

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV083021\
 Data File : VV021994.D
 Acq On : 30 Aug 2021 11:01
 Operator : SY/MD
 Sample : M3573-01
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 ESQK5

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: VV021994.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	96	rVB	178809	178873	13.96%	1.804%
2	1.565	156	163	177	rVB	144606	166208	12.98%	1.676%
3	2.105	321	331	345	rBV	287138	420154	32.80%	4.237%
4	2.327	398	400	403	rVB3	708	319	0.02%	0.003%
5	2.503	449	455	457	rBV3	1139	1205	0.09%	0.012%
6	2.696	512	515	519	rBV	414	304	0.02%	0.003%
7	2.745	527	530	532	rBV2	219	157	0.01%	0.002%
8	2.761	533	535	536	rBV2	392	136	0.01%	0.001%
9	2.857	563	565	569	rBV	301	214	0.02%	0.002%
10	2.921	584	585	587	rVB	301	99	0.01%	0.001%
11	2.950	592	594	598	rVB4	361	191	0.01%	0.002%
12	2.992	605	607	610	rVB2	275	147	0.01%	0.001%
13	3.015	612	614	617	rBV2	226	160	0.01%	0.002%
14	3.208	668	674	677	rBV2	237	261	0.02%	0.003%
15	3.285	696	698	701	rVB2	333	142	0.01%	0.001%
16	3.468	753	755	757	rVB2	240	132	0.01%	0.001%
17	3.516	765	770	774	rBV2	373	347	0.03%	0.003%
18	3.548	777	780	781	rBV2	181	117	0.01%	0.001%
19	3.706	826	829	830	rBV	229	98	0.01%	0.001%
20	3.812	860	862	868	rVB2	406	288	0.02%	0.003%
21	3.876	872	882	919	rBV	103770	285824	22.31%	2.882%
