

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV090821\
 Data File : VV022120.D
 Acq On : 08 Sep 2021 11:31
 Operator : SY/MD
 Sample : VV0908WBL01
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VBLK252

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: VV022120.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	75	82	98	rBV	194993	201971	14.94%	2.049%
2	1.561	155	162	173	rVB	158420	180371	13.34%	1.830%
3	2.105	321	331	359	rVB	338879	509257	37.66%	5.166%
4	2.400	420	423	424	rBV	285	201	0.01%	0.002%
5	2.503	449	455	471	rVB	6735	11336	0.84%	0.115%
6	2.706	514	518	519	rBV3	328	243	0.02%	0.002%
7	2.982	599	604	606	rVB3	262	189	0.01%	0.002%
8	2.995	606	608	611	rVB2	353	181	0.01%	0.002%
9	3.018	611	615	617	rVB2	355	202	0.01%	0.002%
10	3.034	618	620	626	rVB2	403	256	0.02%	0.003%
11	3.117	643	646	648	rBV	289	175	0.01%	0.002%
12	3.233	679	682	685	rBV	334	250	0.02%	0.003%
13	3.391	724	731	732	rBV3	351	252	0.02%	0.003%
14	3.683	819	822	828	rVB2	390	350	0.03%	0.004%
15	3.873	871	881	913	rBV2	103169	277371	20.51%	2.813%
16	4.346	1011	1028	1058	rBV	215042	530386	39.23%	5.380%
17	4.770	1159	1160	1164	rBV2	264	177	0.01%	0.002%
18	4.908	1200	1203	1206	rBV2	277	231	0.02%	0.002%
19	4.950	1213	1216	1222	rBV2	368	269	0.02%	0.003%
20	5.043	1228	1245	1276	rBV3	531924	1352075	100.00%	13.715%
21	5.400	1353	1356	1359	rBV	268	180	0.01%	0.002%
