

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV081721\
 Data File : VV021817.D
 Acq On : 17 Aug 2021 16:10
 Operator : SY/MD
 Sample : M3365-12ME
 Misc : 6.04g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DBKB6ME

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: VV021817.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	102	rBV	140202	188272	12.95%	1.599%
2	2.076	312	322	334	rBV	272799	392634	27.01%	3.335%
3	2.709	517	519	523	rBV3	503	374	0.03%	0.003%
4	2.741	523	529	541	rVV7	1849	3738	0.26%	0.032%
5	2.815	549	552	556	rVB3	509	352	0.02%	0.003%
6	2.902	577	579	583	rBV	598	435	0.03%	0.004%
7	3.150	652	656	659	rBV3	593	417	0.03%	0.004%
8	3.178	659	665	667	rBV3	594	653	0.04%	0.006%
9	3.246	683	686	689	rBV2	721	520	0.04%	0.004%
10	3.339	713	715	717	rVB2	519	170	0.01%	0.001%
11	3.371	722	725	728	rBV2	379	247	0.02%	0.002%
12	3.426	741	742	747	rBV2	185	152	0.01%	0.001%
13	3.535	774	776	779	rVB2	535	271	0.02%	0.002%
14	3.606	796	798	803	rVB2	378	162	0.01%	0.001%
15	3.680	820	821	826	rVB2	416	160	0.01%	0.001%
16	3.706	826	829	831	rBV	298	195	0.01%	0.002%
17	3.725	831	835	838	rBV2	398	348	0.02%	0.003%
18	3.841	868	871	876	rBV3	311	224	0.02%	0.002%
19	3.892	876	887	923	rBV	91407	336331	23.13%	2.857%
20	4.346	1011	1028	1060	rBV	220226	578806	39.81%	4.917%
21	4.600	1105	1107	1113	rVB5	489	441	0.03%	0.004%
22	4.661	1122	1126	1130	rVV7	807	739	0.05%	0.006%
23	4.693	1133	1136	1144	rVB2	463	541	0.04%	0.005%
24	4.773	1158	1161	1166	rVB3	582	449	0.03%	0.004%
25	4.834	1178	1180	1181	rBV	558	272	0.02%	0.002%
26	4.873	1190	1192	1196	rVB	283	183	0.01%	0.002%
27	4.899	1196	1200	1202	rBV2	271	151	0.01%	0.001%
28	4.924	1206	1208	1210	rBV	360	194	0.01%	0.002%
29	4.960	1217	1219	1220	rBV	426	150	0.01%	0.001%
30	5.040	1227	1244	1283	rBV2	587037	1453897	100.00%	12.350%
31	5.612	1409	1422	1453	rBV	466758	981806	67.53%	8.340%
32	5.905	1501	1513	1532	rBV2	25412	58274	4.01%	0.495%
33	6.069	1552	1564	1591	rVB	310941	653939	44.98%	5.555%
34	6.320	1638	1642	1643	rBV	587	339	0.02%	0.003%
35	6.336	1645	1647	1649	rBV2	409	220	0.02%	0.002%
36	6.474	1685	1690	1693	rBV2	437	291	0.02%	0.002%