22	4.352	1011	1030	1059	rBV	191691	506949	39.58%	5.112%
23	4.802	1167	1170	1175	rBV2	413	418	0.03%	0.004%
24	4.870	1188	1191	1195	rBV3	577	366	0.03%	0.004%
25	4.915	1203	1205	1207	rBV2	325	118	0.01%	0.001%
26	5.047	1226	1246	1270	rBV2	504529	1280890	100.00%	12.916%
27	5.416	1359	1361	1365	rVB3	658	406	0.03%	0.004%
28	5.445	1368	1370	1372	rBV	370	157	0.01%	0.002%
29	5.487	1378	1383	1385	rBV2	565	350	0.03%	0.004%
30	5.513	1390	1391	1393	rVB	468	115	0.01%	0.001%
31	5.619	1411	1424	1453	rBV	383982	787773	61.50%	7.943%
32	5.870	1500	1502	1503	rBV2	593	228	0.02%	0.002%
33	5.908	1504	1514	1535	rVB4	22083	47913	3.74%	0.483%
34	5.998	1540	1542	1549	rBV2	301	245	0.02%	0.002%
35	6.072	1551	1565	1587	rBV	279201	574456	44.85%	5.792%
36	6.336	1643	1647	1648	rBV3	246	173	0.01%	0.002%

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 Title : VOC Analysis

37	6.381	1655	1661	1667	rBV5	544	761	0.06%	0.008%
38	6.426	1672	1675	1677	rBV3	503	294	0.02%	0.003%
39	6.458	1683	1685	1687	rBV3	366	120	0.01%	0.001%
40	6.613	1728	1733	1736	rBV	489	398	0.03%	0.004%
41	6.635	1738	1740	1741	rBV	525	240	0.02%	0.002%
42	6.712	1763	1764	1766	rBV2	329	141	0.01%	0.001%
43	6.777	1781	1784	1785	rBV2	179	113	0.01%	0.001%
44	6.793	1785	1789	1796	rVB3	599	515	0.04%	0.005%
45	6.834	1798	1802	1805	rBV3	385	285	0.02%	0.003%
46	6.937	1832	1834	1837	rVB	431	218	0.02%	0.002%
