

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082621\
 Data File : VV021958.D
 Acq On : 26 Aug 2021 14:02
 Operator : SY/MD
 Sample : M3526-14ME
 Misc : 3.80g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 EW7C4ME

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\SFAMVLM081621WMA.M
 Title : VOC Analysis

Signal : TIC: VV021958.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.301	75	81	112	rVB	119849	175226	12.61%	1.486%
2	1.532	148	153	160	rBV	40959	42320	3.05%	0.359%
3	2.079	312	323	334	rBV	275681	398097	28.66%	3.376%
4	2.256	375	378	380	rBV2	854	602	0.04%	0.005%
5	2.314	393	396	398	rBV3	821	497	0.04%	0.004%
6	2.400	420	423	425	rVB2	606	294	0.02%	0.002%
7	2.433	425	433	434	rBV2	1490	1587	0.11%	0.013%
8	2.490	442	451	466	rVB	15838	28049	2.02%	0.238%
9	2.571	475	476	479	rBV2	418	307	0.02%	0.003%
10	2.613	479	489	496	rVV3	4604	8922	0.64%	0.076%
11	2.873	566	570	573	rBV2	293	312	0.02%	0.003%
12	3.011	604	613	625	rVB8	2089	4599	0.33%	0.039%
13	3.169	655	662	663	rBV2	1322	1093	0.08%	0.009%
14	3.179	663	665	666	rBV2	657	292	0.02%	0.002%
15	3.343	711	716	719	rVB	351	267	0.02%	0.002%
16	3.735	827	838	841	rBV3	1968	2885	0.21%	0.024%
17	3.883	872	884	948	rBV	67961	300364	21.62%	2.547%
18	4.339	1004	1026	1057	rBV	195247	542882	39.08%	4.604%
19	4.658	1119	1125	1136	rVB8	2294	4779	0.34%	0.041%
20	4.735	1144	1149	1150	rBV2	466	262	0.02%	0.002%
21	4.870	1186	1191	1192	rBV3	395	338	0.02%	0.003%
22	4.899	1194	1200	1202	rBV5	779	778	0.06%	0.007%
23	4.931	1207	1210	1212	rVB2	538	296	0.02%	0.003%
24	4.950	1212	1216	1220	rVB2	379	358	0.03%	0.003%
25	5.034	1220	1242	1279	rBV2	549716	1389073	100.00%	11.779%
26	5.333	1320	1335	1345	rBV10	4852	13972	1.01%	0.118%
27	5.487	1373	1383	1392	rVV5	2219	4547	0.33%	0.039%
28	5.609	1407	1421	1453	rVV	432819	919071	66.16%	7.794%
29	5.783	1472	1475	1482	rVB3	463	479	0.03%	0.004%
30	5.899	1499	1511	1526	rBV2	30639	68507	4.93%	0.581%
31	5.989	1533	1539	1548	rVB6	1692	2689	0.19%	0.023%
32	6.063	1548	1562	1596	rBV	288434	640330	46.10%	5.430%
33	6.330	1640	1645	1648	rBV	671	600	0.04%	0.005%
34	6.362	1651	1655	1662	rVB4	918	800	0.06%	0.007%
35	6.455	1679	1684	1687	rBV4	602	591	0.04%	0.005%
36	6.625	1732	1737	1738	rBV3	1306	1033	0.07%	0.009%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
 Title : VOC Analysis

