

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011322\
 Data File : VV024346.D
 Acq On : 13 Jan 2022 11:38
 Operator : SY/MD
 Sample : VV0113WBL01
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VBLK293

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\SFAMVLM123121WMA.M
 Title : VOC Analysis

Signal : TIC: VV024346.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.307	76	83	98	rVB	127404	130344	14.48%	1.925%
2	1.568	157	164	176	rBV	106689	119058	13.23%	1.758%
3	2.005	298	300	301	rBV	394	187	0.02%	0.003%
4	2.108	321	332	359	rBV	234291	347871	38.65%	5.136%
5	2.285	382	387	388	rBV	257	220	0.02%	0.003%
6	2.452	436	439	443	rBV2	228	199	0.02%	0.003%
7	2.510	451	457	462	rVB5	933	1091	0.12%	0.016%
8	2.558	470	472	475	rBV2	304	231	0.03%	0.003%
9	2.619	485	491	495	rBV4	555	775	0.09%	0.011%
10	2.728	523	525	529	rVB2	387	277	0.03%	0.004%
11	2.902	575	579	582	rBB	240	178	0.02%	0.003%
12	2.921	582	585	589	rBV	206	200	0.02%	0.003%
13	2.989	600	606	609	rBV2	277	321	0.04%	0.005%
14	3.008	610	612	616	rVB	289	179	0.02%	0.003%
15	3.056	625	627	629	rBV	271	170	0.02%	0.003%
16	3.326	708	711	715	rBV	177	197	0.02%	0.003%
17	3.722	831	834	837	rBV	171	175	0.02%	0.003%
18	3.886	875	885	918	rBV	52606	165685	18.41%	2.446%
19	4.243	994	996	1001	rVB2	387	210	0.02%	0.003%
20	4.346	1011	1028	1059	rBV	155473	380341	42.26%	5.616%
21	4.506	1077	1078	1083	rVB2	335	199	0.02%	0.003%
22	4.571	1095	1098	1099	rBV	359	164	0.02%	0.002%
23	4.654	1120	1124	1130	rBV	184	290	0.03%	0.004%
24	4.838	1177	1181	1187	rBB2	393	424	0.05%	0.006%
25	5.043	1225	1245	1282	rBV2	346045	899947	100.00%	13.288%
26	5.317	1327	1330	1331	rBV2	346	160	0.02%	0.002%
27	5.458	1371	1374	1376	rBV2	238	157	0.02%	0.002%
28	5.571	1407	1409	1410	rBV	415	203	0.02%	0.003%
29	5.616	1411	1423	1457	rBV	244894	492643	54.74%	7.274%
30	5.834	1489	1491	1496	rVB3	435	255	0.03%	0.004%
31	5.908	1504	1514	1528	rBV5	13601	28034	3.12%	0.414%
32	6.066	1551	1563	1584	rBV	194315	393648	43.74%	5.812%
33	6.249	1616	1620	1624	rBV2	431	377	0.04%	0.006%
34	6.362	1654	1655	1659	rVB	425	194	0.02%	0.003%
35	6.387	1660	1663	1667	rBV	232	192	0.02%	0.003%
36	6.423	1667	1674	1679	rBV2	199	280	0.03%	0.004%