47	6.989	1838	1850	1871	rBV	156903	283510	22.13%	2.859%
48	7.275	1936	1939	1940	rBV2	500	240	0.02%	0.002%
49	7.317	1941	1952	1972	rBV	611965	1060881	82.82%	10.697%
50	7.580	2032	2034	2037	rBV3	347	259	0.02%	0.003%
51	7.625	2037	2048	2069	rBV	106526	186943	14.59%	1.885%
52	7.857	2116	2120	2121	rBV2	382	250	0.02%	0.003%
53	7.899	2128	2133	2134	rBV2	446	265	0.02%	0.003%
54	7.912	2134	2137	2139	rVV	312	153	0.01%	0.002%
55	7.947	2143	2148	2149	rBV2	349	244	0.02%	0.002%
56	7.989	2156	2161	2165	rBV5	553	534	0.04%	0.005%
57	8.031	2171	2174	2178	rBV2	276	220	0.02%	0.002%
58	8.092	2182	2193	2229	rBV2	310751	595265	46.47%	6.002%
59	8.564	2338	2340	2342	rVB2	651	204	0.02%	0.002%
60	8.741	2394	2395	2397	rVV	332	158	0.01%	0.002%
61	8.767	2401	2403	2406	rVV2	335	165	0.01%	0.002%
62	8.854	2418	2430	2454	rBV	582376	957109	74.72%	9.651%
63	9.098	2505	2506	2508	rBV	355	138	0.01%	0.001%
64	9.140	2516	2519	2520	rBV	786	422	0.03%	0.004%
65	9.214	2538	2542	2546	rBV	354	344	0.03%	0.003%
66	9.239	2549	2550	2553	rVV2	277	138	0.01%	0.001%
67	9.284	2562	2564	2568	rVB	386	206	0.02%	0.002%
68	9.317	2572	2574	2578	rVB2	250	183	0.01%	0.002%
69	9.381	2591	2594	2597	rVB	320	169	0.01%	0.002%
70	9.429	2606	2609	2610	rBV2	261	153	0.01%	0.002%
71	9.551	2645	2647	2648	rBV2	488	229	0.02%	0.002%
72	9.577	2653	2655	2658	rVB	340	180	0.01%	0.002%