37	6.712	1762	1764	1768	rVB2	763	489	0.04%	0.004%
38	6.796	1786	1790	1792	rVV3	345	275	0.02%	0.002%
39	6.834	1797	1802	1804	rBV2	386	276	0.02%	0.002%
40	6.982	1837	1848	1876	rBV	162956	322841	23.24%	2.738%
41	7.252	1924	1932	1934	rBV5	2114	2232	0.16%	0.019%
42	7.310	1938	1950	1965	rVV	662720	1182331	85.12%	10.026%
43	7.387	1966	1974	2000	rVB	118180	228879	16.48%	1.941%
44	7.567	2023	2030	2036	rBV6	3466	4416	0.32%	0.037%
45	7.622	2037	2047	2074	rVV	109564	215012	15.48%	1.823%
46	7.783	2092	2097	2100	rBV3	861	741	0.05%	0.006%
47	7.850	2116	2118	2123	rVB	374	297	0.02%	0.003%
48	7.915	2133	2138	2143	rVB3	380	442	0.03%	0.004%
49	7.979	2155	2158	2162	rVB3	897	631	0.05%	0.005%
50	8.101	2183	2196	2230	rBV2	281461	647641	46.62%	5.492%
51	8.284	2248	2253	2261	rVB7	2707	3794	0.27%	0.032%
52	8.349	2266	2273	2282	rVB5	2559	3975	0.29%	0.034%
53	8.394	2282	2287	2291	rBV5	948	950	0.07%	0.008%
54	8.429	2295	2298	2300	rBV3	689	349	0.03%	0.003%
55	8.448	2301	2304	2307	rVB3	807	483	0.03%	0.004%
56	8.497	2316	2319	2325	rVB3	661	606	0.04%	0.005%
57	8.548	2330	2335	2338	rBV4	680	482	0.03%	0.004%
58	8.571	2338	2342	2343	rBV	827	501	0.04%	0.004%
59	8.590	2346	2348	2353	rVB6	655	503	0.04%	0.004%
60	8.667	2369	2372	2376	rBV3	681	581	0.04%	0.005%
61	8.786	2403	2409	2410	rBV2	881	622	0.04%	0.005%
62	8.854	2417	2430	2452	rBV	660418	1145040	82.43%	9.710%
63	8.989	2470	2472	2475	rBV3	562	413	0.03%	0.004%
64	9.018	2477	2481	2489	rVB5	2608	3213	0.23%	0.027%
65	9.088	2498	2503	2504	rBV2	404	295	0.02%	0.003%
66	9.104	2504	2508	2511	rBV3	1438	1494	0.11%	0.013%
67	9.146	2512	2521	2533	rVV2	15177	28518	2.05%	0.242%
68	9.207	2533	2540	2547	rVB7	3750	5876	0.42%	0.050%
69	9.313	2571	2573	2576	rVV2	478	305	0.02%	0.003%
70	9.445	2608	2614	2615	rBV3	953	780	0.06%	0.007%
71	9.481	2620	2625	2630	rVB7	1399	1627	0.12%	0.014%
72	9.548	2639	2646	2661	rVV3	9548	15978	1.15%	0.135%
73	9.677	2677	2686	2687	rBV6	1631	1945	0.14%	0.016%
74	9.709	2691	2696	2705	rVB7	2371	3075	0.22%	0.026%
75	9.763	2710	2713	2718	rBV3	661	702	0.05%	0.006%
76	9.796	2719	2723	2724	rBV3	1293	879	0.06%	0.007%

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 ClientSampleId :
 EW7C4ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
 Title : VOC Analysis

77	9.844	2735	2738	2748	rVB8	2038	3206	0.23%	0.027%
78	9.937	2761	2767	2773	rBV3	1594	2384	0.17%	0.020%
79	10.017	2785	2792	2793	rBV4	1019	949	0.07%	0.008%
80	10.072	2802	2809	2811	rBV4	820	936	0.07%	0.008%
81	10.127	2819	2826	2836	rVB5	7517	12560	0.90%	0.107%
82	10.220	2841	2855	2874	rBV	414372	666860	48.01%	5.655%
83	10.358	2893	2898	2905	rBV2	3865	4997	0.36%	0.042%
84	10.455	2917	2928	2934	rBV2	9079	17894	1.29%	0.152%
85	10.542	2950	2955	2961	rBV3	5124	6995	0.50%	0.059%
86	10.657	2988	2991	2994	rBV5	494	371	0.03%	0.003%
87	10.744	3010	3018	3026	rVV3	4190	7112	0.51%	0.060%
88	10.831	3040	3045	3048	rBV5	1542	1359	0.10%	0.012%
89	10.860	3052	3054	3055	rBV2	707	263	0.02%	0.002%
90	10.921	3064	3073	3090	rVB	33389	55437	3.99%	0.470%
91	10.998	3095	3097	3100	rVB2	582	302	0.02%	0.003%
92	11.156	3136	3146	3153	rBV8	4323	7912	0.57%	0.067%
93	11.198	3154	3159	3165	rVV6	2513	2857	0.21%	0.024%
94	11.252	3165	3176	3196	rBV	833690	1308231	94.18%	11.094%
95	11.545	3257	3267	3269	rBV6	4472	5772	0.42%	0.049%
96	11.628	3282	3293	3315	rVB	783674	1256525	90.46%	10.655%
97	11.789	3335	3343	3350	rBV	4704	8856	0.64%	0.075%
98	12.371	3516	3524	3525	rBV6	5411	6000	0.43%	0.051%
99	12.468	3548	3554	3568	rBV9	10129	19761	1.42%	0.168%
100	12.558	3574	3582	3589	rBV9	5407	8194	0.59%	0.069%

