

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082721\
 Data File : VV021969.D
 Acq On : 27 Aug 2021 12:27
 Operator : SY/MD
 Sample : VV0827MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VBLK241

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: VV021969.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	100	rVB	203756	209550	14.79%	1.904%
2	1.564	156	163	180	rVB	160087	186331	13.15%	1.693%
3	2.105	321	331	360	rVB	325078	486088	34.31%	4.417%
4	2.510	448	457	468	rVB3	7442	12376	0.87%	0.112%
5	2.719	518	522	525	rBV3	473	408	0.03%	0.004%
6	2.767	529	537	545	rVB6	1440	2642	0.19%	0.024%
7	2.908	578	581	583	rBV	216	130	0.01%	0.001%
8	3.413	736	738	741	rBV	254	124	0.01%	0.001%
9	3.465	752	754	755	rBV2	308	120	0.01%	0.001%
10	3.561	781	784	786	rBV	193	128	0.01%	0.001%
11	3.616	798	801	803	rBV	174	116	0.01%	0.001%
12	3.693	822	825	827	rBV	137	93	0.01%	0.001%
13	3.712	828	831	837	rVB2	506	451	0.03%	0.004%
14	3.838	868	870	872	rVB2	237	96	0.01%	0.001%
15	3.876	872	882	925	rBV	119436	318089	22.45%	2.890%
16	4.349	1013	1029	1061	rBV	211796	545936	38.54%	4.960%
17	4.667	1124	1128	1130	rBV2	579	526	0.04%	0.005%
18	4.715	1140	1143	1148	rBV3	454	379	0.03%	0.003%
19	4.744	1151	1152	1156	rVB2	267	136	0.01%	0.001%
20	4.796	1166	1168	1172	rBV	245	170	0.01%	0.002%
21	4.838	1177	1181	1182	rBV	393	275	0.02%	0.002%
22	4.847	1182	1184	1186	rBV2	317	159	0.01%	0.001%
23	4.892	1197	1198	1200	rVB	257	93	0.01%	0.001%
24	4.921	1206	1207	1210	rVB	446	145	0.01%	0.001%
25	4.963	1216	1220	1221	rBV	233	150	0.01%	0.001%
26	5.047	1230	1246	1282	rBV2	553824	1416704	100.00%	12.872%
27	5.349	1338	1340	1344	rBV2	393	288	0.02%	0.003%
28	5.516	1390	1392	1396	rBV3	363	241	0.02%	0.002%
29	5.535	1396	1398	1401	rVB2	442	218	0.02%	0.002%
30	5.619	1412	1424	1453	rBV	418383	840571	59.33%	7.637%
31	5.908	1503	1514	1530	rBV3	35965	77097	5.44%	0.701%
32	6.072	1551	1565	1600	rBV	305546	631209	44.55%	5.735%
33	6.365	1653	1656	1658	rBV	427	243	0.02%	0.002%
34	6.397	1664	1666	1669	rVB	276	127	0.01%	0.001%
35	6.461	1683	1686	1689	rVB2	390	234	0.02%	0.002%
36	6.516	1700	1703	1704	rBV2	441	212	0.01%	0.002%