22	5.416	1359	1361	1365	rBV3	473	304	0.02%	0.003%
23	5.494	1381	1385	1389	rBV2	382	295	0.02%	0.003%
24	5.522	1389	1394	1395	rBV2	644	499	0.04%	0.005%
25	5.548	1399	1402	1406	rBV5	446	379	0.03%	0.004%
26	5.616	1409	1423	1453	rBV	358931	733546	54.25%	7.441%
27	5.905	1502	1513	1532	rBV3	22417	48543	3.59%	0.492%
28	6.069	1550	1564	1585	rBV	295038	602387	44.55%	6.110%
29	6.426	1669	1675	1678	rBV2	213	176	0.01%	0.002%
30	6.542	1705	1711	1712	rBV2	374	265	0.02%	0.003%
31	6.580	1720	1723	1724	rBV	304	163	0.01%	0.002%
32	6.632	1735	1739	1741	rBV2	404	338	0.02%	0.003%
33	6.670	1748	1751	1755	rBV2	414	257	0.02%	0.003%
34	6.799	1786	1791	1795	rBV2	167	164	0.01%	0.002%
35	6.847	1803	1806	1810	rVB2	406	281	0.02%	0.003%
36	6.870	1810	1813	1820	rBV2	278	228	0.02%	0.002%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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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

37	6.985	1838	1849	1874	rBV	159303	293166	21.68%	2.974%
38	7.214	1918	1920	1923	rBV2	301	237	0.02%	0.002%
39	7.233	1923	1926	1928	rBV	399	235	0.02%	0.002%
40	7.249	1928	1931	1932	rBV2	463	208	0.02%	0.002%
41	7.317	1939	1952	1969	rBV	636144	1101820	81.49%	11.176%
42	7.622	2036	2047	2075	rBV	109733	191422	14.16%	1.942%
43	7.789	2096	2099	2104	rVB3	438	412	0.03%	0.004%
44	7.960	2145	2152	2153	rBV3	280	270	0.02%	0.003%