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Integrator: RTE

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

37	6.522	1700	1705	1707	rBV4	702	583	0.04%	0.005%
38	6.551	1712	1714	1716	rVB2	747	347	0.02%	0.003%
39	6.616	1731	1734	1735	rBV2	339	189	0.01%	0.002%
40	6.728	1766	1769	1775	rVB4	739	637	0.04%	0.005%
41	6.773	1778	1783	1785	rBV4	506	444	0.03%	0.004%
42	6.802	1790	1792	1795	rVB	344	218	0.01%	0.002%
43	6.818	1795	1797	1800	rBV	274	166	0.01%	0.001%
44	6.841	1800	1804	1809	rBV4	397	451	0.03%	0.004%
45	6.895	1818	1821	1823	rBV	230	161	0.01%	0.001%
46	6.915	1823	1827	1831	rVV4	540	513	0.04%	0.004%
47	6.934	1831	1833	1837	rVB2	573	344	0.02%	0.003%
48	6.989	1837	1850	1877	rBV	175649	348587	23.98%	2.961%
49	7.185	1907	1911	1912	rBV2	597	329	0.02%	0.003%
50	7.317	1940	1952	1967	rBV	656071	1150831	79.15%	9.776%
51	7.625	2037	2048	2076	rBV	116990	231345	15.91%	1.965%
52	7.889	2128	2130	2134	rBV2	430	302	0.02%	0.003%
53	7.915	2134	2138	2140	rBV3	416	303	0.02%	0.003%
54	7.982	2150	2159	2167	rVB6	2517	4049	0.28%	0.034%
55	8.040	2174	2177	2180	rBV3	403	269	0.02%	0.002%
56	8.059	2180	2183	2184	rVB	349	149	0.01%	0.001%
57	8.104	2184	2197	2232	rBV2	316933	718934	49.45%	6.107%
58	8.468	2307	2310	2311	rBV	369	167	0.01%	0.001%
59	8.725	2386	2390	2391	rBV	296	177	0.01%	0.002%
60	8.853	2419	2430	2461	rBV	705446	1214796	83.55%	10.319%
61	9.275	2557	2561	2564	rBV	367	197	0.01%	0.002%
62	9.294	2564	2567	2574	rBV	285	274	0.02%	0.002%
63	9.329	2574	2578	2579	rBV	347	197	0.01%	0.002%
64	9.410	2599	2603	2604	rBV	260	174	0.01%	0.001%
65	9.435	2608	2611	2613	rBV	328	166	0.01%	0.001%
66	9.445	2613	2614	2618	rVB	423	205	0.01%	0.002%
67	9.490	2625	2628	2632	rVB2	392	237	0.02%	0.002%
68	9.558	2643	2649	2654	rVV6	1855	2418	0.17%	0.021%
69	9.751	2708	2709	2712	rVB	680	278	0.02%	0.002%
70	9.847	2736	2739	2741	rBV3	430	244	0.02%	0.002%
71	9.882	2748	2750	2752	rBV	349	199	0.01%	0.002%
72	9.908	2754	2758	2764	rVB3	1827	2172	0.15%	0.018%
73	10.075	2807	2810	2812	rBV2	304	221	0.02%	0.002%
74	10.130	2819	2827	2836	rBV4	2208	3398	0.23%	0.029%
75	10.223	2840	2856	2871	rBV	482848	795311	54.70%	6.756%
76	10.522	2945	2949	2950	rBV	304	213	0.01%	0.002%

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 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DBKB6ME

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

77	10.548	2950	2957	2963	rBV5	2584	3848	0.26%	0.033%
78	10.664	2987	2993	2997	rBV5	543	613	0.04%	0.005%
79	10.686	2997	3000	3001	rBV	346	195	0.01%	0.002%
80	10.718	3007	3010	3012	rBV	336	199	0.01%	0.002%
81	10.734	3012	3015	3018	rBV2	421	397	0.03%	0.003%
82	10.789	3029	3032	3036	rBV2	589	411	0.03%	0.003%
83	10.924	3066	3074	3084	rVB4	5651	8611	0.59%	0.073%
84	11.011	3098	3101	3104	rBV	228	183	0.01%	0.002%
85	11.091	3122	3126	3128	rBV2	501	371	0.03%	0.003%
86	11.191	3151	3157	3165	rBV7	3820	5767	0.40%	0.049%
87	11.252	3165	3176	3201	rVV	833494	1291831	88.85%	10.973%
88	11.484	3245	3248	3252	rVB3	457	351	0.02%	0.003%
89	11.535	3252	3264	3273	rBV	21286	33053	2.27%	0.281%
90	11.628	3281	3293	3315	rBV	809571	1250332	86.00%	10.621%
91	11.940	3388	3390	3392	rBV	411	199	0.01%	0.002%
92	12.017	3411	3414	3418	rVB2	385	237	0.02%	0.002%
93	12.049	3420	3424	3428	rVB2	566	395	0.03%	0.003%
94	12.091	3428	3437	3443	rBV4	1020	1534	0.11%	0.013%
95	12.435	3542	3544	3548	rVB3	878	579	0.04%	0.005%
96	12.561	3580	3583	3584	rBV2	474	240	0.02%	0.002%
97	12.654	3604	3612	3625	rBV4	5927	8449	0.58%	0.072%
98	12.889	3678	3685	3693	rBV6	3031	4072	0.28%	0.035%
99	13.271	3800	3804	3813	rVB6	2306	3121	0.21%	0.027%
100	13.512	3871	3879	3890	rBV	12653	20753	1.43%	0.176%