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Integrator: RTE

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

37	6.641	1739	1742	1744	rBV	381	218	0.02%	0.002%
38	6.735	1767	1771	1772	rBV2	308	149	0.01%	0.001%
39	6.754	1775	1777	1778	rVB	332	96	0.01%	0.001%
40	6.770	1778	1782	1784	rBV	412	237	0.02%	0.002%
41	6.834	1800	1802	1805	rVB	224	108	0.01%	0.001%
42	6.873	1810	1814	1818	rBV	328	296	0.02%	0.003%
43	6.928	1830	1831	1835	rVB2	350	188	0.01%	0.002%
44	6.989	1839	1850	1873	rBV	175410	320323	22.61%	2.910%
45	7.262	1933	1935	1937	rVB2	631	207	0.01%	0.002%
46	7.317	1940	1952	1971	rBV	682804	1191386	84.10%	10.825%
47	7.625	2037	2048	2077	rBV	117491	212103	14.97%	1.927%
48	7.841	2111	2115	2116	rBV3	561	407	0.03%	0.004%
49	7.892	2129	2131	2135	rVB2	270	150	0.01%	0.001%
50	7.937	2139	2145	2148	rBV2	397	417	0.03%	0.004%
51	7.950	2148	2149	2152	rVV2	394	147	0.01%	0.001%
52	7.979	2152	2158	2162	rVV4	1358	1622	0.11%	0.015%
53	8.014	2166	2169	2172	rBV	197	94	0.01%	0.001%
54	8.091	2183	2193	2235	rBV2	336258	666117	47.02%	6.052%
55	8.583	2344	2346	2349	rBV2	250	146	0.01%	0.001%
56	8.628	2354	2360	2362	rBV3	596	588	0.04%	0.005%
57	8.670	2370	2373	2376	rBV2	400	278	0.02%	0.003%
58	8.783	2404	2408	2412	rBV2	245	201	0.01%	0.002%
59	8.853	2419	2430	2451	rBV	616148	1025191	72.36%	9.315%
60	9.249	2550	2553	2555	rVB	406	230	0.02%	0.002%
61	9.368	2588	2590	2593	rVB	212	79	0.01%	0.001%
62	9.384	2593	2595	2598	rBV2	187	119	0.01%	0.001%
63	9.464	2618	2620	2623	rBV	276	183	0.01%	0.002%
64	9.522	2636	2638	2640	rVB	378	175	0.01%	0.002%
65	9.542	2640	2644	2646	rBV2	595	510	0.04%	0.005%
66	9.580	2653	2656	2668	rVB6	1424	1813	0.13%	0.016%
67	9.648	2675	2677	2679	rBV	248	119	0.01%	0.001%
68	9.686	2687	2689	2691	rVB	311	113	0.01%	0.001%
69	9.741	2705	2706	2711	rVB2	228	134	0.01%	0.001%
70	9.879	2747	2749	2750	rBV2	288	114	0.01%	0.001%
71	9.940	2760	2768	2776	rBV4	1145	1938	0.14%	0.018%
72	10.021	2791	2793	2795	rBV	455	234	0.02%	0.002%
73	10.082	2809	2812	2813	rBV	320	132	0.01%	0.001%
74	10.098	2815	2817	2820	rBV3	692	552	0.04%	0.005%
75	10.220	2842	2855	2881	rBV	392674	626454	44.22%	5.692%
76	10.416	2914	2916	2920	rBV	215	118	0.01%	0.001%

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Integration Parameters: LSCINT.P

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Peak Location: TOP

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Title : VOC Analysis

77	10.448	2925	2926	2929	rBV	209	91	0.01%	0.001%
78	10.477	2931	2935	2938	rBV2	548	458	0.03%	0.004%
79	10.664	2987	2993	2998	rBV3	679	772	0.05%	0.007%
80	10.738	3014	3016	3018	rBV	337	185	0.01%	0.002%
81	10.818	3040	3041	3044	rBV	389	204	0.01%	0.002%
82	10.892	3062	3064	3065	rBV	331	113	0.01%	0.001%
83	10.924	3066	3074	3083	rVB4	4432	6889	0.49%	0.063%
84	11.037	3104	3109	3117	rBV5	647	1126	0.08%	0.010%
85	11.152	3138	3145	3151	rBV3	1596	2183	0.15%	0.020%
86	11.194	3151	3158	3165	rBV5	2533	3578	0.25%	0.033%
87	11.252	3165	3176	3196	rBV	685995	1068209	75.40%	9.706%
88	11.474	3242	3245	3246	rBV	356	191	0.01%	0.002%
89	11.535	3261	3264	3266	rBV2	429	305	0.02%	0.003%
90	11.628	3280	3293	3315	rBV	698645	1105672	78.05%	10.046%
91	12.522	3569	3571	3573	rBV	257	142	0.01%	0.001%
92	12.654	3606	3612	3622	rVB7	3049	4628	0.33%	0.042%
93	12.869	3676	3679	3681	rBV2	342	187	0.01%	0.002%
94	12.918	3690	3694	3696	rBV	244	196	0.01%	0.002%
95	12.940	3699	3701	3702	rBV	372	149	0.01%	0.001%
96	13.030	3726	3729	3731	rBV2	381	232	0.02%	0.002%
97	13.271	3791	3804	3812	rBV5	4747	7530	0.53%	0.068%
98	13.413	3847	3848	3849	rBV5	254	90	0.01%	0.001%
99	13.512	3872	3879	3889	rBV2	6586	10404	0.73%	0.095%
100	13.747	3947	3952	3963	rVB5	4147	6879	0.49%	0.063%