45	8.050	2178	2180	2181	rVB3	401	146	0.01%	0.001%
46	8.088	2181	2192	2224	rBV	306237	573757	42.44%	5.820%
47	8.378	2279	2282	2285	rVB2	460	294	0.02%	0.003%
48	8.526	2325	2328	2329	rBV	556	319	0.02%	0.003%
49	8.571	2340	2342	2343	rBV	352	148	0.01%	0.002%
50	8.612	2351	2355	2360	rBV2	692	598	0.04%	0.006%
51	8.715	2384	2387	2390	rBV	233	188	0.01%	0.002%
52	8.854	2417	2430	2468	rBV	532857	877004	64.86%	8.896%
53	9.018	2479	2481	2485	rVB3	562	443	0.03%	0.004%
54	9.098	2501	2506	2507	rBV3	512	329	0.02%	0.003%
55	9.143	2518	2520	2528	rVB4	858	865	0.06%	0.009%
56	9.227	2543	2546	2549	rVV	273	172	0.01%	0.002%
57	9.246	2549	2552	2554	rVV	318	169	0.01%	0.002%
58	9.384	2593	2595	2600	rVB2	402	265	0.02%	0.003%
59	9.477	2621	2624	2627	rBV	333	263	0.02%	0.003%
60	9.509	2632	2634	2638	rVB2	318	168	0.01%	0.002%
61	9.558	2644	2649	2651	rBV	490	321	0.02%	0.003%
62	9.596	2658	2661	2667	rBV2	184	193	0.01%	0.002%
63	9.638	2667	2674	2679	rVB2	334	429	0.03%	0.004%
64	9.673	2679	2685	2688	rBV2	476	339	0.03%	0.003%
65	9.709	2694	2696	2704	rVB	302	231	0.02%	0.002%
66	9.937	2761	2767	2771	rBV	420	378	0.03%	0.004%
67	10.001	2785	2787	2791	rVB2	355	165	0.01%	0.002%
68	10.133	2817	2828	2839	rBV3	3276	5949	0.44%	0.060%
69	10.217	2842	2854	2874	rBV	377550	583830	43.18%	5.922%
70	10.564	2960	2962	2963	rBV	323	175	0.01%	0.002%
71	10.577	2963	2966	2968	rBV2	617	438	0.03%	0.004%