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 Title : VOC Analysis

37	6.548	1708	1713	1716	rBV2	357	255	0.03%	0.004%
38	6.606	1724	1731	1734	rBB2	279	292	0.03%	0.004%
39	6.854	1805	1808	1812	rBV	270	303	0.03%	0.004%
40	6.899	1817	1822	1826	rBV	179	247	0.03%	0.004%
41	6.985	1837	1849	1869	rBV	113271	203957	22.66%	3.011%
42	7.127	1891	1893	1896	rVB	322	187	0.02%	0.003%
43	7.313	1939	1951	1971	rBV	433494	744096	82.68%	10.986%
44	7.587	2032	2036	2037	rBV2	307	245	0.03%	0.004%
45	7.619	2037	2046	2068	rVV	79339	140825	15.65%	2.079%
46	7.834	2108	2113	2115	rBB	327	217	0.02%	0.003%
47	7.853	2116	2119	2123	rBV	253	223	0.02%	0.003%
48	7.911	2135	2137	2140	rVB	399	224	0.02%	0.003%
49	7.940	2140	2146	2153	rBB2	451	700	0.08%	0.010%
50	7.985	2158	2160	2163	rBV	289	196	0.02%	0.003%
51	8.024	2169	2172	2177	rBV2	258	282	0.03%	0.004%
52	8.088	2182	2192	2227	rBV	198858	385309	42.81%	5.689%
53	8.362	2274	2277	2280	rBV2	374	239	0.03%	0.004%
54	8.423	2289	2296	2304	rVB4	1743	2569	0.29%	0.038%
55	8.571	2340	2342	2344	rBV4	334	159	0.02%	0.002%
56	8.625	2354	2359	2363	rBB	316	302	0.03%	0.004%
57	8.644	2363	2365	2367	rBV	284	182	0.02%	0.003%
58	8.850	2418	2429	2453	rBV	373176	603366	67.04%	8.909%
59	9.030	2481	2485	2491	rVB4	515	573	0.06%	0.008%
60	9.120	2510	2513	2515	rBV2	267	176	0.02%	0.003%
61	9.133	2515	2517	2518	rBV	399	185	0.02%	0.003%
62	9.220	2540	2544	2547	rVB2	378	204	0.02%	0.003%
63	9.770	2712	2715	2720	rVB2	287	297	0.03%	0.004%
64	9.808	2721	2727	2731	rBB	227	254	0.03%	0.004%
65	9.857	2737	2742	2745	rVB	192	192	0.02%	0.003%
66	9.937	2763	2767	2769	rVB	347	273	0.03%	0.004%
67	9.963	2769	2775	2778	rBV	176	249	0.03%	0.004%
68	9.985	2779	2782	2784	rVV2	222	157	0.02%	0.002%
69	10.088	2811	2814	2817	rBV	215	180	0.02%	0.003%
70	10.130	2818	2827	2834	rVB4	1880	2661	0.30%	0.039%
71	10.214	2841	2853	2877	rVB	256673	404562	44.95%	5.973%
72	10.304	2879	2881	2883	rVV2	398	189	0.02%	0.003%
73	10.323	2885	2887	2891	rVB3	482	320	0.04%	0.005%
74	10.477	2933	2935	2940	rVB	316	182	0.02%	0.003%
75	10.522	2942	2949	2951	rBV2	307	316	0.04%	0.005%
76	10.574	2960	2965	2966	rBV2	282	232	0.03%	0.003%

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 Title : VOC Analysis

77	10.583	2966	2968	2975	rVB5	702	692	0.08%	0.010%
78	10.911	3065	3070	3071	rBV2	1201	830	0.09%	0.012%
79	11.149	3138	3144	3150	rVB5	939	1210	0.13%	0.018%
80	11.249	3163	3175	3196	rBV	381705	586138	65.13%	8.654%
81	11.426	3225	3230	3237	rVB5	1781	2089	0.23%	0.031%
82	11.583	3274	3279	3280	rBV2	219	165	0.02%	0.002%
83	11.622	3280	3291	3311	rVV	459565	715651	79.52%	10.566%
84	11.789	3340	3343	3351	rVB5	754	709	0.08%	0.010%
85	11.853	3359	3363	3366	rBV2	591	373	0.04%	0.006%
86	12.066	3425	3429	3434	rBV	363	324	0.04%	0.005%
87	12.516	3563	3569	3573	rBV2	402	476	0.05%	0.007%
88	12.593	3591	3593	3596	rBV2	344	221	0.02%	0.003%
89	12.631	3602	3605	3608	rBV2	249	209	0.02%	0.003%
90	13.268	3799	3803	3809	rVB3	629	695	0.08%	0.010%
91	13.429	3849	3853	3855	rBV	254	188	0.02%	0.003%
92	13.493	3871	3873	3874	rBV	359	164	0.02%	0.002%
93	13.744	3949	3951	3952	rBV2	459	179	0.02%	0.003%
94	14.040	4041	4043	4045	rBV	427	247	0.03%	0.004%
95	14.155	4076	4079	4083	rBV2	434	324	0.04%	0.005%
96	14.204	4091	4094	4096	rBV2	250	157	0.02%	0.002%
97	14.274	4113	4116	4122	rBV3	300	357	0.04%	0.005%
98	14.326	4130	4132	4135	rBV	318	173	0.02%	0.003%
99	14.348	4135	4139	4142	rBV3	351	375	0.04%	0.006%
100	14.413	4157	4159	4162	rBV	369	249	0.03%	0.004%