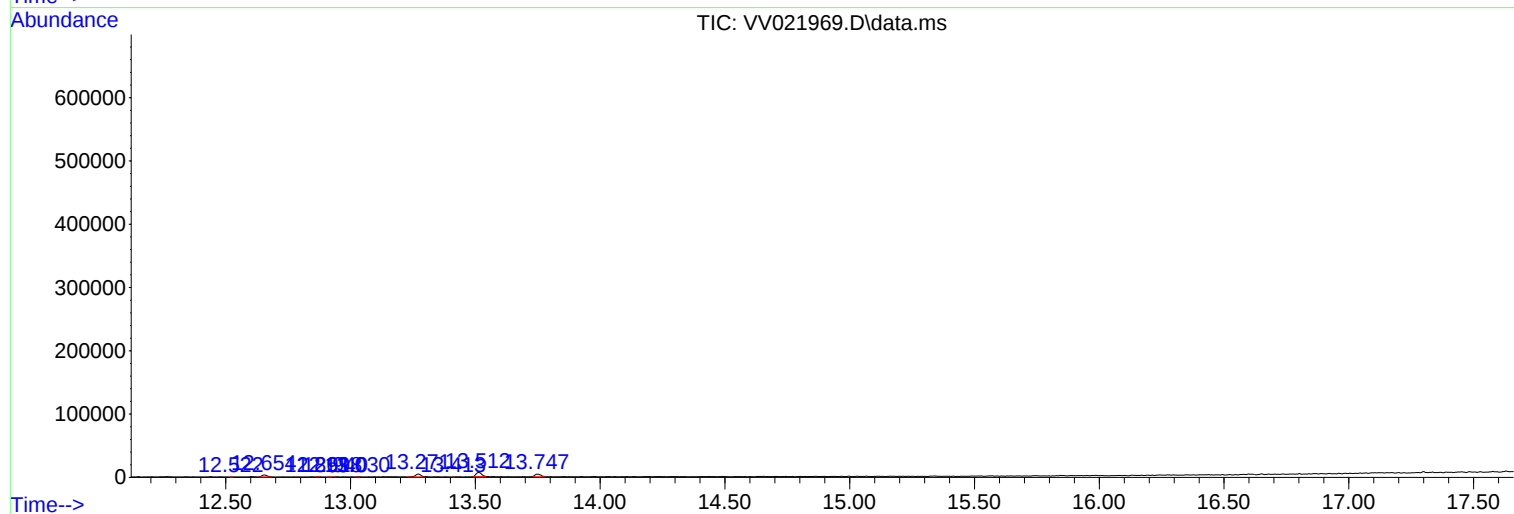
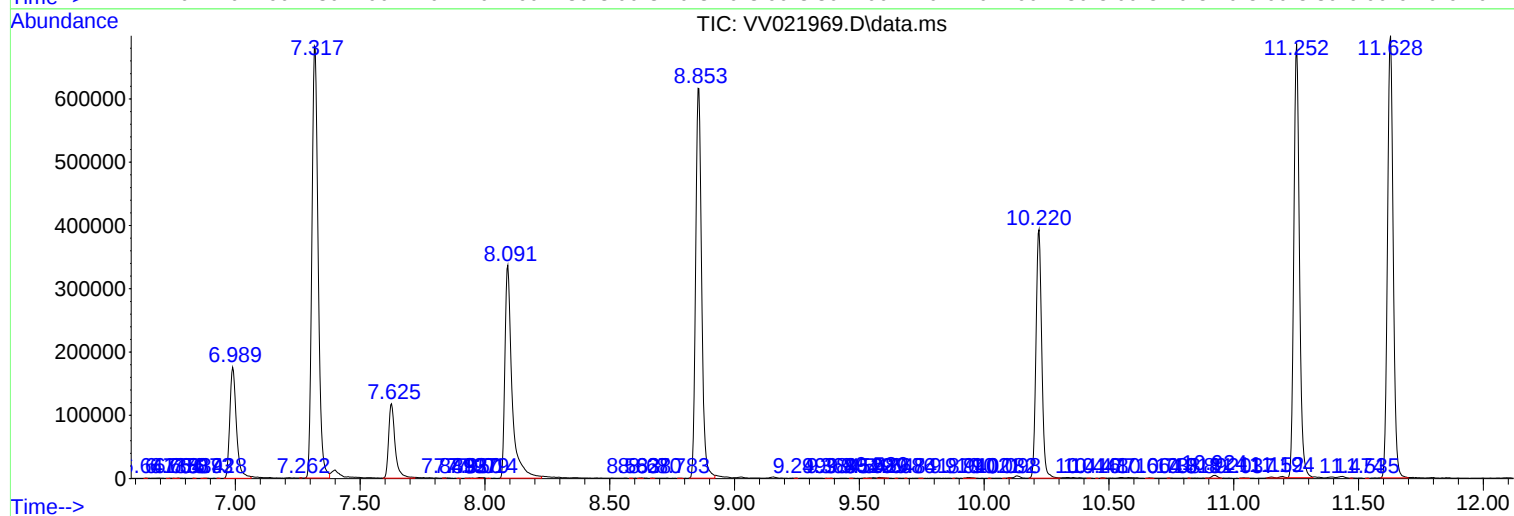