72	10.760	3020	3023	3026	rBV	273	153	0.01%	0.002%
73	10.792	3027	3033	3037	rBV	517	493	0.04%	0.005%
74	10.837	3045	3047	3051	rVB2	411	218	0.02%	0.002%
75	10.882	3058	3061	3064	rBV3	429	315	0.02%	0.003%
76	11.040	3103	3110	3111	rBV3	443	445	0.03%	0.005%

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 ClientSampleId :
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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

77	11.111	3130	3132	3134	rBV	261	155	0.01%	0.002%
78	11.152	3139	3145	3153	rVB4	1521	1854	0.14%	0.019%
79	11.188	3153	3156	3160	rBV3	464	294	0.02%	0.003%
80	11.249	3164	3175	3195	rBV	517098	808511	59.80%	8.201%
81	11.384	3212	3217	3225	rBV5	1739	2594	0.19%	0.026%
82	11.497	3248	3252	3256	rBV	390	313	0.02%	0.003%
83	11.522	3256	3260	3264	rVB3	368	305	0.02%	0.003%
84	11.548	3264	3268	3272	rBV4	632	647	0.05%	0.007%
85	11.570	3273	3275	3280	rVB2	406	279	0.02%	0.003%
86	11.625	3280	3292	3316	rBV	601791	949666	70.24%	9.633%
87	11.831	3353	3356	3360	rBV2	524	374	0.03%	0.004%
88	11.934	3386	3388	3391	rBV	284	159	0.01%	0.002%
89	12.230	3476	3480	3487	rVB2	283	328	0.02%	0.003%
90	12.394	3529	3531	3535	rBV	393	235	0.02%	0.002%
91	12.439	3543	3545	3547	rBV2	365	189	0.01%	0.002%
92	12.471	3554	3555	3559	rBV2	259	173	0.01%	0.002%
93	12.587	3589	3591	3592	rBV	363	152	0.01%	0.002%
94	12.660	3609	3614	3615	rBV2	419	264	0.02%	0.003%