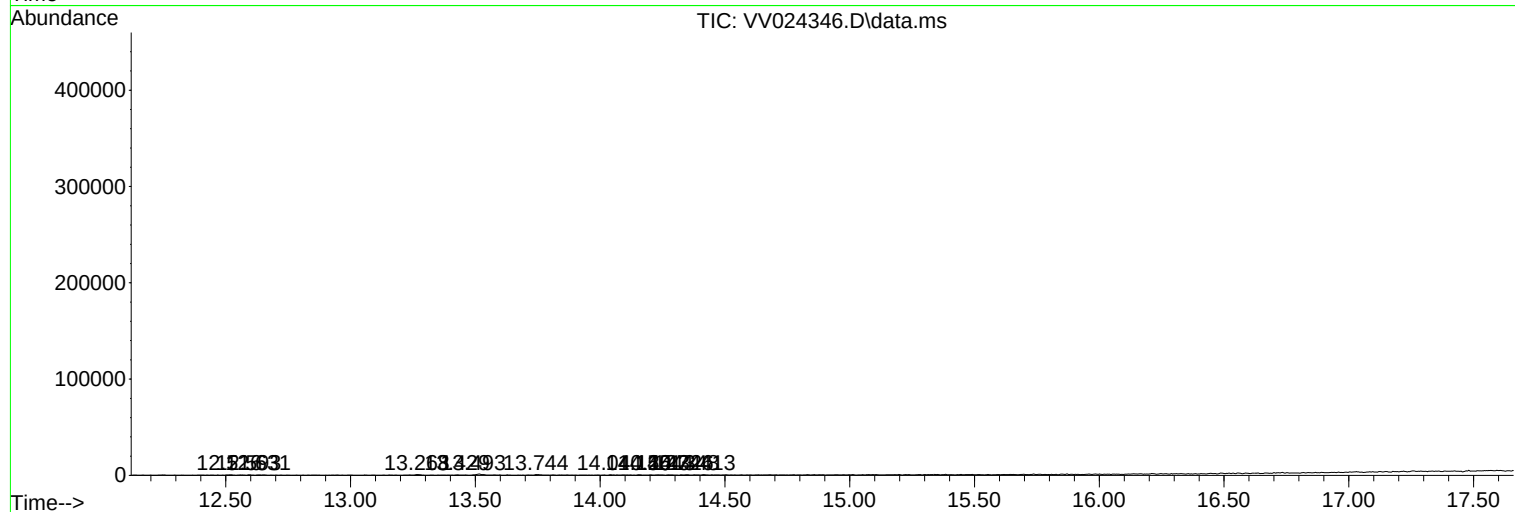
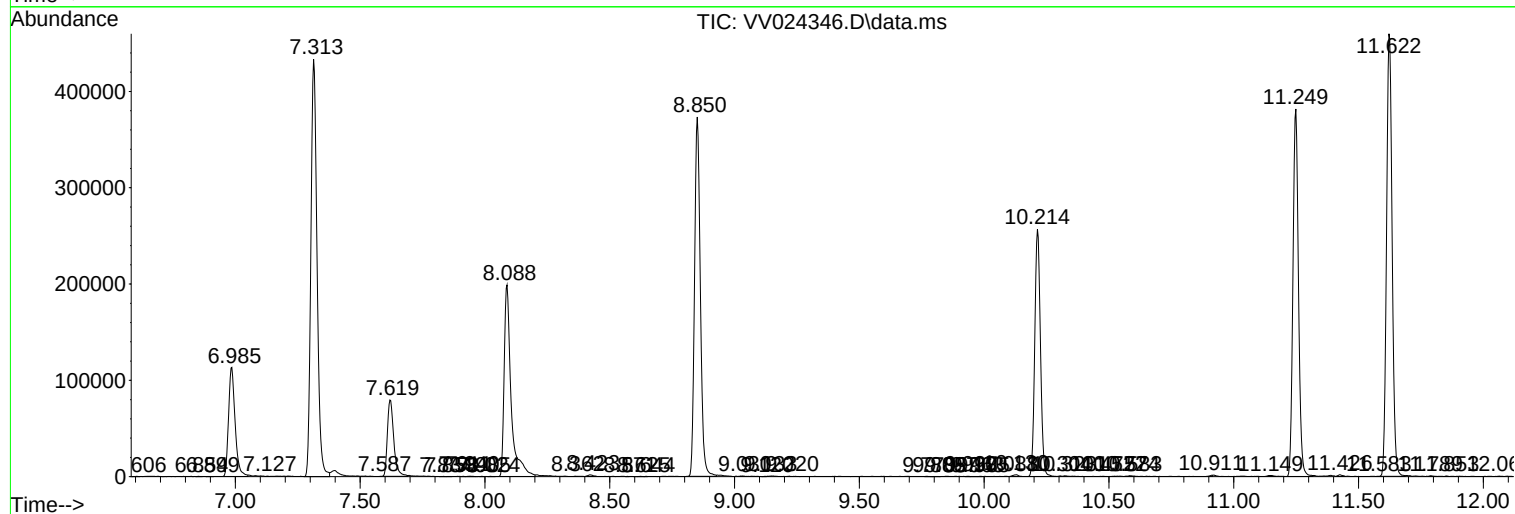