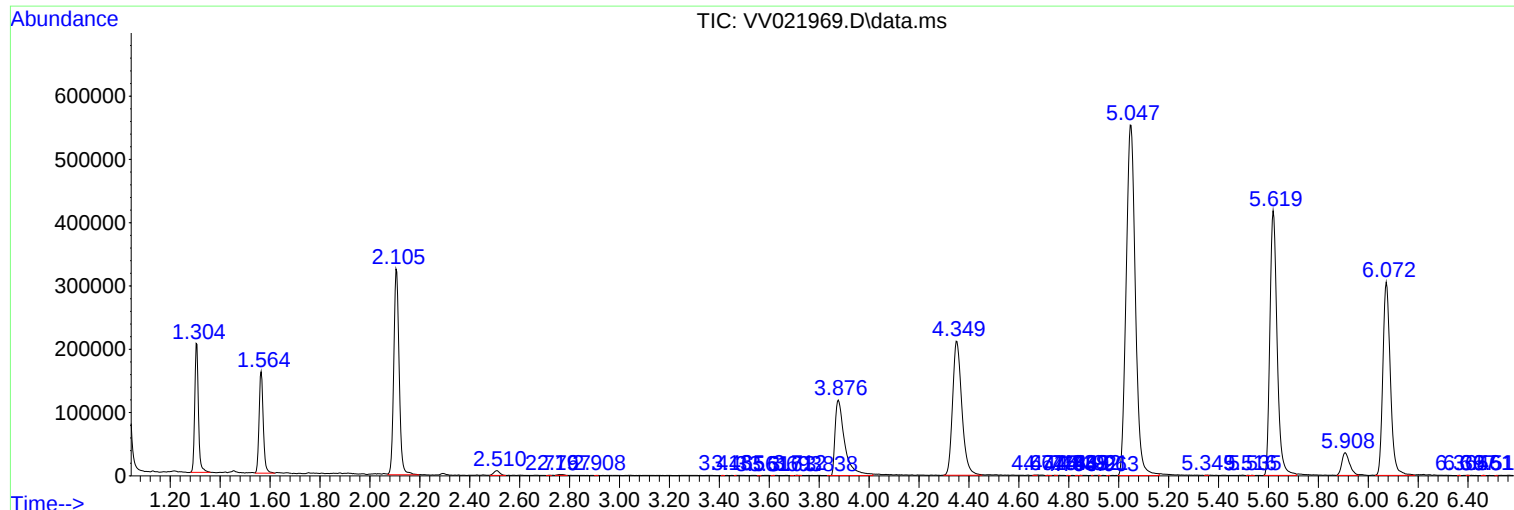
Sum of corrected areas: 11005954