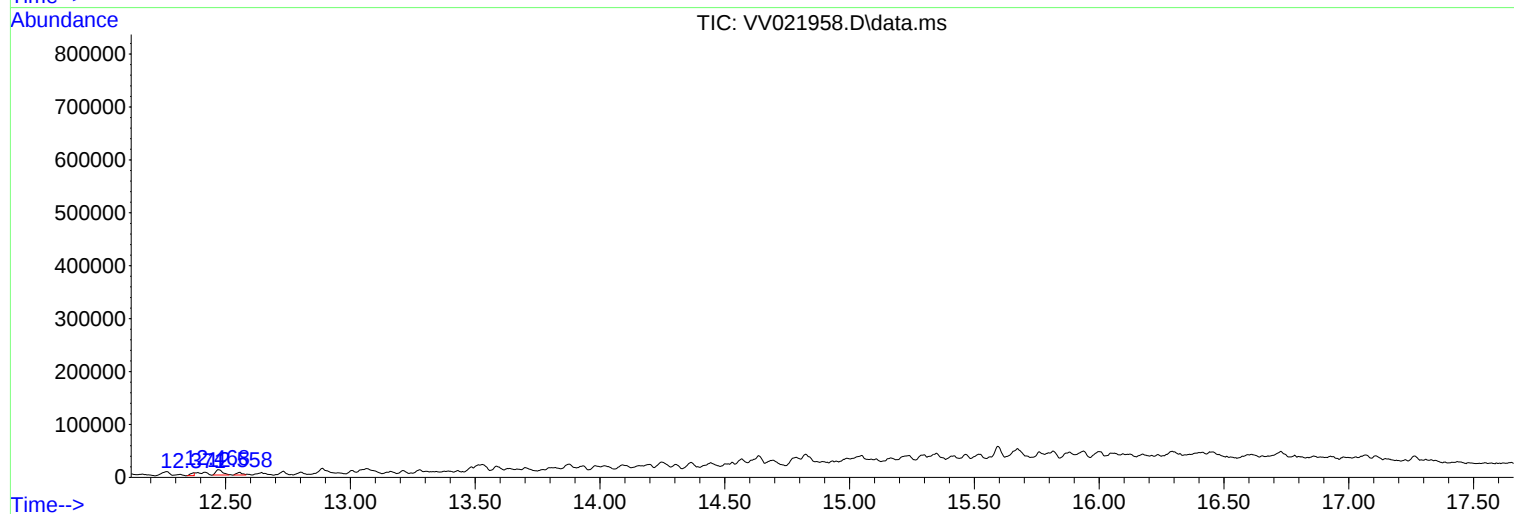
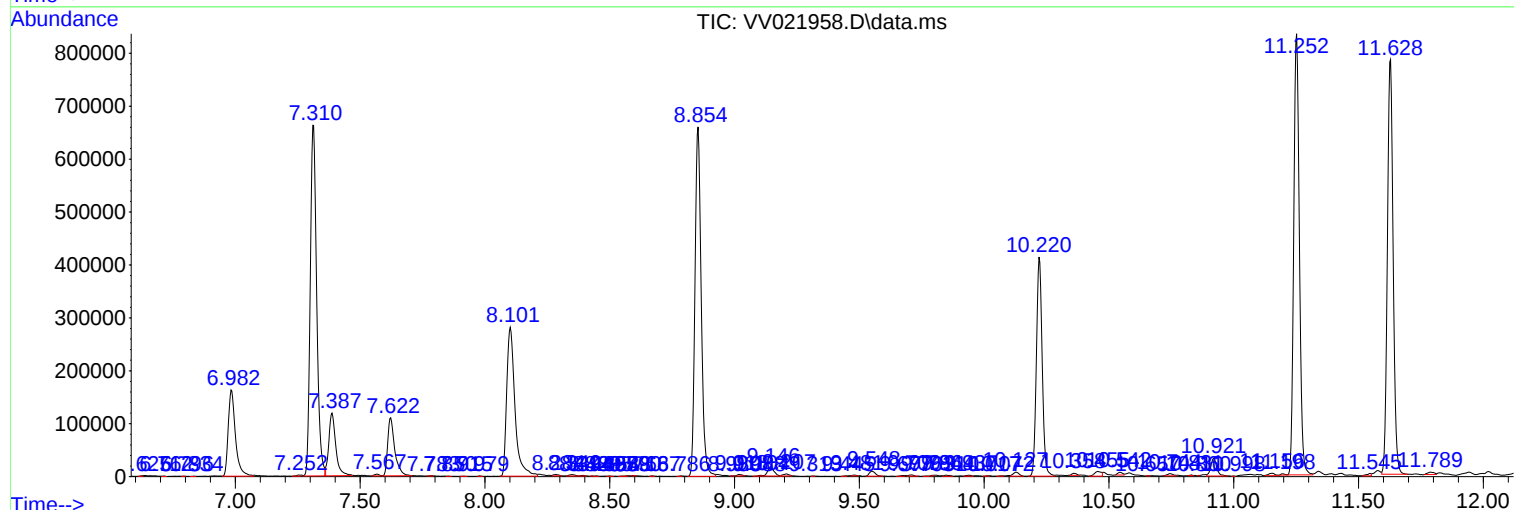
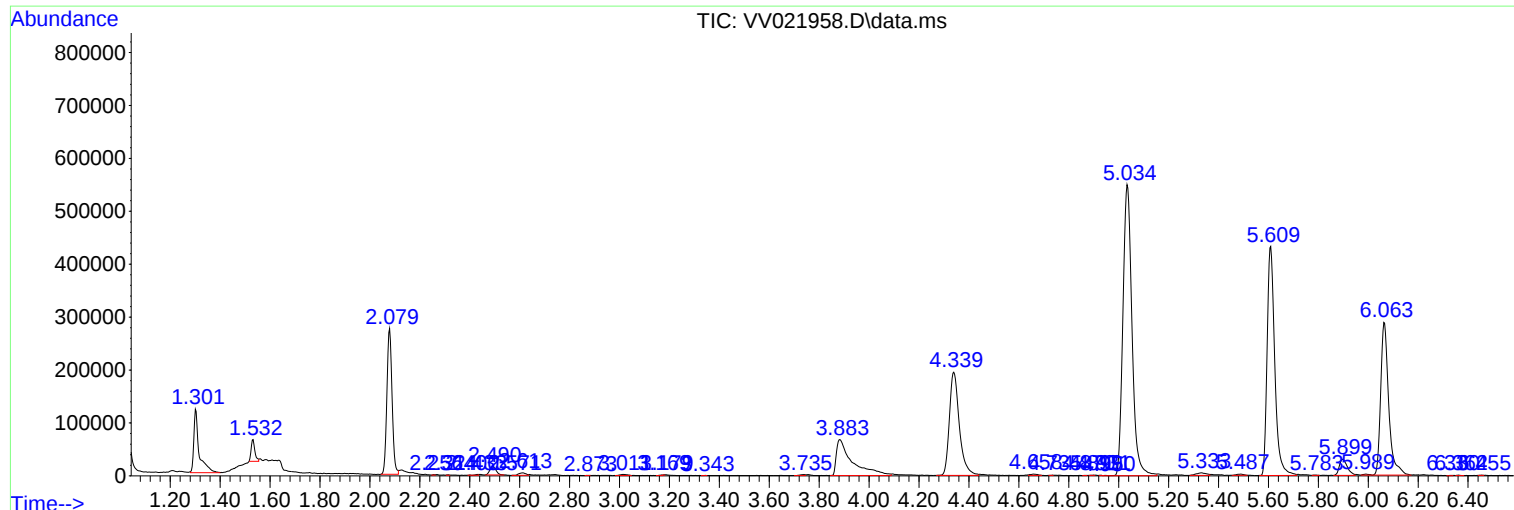
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ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampled :
EW7C4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EW7C4ME