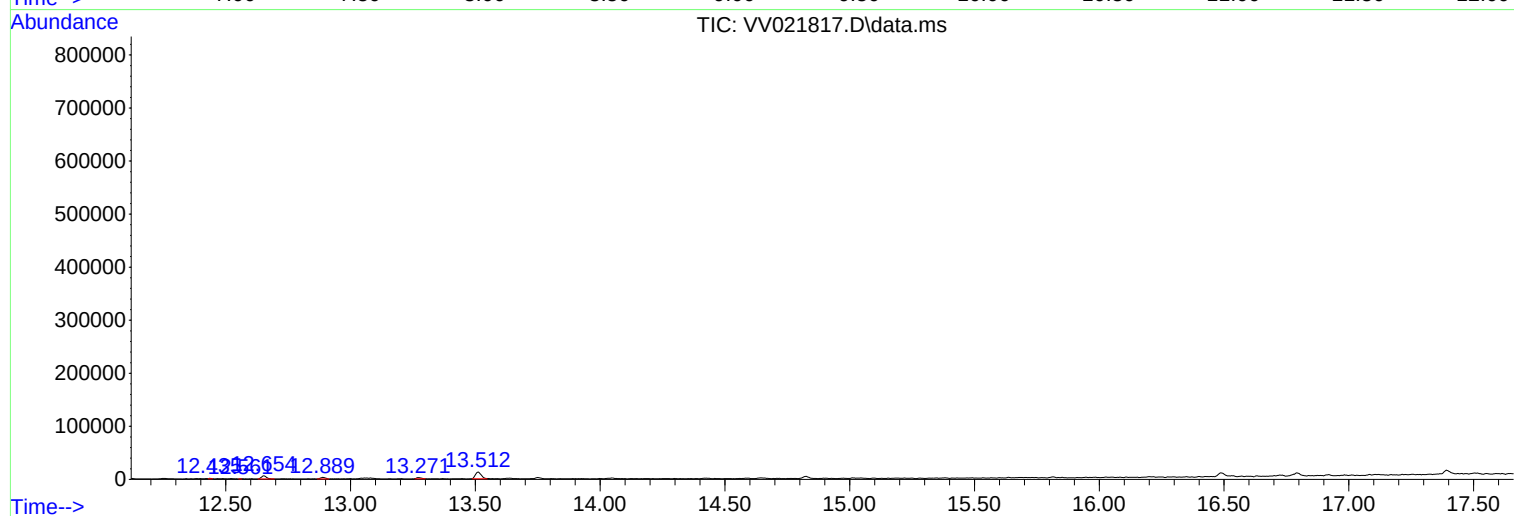
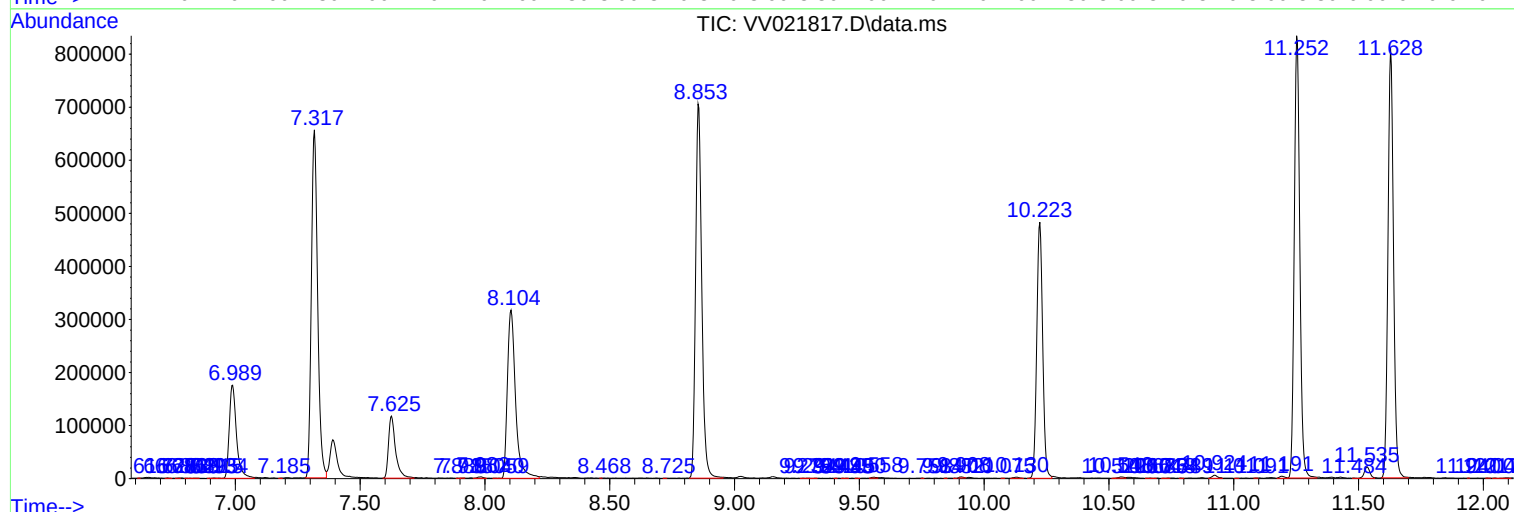