73	9.680	2683	2687	2692	rVV4	443	338	0.03%	0.003%
74	9.702	2692	2694	2699	rVB	297	247	0.02%	0.002%
75	9.731	2701	2703	2708	rVB2	344	150	0.01%	0.002%
76	9.805	2722	2726	2727	rBV	514	248	0.02%	0.003%

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77	9.934	2763	2766	2768	rBV2	200	119	0.01%	0.001%
78	10.008	2785	2789	2790	rBV	346	178	0.01%	0.002%
79	10.130	2817	2827	2839	rBV5	2547	4326	0.34%	0.044%
80	10.217	2843	2854	2878	rBV	378228	603326	47.10%	6.084%
81	10.548	2953	2957	2962	rBV3	605	639	0.05%	0.006%
82	10.580	2963	2967	2972	rVV4	485	544	0.04%	0.005%
83	10.657	2989	2991	2992	rBV	258	131	0.01%	0.001%
84	10.918	3065	3072	3084	rBV6	2730	4537	0.35%	0.046%
85	11.149	3141	3144	3153	rVB5	1191	1323	0.10%	0.013%
86	11.252	3164	3176	3200	rBV	618016	964528	75.30%	9.726%
87	11.548	3260	3268	3270	rBV4	1819	2297	0.18%	0.023%
88	11.625	3280	3292	3313	rBV	608147	983671	76.80%	9.919%
89	11.850	3358	3362	3368	rVB2	591	527	0.04%	0.005%
90	12.468	3552	3554	3556	rBV2	266	97	0.01%	0.001%
91	12.497	3560	3563	3564	rBV	301	149	0.01%	0.002%
92	12.513	3567	3568	3573	rVV	302	102	0.01%	0.001%
93	12.587	3588	3591	3595	rBV2	332	229	0.02%	0.002%
94	12.648	3607	3610	3611	rBV2	558	277	0.02%	0.003%
95	12.693	3620	3624	3626	rBV2	347	231	0.02%	0.002%
96	12.738	3635	3638	3642	rBV3	372	341	0.03%	0.003%