95	12.828	3664	3666	3668	rVB	355	167	0.01%	0.002%
96	12.873	3678	3680	3684	rVB	359	201	0.01%	0.002%
97	12.956	3704	3706	3709	rBV	419	185	0.01%	0.002%
98	13.037	3727	3731	3737	rVB3	652	468	0.03%	0.005%
99	13.066	3737	3740	3742	rBV2	295	163	0.01%	0.002%
100	14.705	4248	4250	4254	rBV2	345	223	0.02%	0.002%

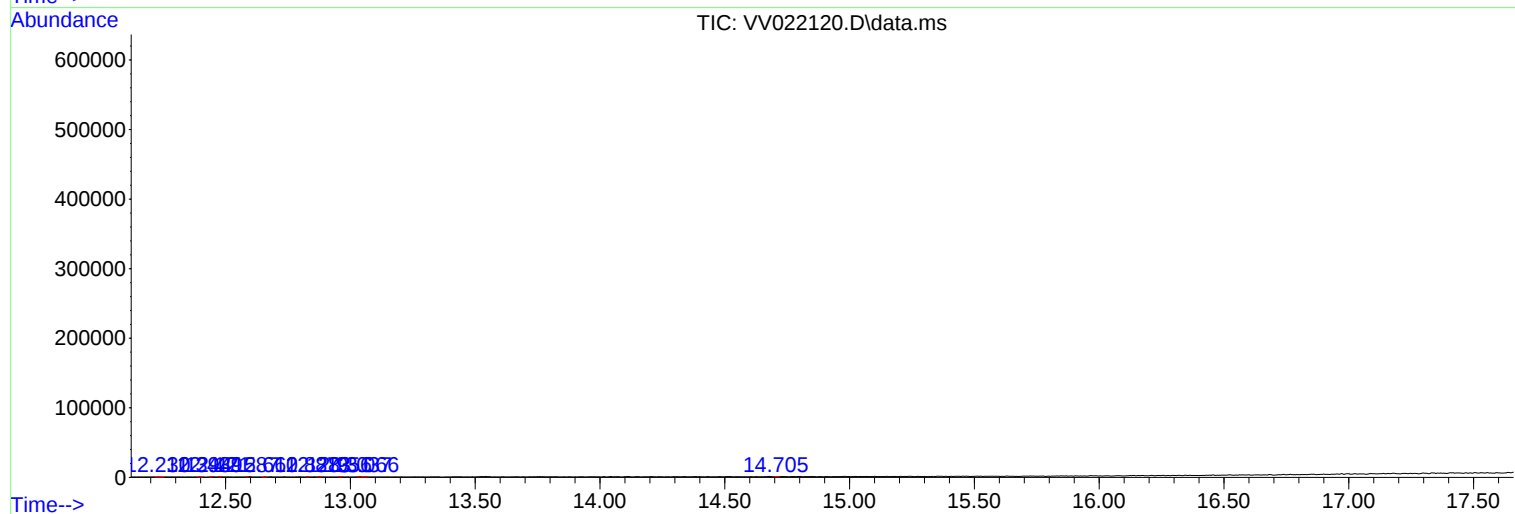
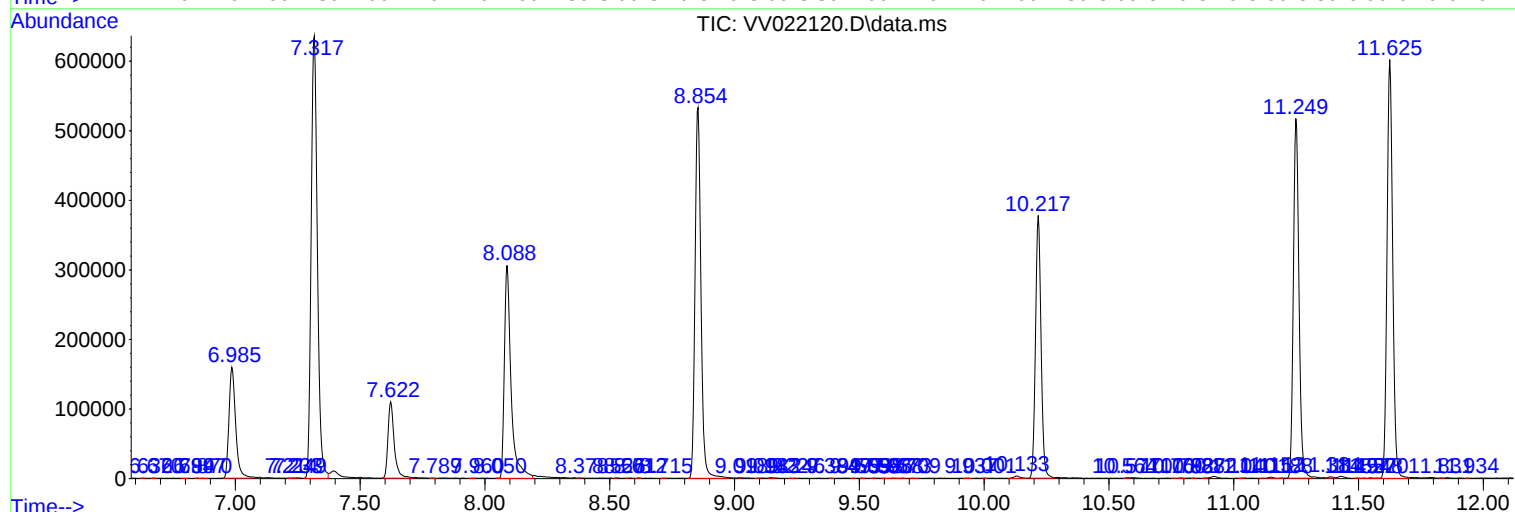
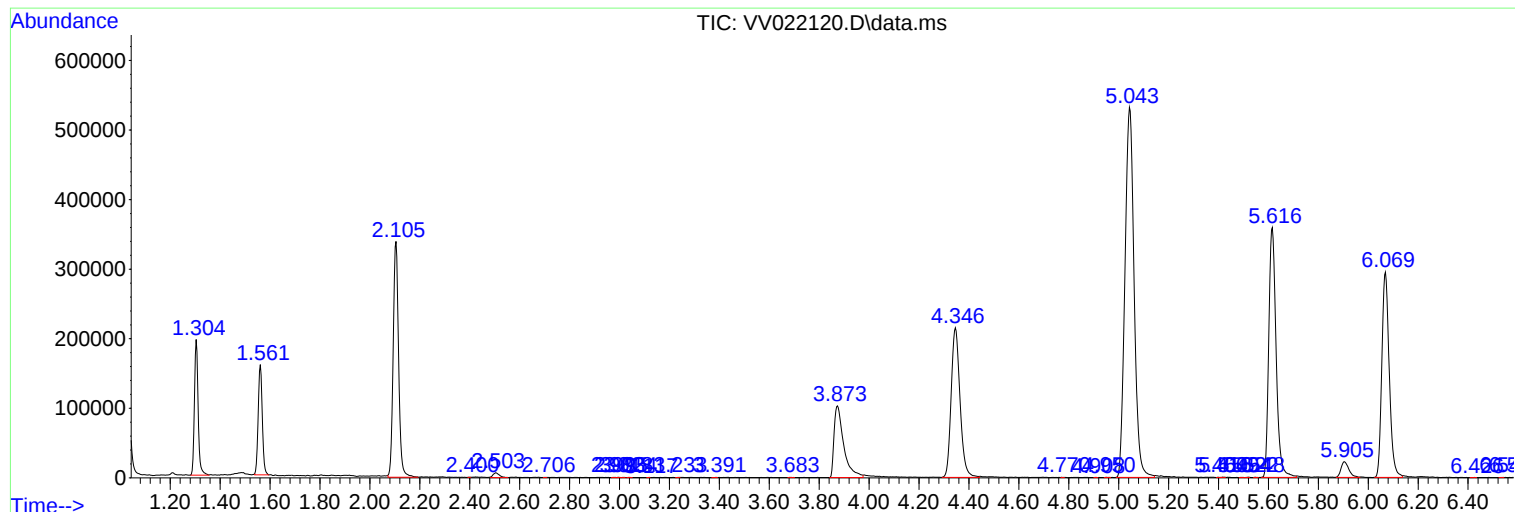
Sum of corrected areas: 9858617

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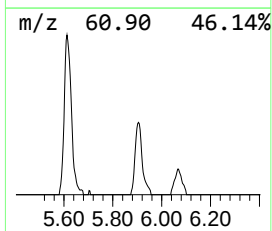
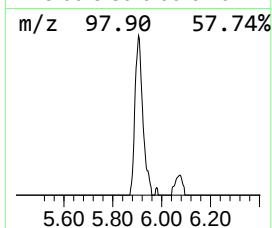
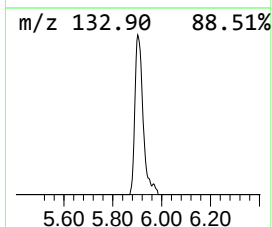
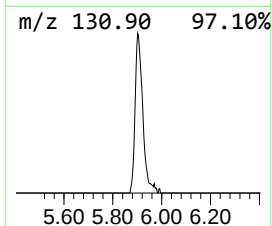
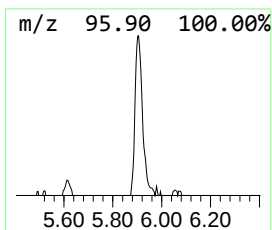
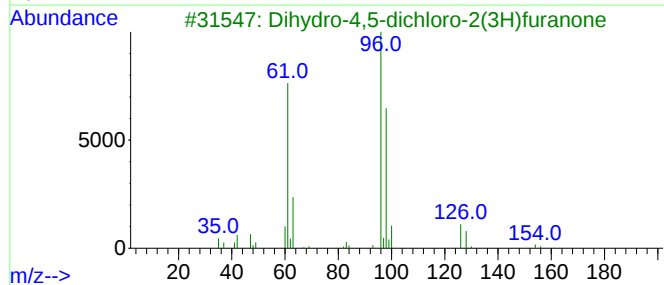
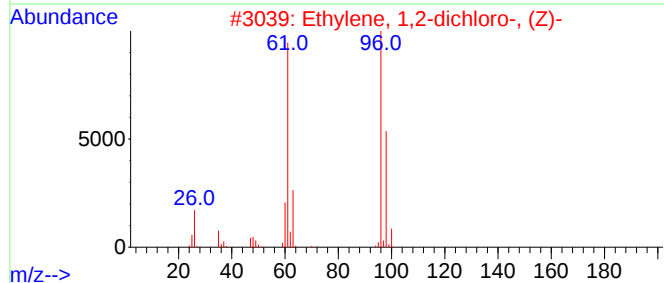
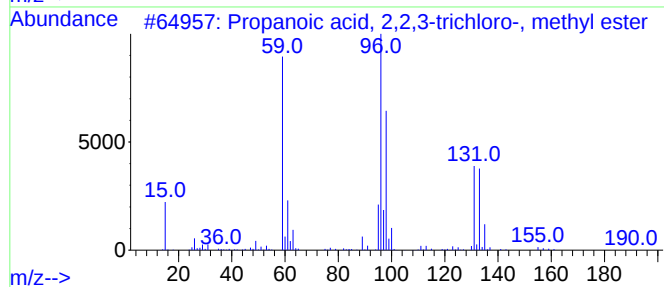
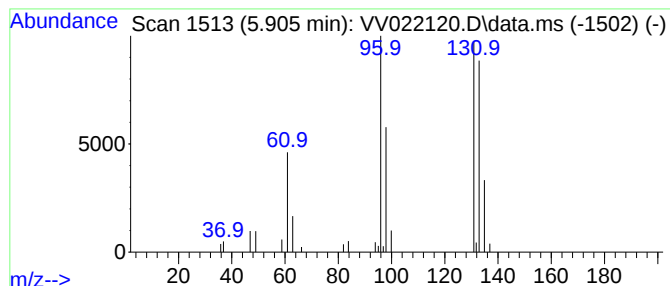
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082721WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.905	3.31 ug/L	48543	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	38
3			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	35
4			2-Chloro-5-methylthiazole	133	C4H4ClNS	033342-65-3	25
5			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	23



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	5.905	3.3	ug/L	48543	1	5.616	733546	50.0