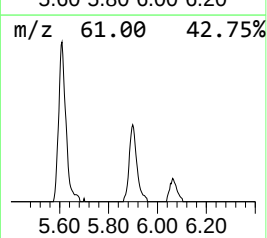
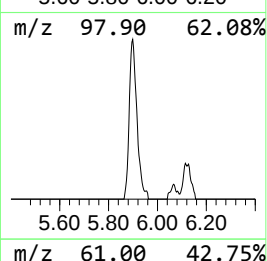
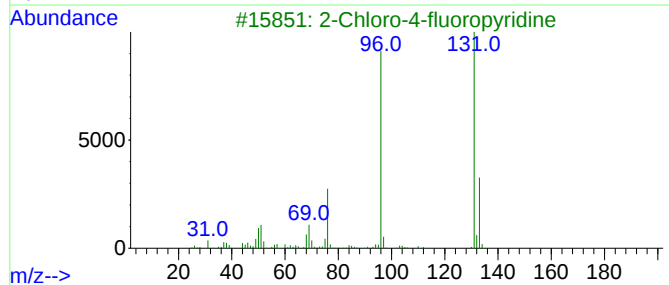
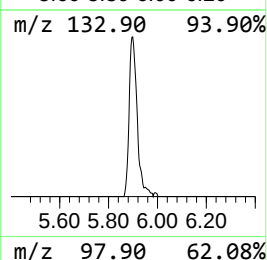
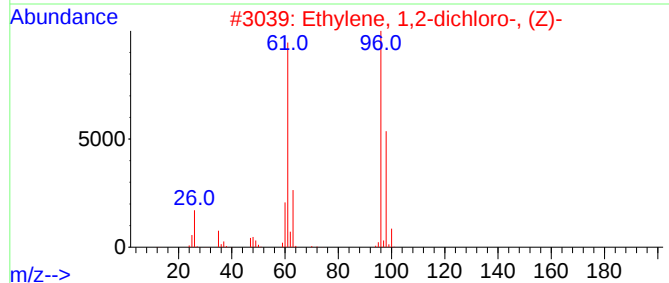
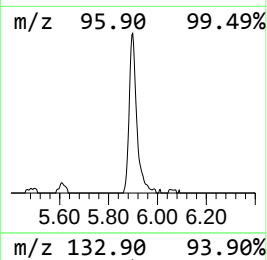
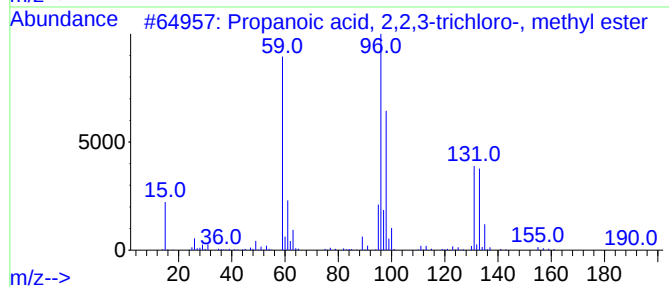
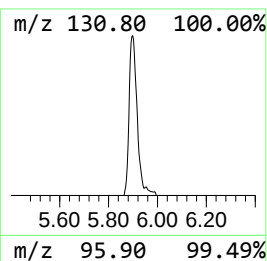
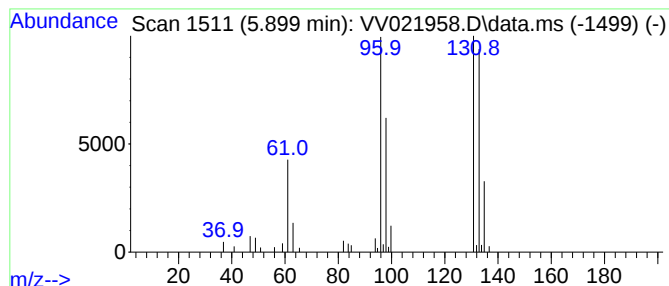
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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.
5.899	3.73 ug/L	68507	1,4-Difluorobenzene	5.609

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	38
3			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	23
4			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	23
5			2-Chloro-5-methylthiazole	133	C4H4ClNS	033342-65-3	16



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	5.899	3.7	ug/L	68507	1	5.609	919071	50.0