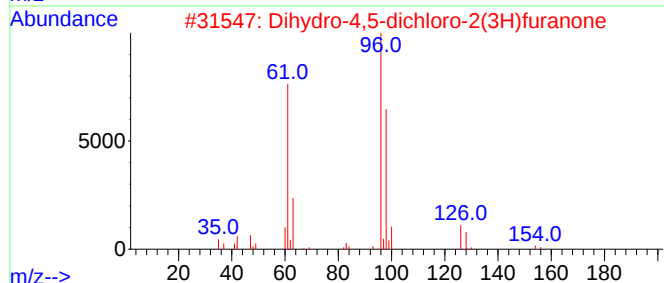
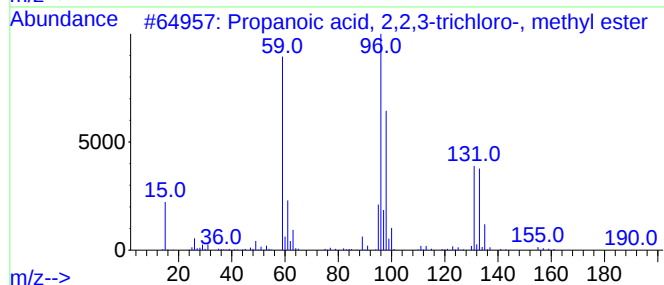
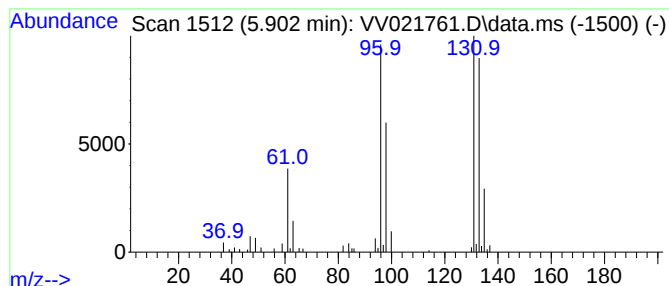
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM080221WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.902	5.02 ug/L	103136	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			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	35
3			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	35
4			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	32
5			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	5.902	5.0	ug/L	103136	1	5.616	1026930	50.0