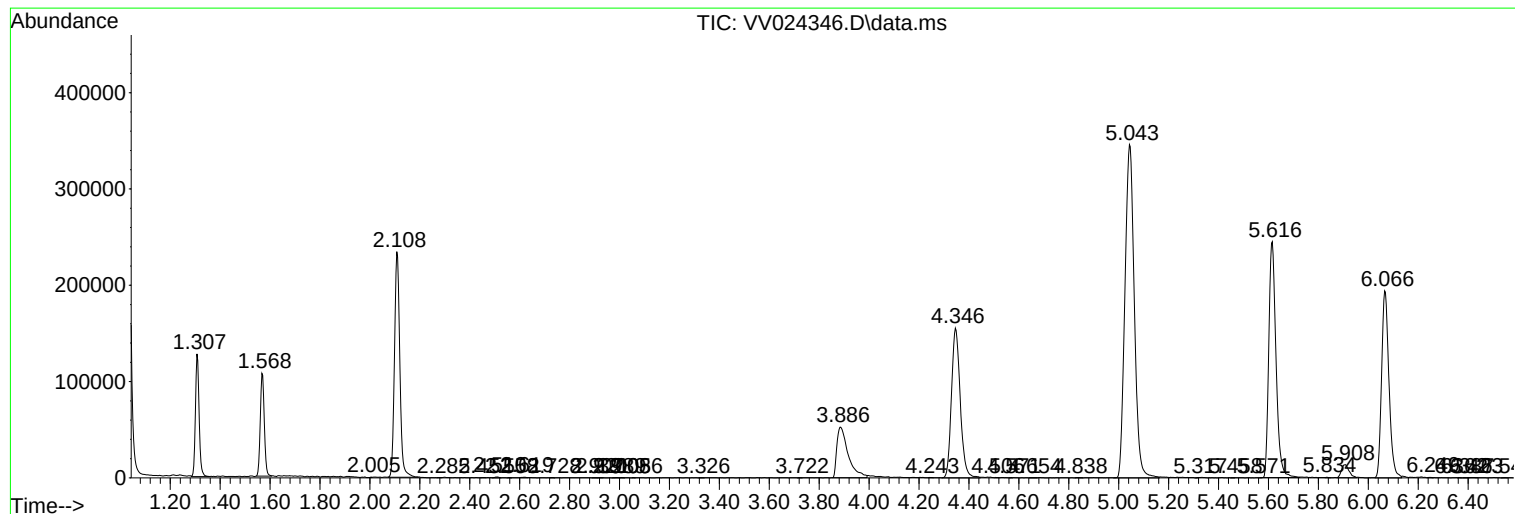
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
Quant Title : VOC Analysis