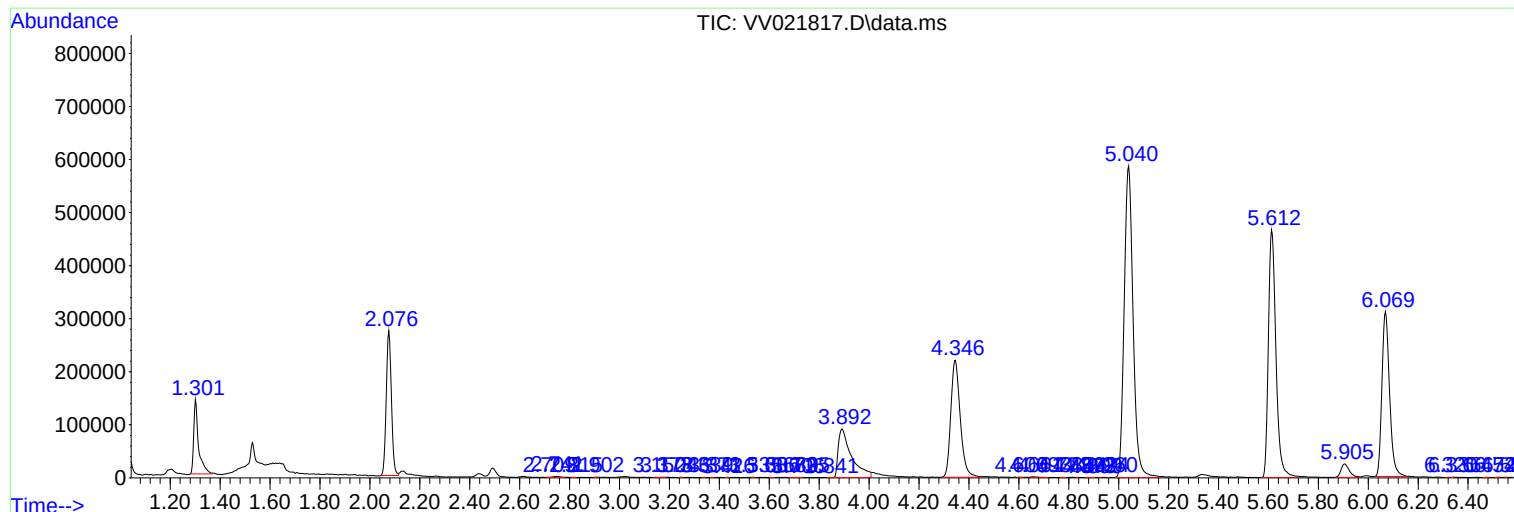
Sum of corrected areas: 11772283