97	12.841	3667	3670	3673	rBV2	375	250	0.02%	0.003%
98	12.902	3687	3689	3691	rBV3	326	149	0.01%	0.002%
99	13.419	3847	3850	3854	rBV2	360	374	0.03%	0.004%
100	13.458	3860	3862	3870	rVB2	587	451	0.04%	0.005%

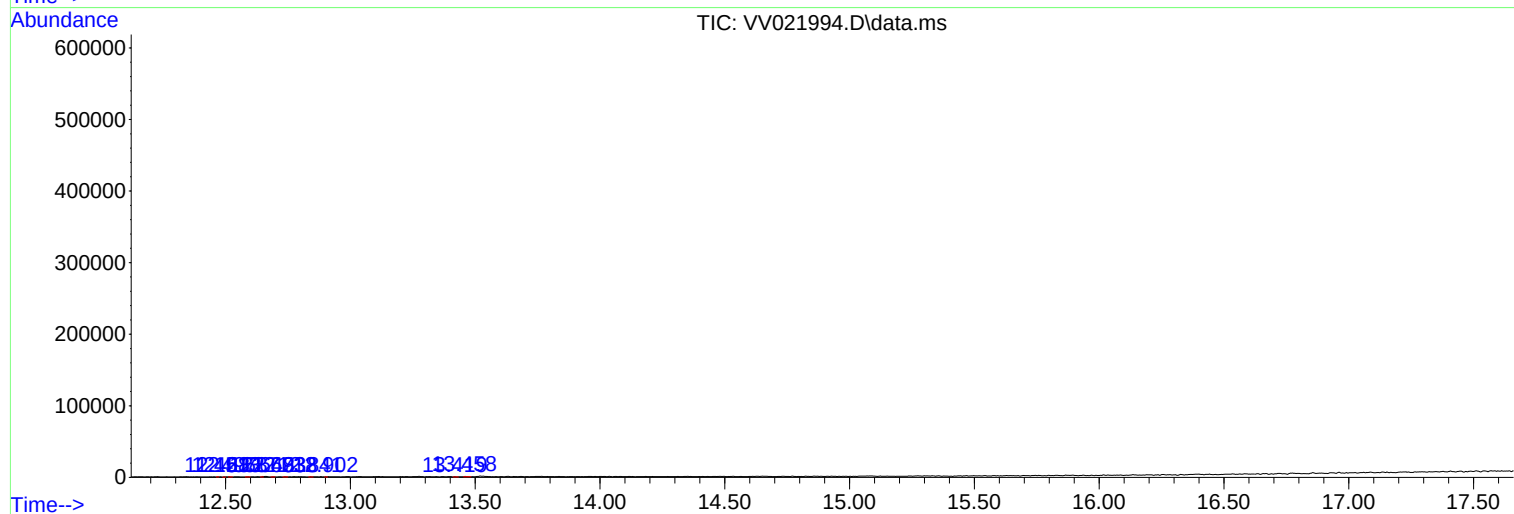
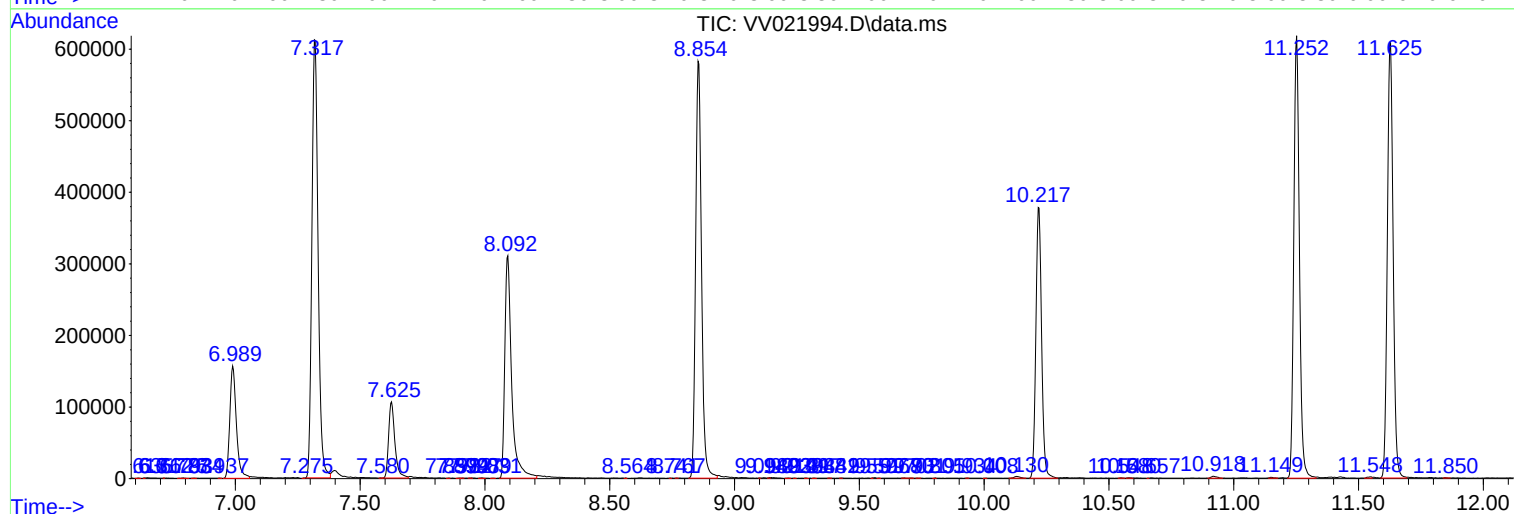
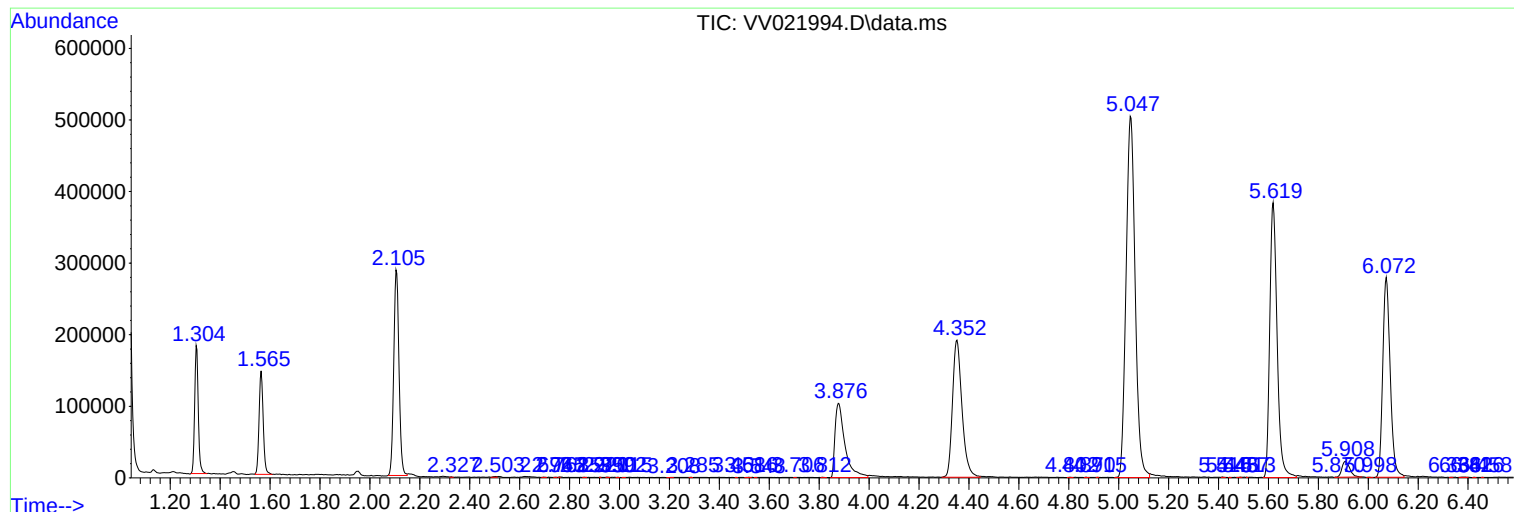
Sum of corrected areas: 9917359

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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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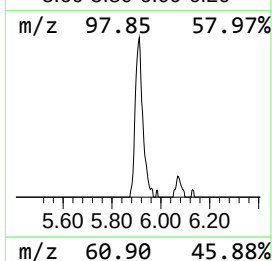
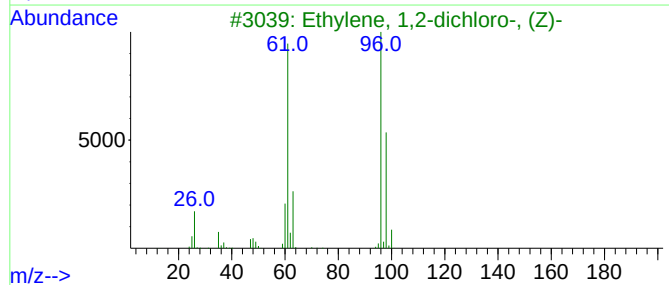
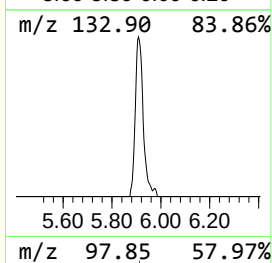
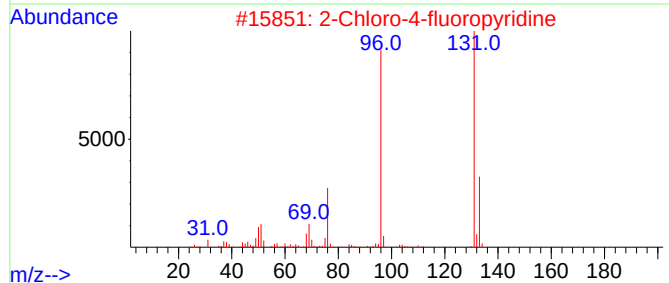
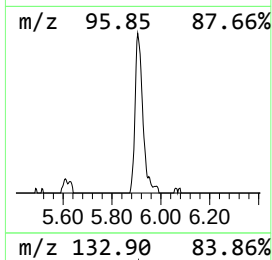
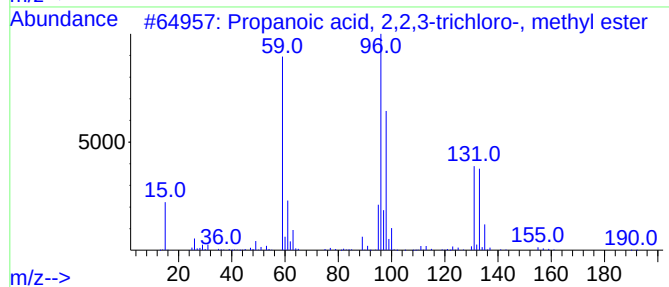
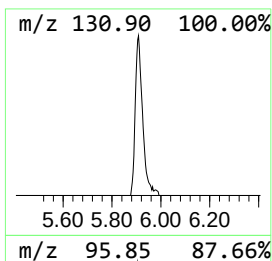
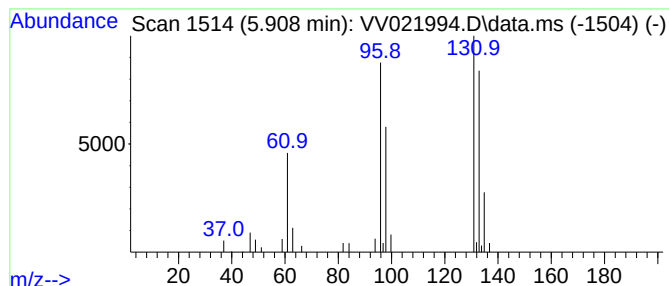
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 Propanoic acid, 2,2,3-trich... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.908	3.04 ug/L	47913	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	50
2			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	38
3			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	35
4			2-Chloro-5-methylthiazole	133	C4H4ClNS	033342-65-3	27
5			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	5.908	3.0	ug/L	47913	1	5.619	787773	50.0