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



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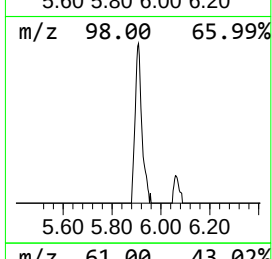
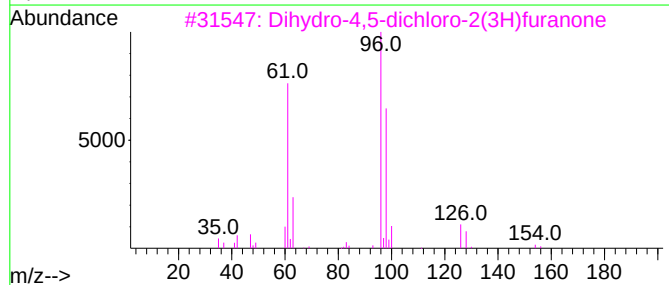
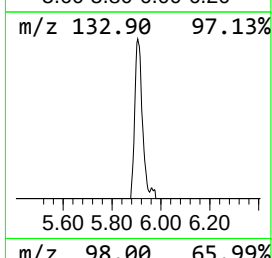
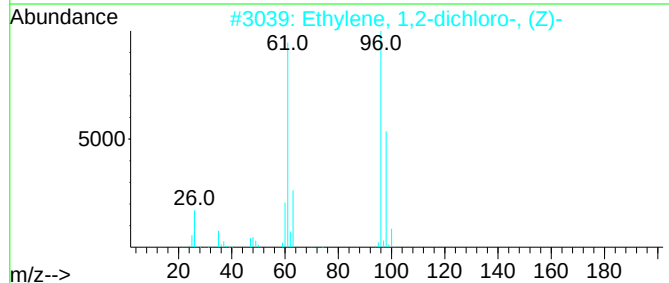
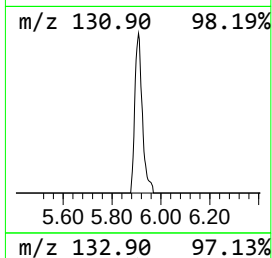
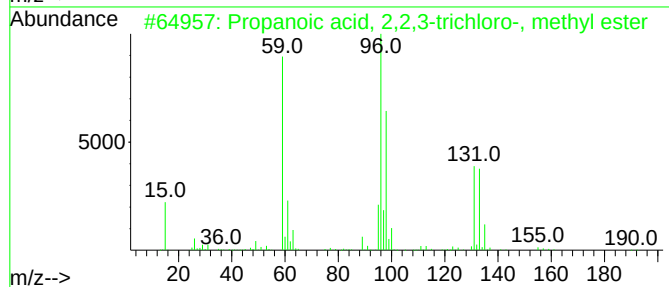
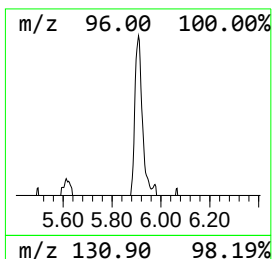
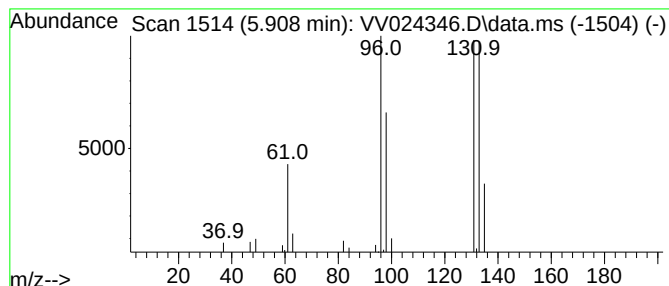
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Peak Number 1 Propanoic acid, 2,2,3-trich... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.908	2.85 ug/L	28034	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	56
2			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	35
3			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	35
4			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	32
5			2-Chloro-5-methylthiazole	133	C4H4ClNS	033342-65-3	30



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	5.908	2.9	ug/L	28034	1	5.616	492643	50.0