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ALS Vial : 9 Sample Multiplier: 1

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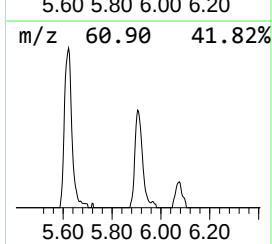
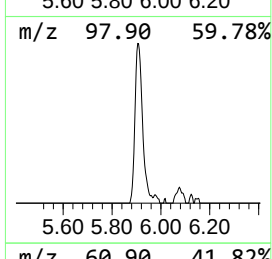
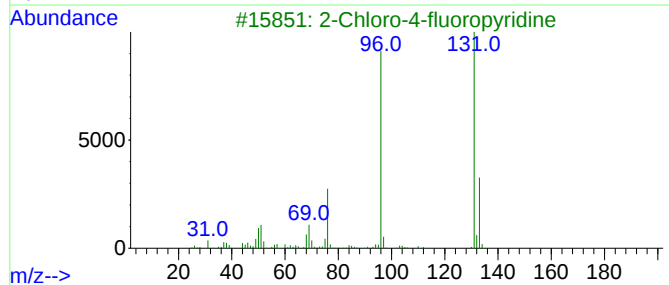
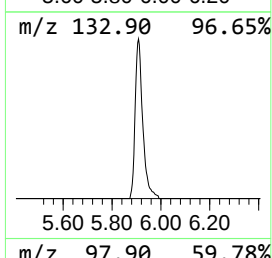
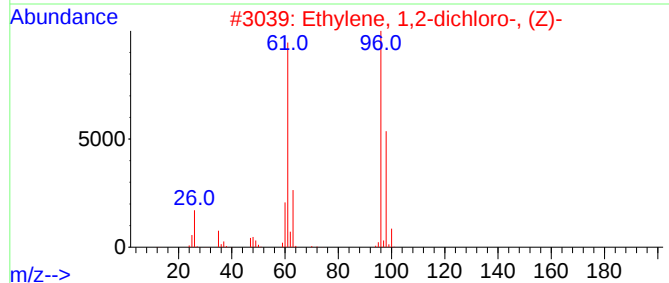
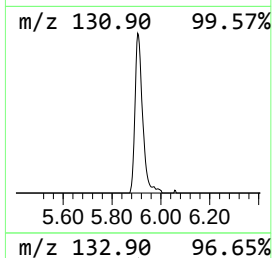
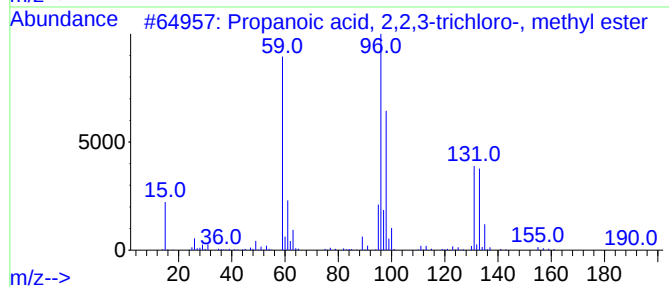
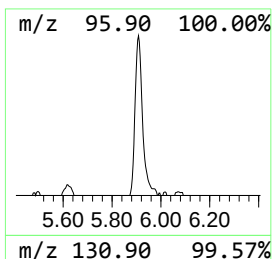
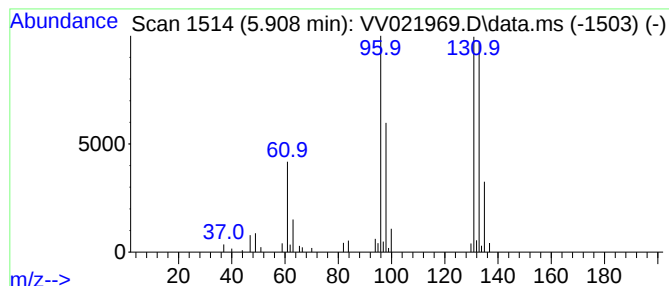
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082721WMA.M
Quant Title : VOC Analysis

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.
5.908	4.59 ug/L	77097	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	56
2			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	41
3			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	38
4			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	27
5			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	5.908	4.6	ug/L	77097	1	5.619	840571	50.0