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Misc : 6.04g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampled :
DBKB6ME

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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Instrument :
MSVOA_V
ClientSampleId :
DBKB6ME

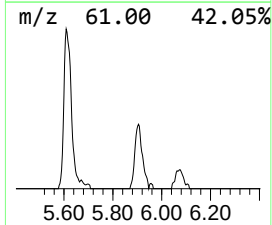
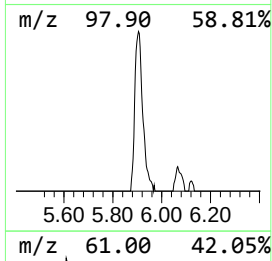
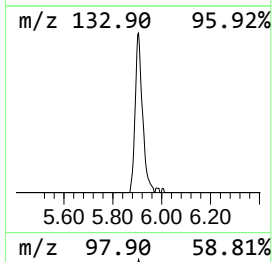
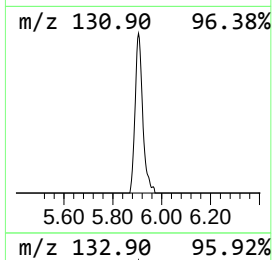
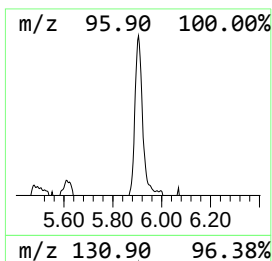
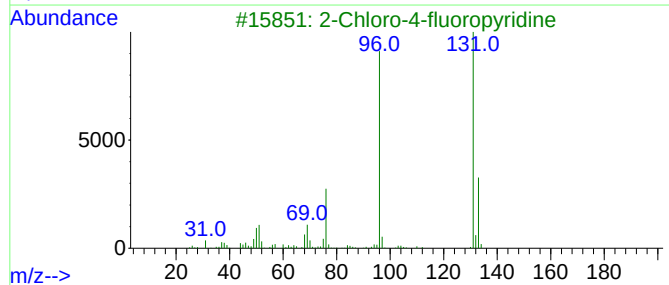
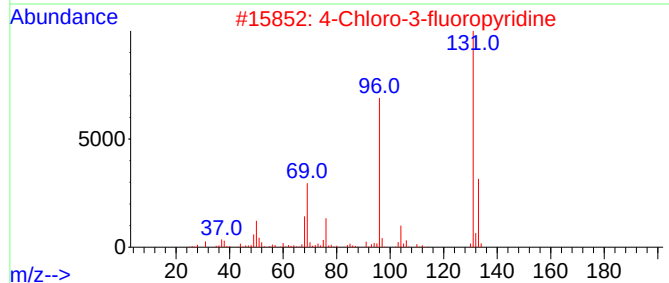
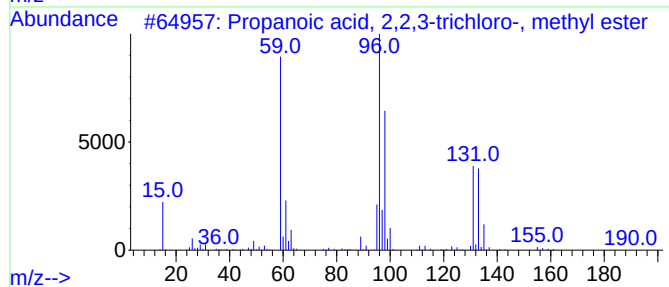
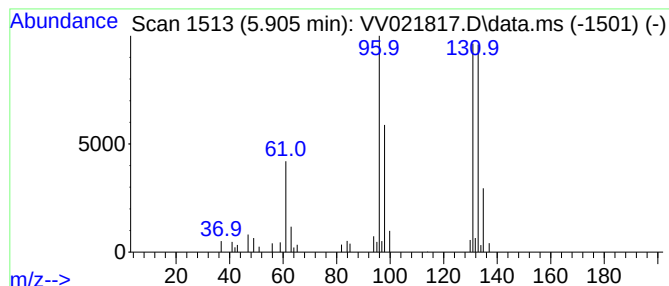
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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.
5.905	2.97 ug/L	58274	1,4-Difluorobenzene	5.612

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	56
2			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	43
3			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	43
4			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
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,...	5.905	3.0	ug/L	58274	1	5.612	981806	50.0