

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082021\
 Data File : VV021916.D
 Acq On : 20 Aug 2021 15:47
 Operator : SY/MD
 Sample : M3458-11ME
 Misc : 5.03g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AT7ME

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: VV021916.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	111	rBV	120682	183903	14.28%	1.763%
2	2.069	311	320	335	rVB	278624	393899	30.58%	3.777%
3	2.490	441	451	465	rBV	21743	39656	3.08%	0.380%
4	2.741	526	529	533	rVB4	638	420	0.03%	0.004%
5	2.764	533	536	538	rBV4	671	341	0.03%	0.003%
6	2.805	546	549	552	rVB	491	260	0.02%	0.002%
7	2.854	562	564	567	rVB2	561	272	0.02%	0.003%
8	2.889	571	575	578	rBV2	415	369	0.03%	0.004%
9	3.011	604	613	614	rBV6	1025	1251	0.10%	0.012%
10	3.056	625	627	631	rVB2	470	190	0.01%	0.002%
11	3.104	638	642	645	rBV3	423	334	0.03%	0.003%
12	3.291	696	700	702	rVB2	362	232	0.02%	0.002%
13	3.375	718	726	728	rBV2	285	325	0.03%	0.003%
14	3.490	759	762	765	rBV	263	203	0.02%	0.002%
15	3.603	793	797	801	rBV3	422	357	0.03%	0.003%
16	3.638	806	808	811	rVV3	364	231	0.02%	0.002%
17	3.709	826	830	836	rBV3	558	581	0.05%	0.006%
18	3.738	836	839	841	rBV2	342	195	0.02%	0.002%
19	3.786	850	854	860	rBV2	382	373	0.03%	0.004%
20	3.822	863	865	870	rVB	383	201	0.02%	0.002%
21	3.863	874	878	879	rBV	357	187	0.01%	0.002%
22	3.902	879	890	928	rBV3	63758	259434	20.14%	2.488%
23	4.346	1013	1028	1056	rBV	183221	485143	37.66%	4.652%
24	4.600	1105	1107	1109	rBV2	609	309	0.02%	0.003%
25	4.764	1154	1158	1160	rVB3	487	300	0.02%	0.003%
26	5.040	1228	1244	1289	rBV2	517606	1288111	100.00%	12.352%
27	5.336	1324	1336	1347	rBV4	5620	14535	1.13%	0.139%
28	5.471	1375	1378	1380	rBV3	712	469	0.04%	0.004%
29	5.612	1407	1422	1457	rBV	457707	968614	75.20%	9.288%
30	5.837	1489	1492	1494	rBV3	452	299	0.02%	0.003%
31	5.905	1501	1513	1530	rBV2	24184	53470	4.15%	0.513%
32	6.069	1552	1564	1594	rVB	262889	564510	43.82%	5.413%
33	6.301	1634	1636	1638	rBV2	351	221	0.02%	0.002%
34	6.333	1644	1646	1649	rBV3	479	249	0.02%	0.002%
35	6.548	1709	1713	1715	rBV2	444	306	0.02%	0.003%
36	6.583	1719	1724	1726	rBV2	487	341	0.03%	0.003%

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 Title : VOC Analysis

37	6.645	1733	1743	1745	rBV5	1319	1555	0.12%	0.015%
38	6.754	1774	1777	1780	rBV3	325	233	0.02%	0.002%
39	6.825	1797	1799	1803	rVB	522	261	0.02%	0.003%
40	6.934	1829	1833	1834	rBV2	416	290	0.02%	0.003%
41	6.989	1839	1850	1873	rBV	141149	276853	21.49%	2.655%
42	7.201	1912	1916	1919	rBV4	693	563	0.04%	0.005%
43	7.317	1939	1952	1971	rBV	595083	1070138	83.08%	10.262%
44	7.625	2038	2048	2080	rBV	93353	185850	14.43%	1.782%
45	7.886	2126	2129	2131	rBV2	398	245	0.02%	0.002%
46	7.979	2155	2158	2159	rBV	632	371	0.03%	0.004%
47	8.011	2166	2168	2172	rVB	335	208	0.02%	0.002%
48	8.107	2185	2198	2244	rBV2	228172	559183	43.41%	5.362%
49	8.503	2318	2321	2325	rBV4	593	438	0.03%	0.004%
50	8.548	2332	2335	2337	rBV3	398	254	0.02%	0.002%
51	8.577	2342	2344	2346	rVB	469	186	0.01%	0.002%
52	8.632	2357	2361	2365	rVV	359	291	0.02%	0.003%
53	8.712	2378	2386	2389	rBV4	561	599	0.05%	0.006%
54	8.792	2405	2411	2413	rVB5	712	391	0.03%	0.004%
55	8.808	2413	2416	2418	rBV2	333	190	0.01%	0.002%
56	8.857	2418	2431	2456	rBV	660406	1186259	92.09%	11.375%
57	9.140	2515	2519	2521	rBV3	782	686	0.05%	0.007%
58	9.217	2540	2543	2545	rBV3	342	281	0.02%	0.003%
59	9.487	2625	2627	2630	rBV2	321	222	0.02%	0.002%
60	9.551	2643	2647	2649	rBV4	841	686	0.05%	0.007%
61	9.606	2660	2664	2666	rVB3	434	289	0.02%	0.003%
62	9.628	2666	2671	2672	rBV2	361	264	0.02%	0.003%
63	9.670	2681	2684	2687	rBV3	422	243	0.02%	0.002%
64	9.689	2687	2690	2693	rVV2	373	273	0.02%	0.003%
65	9.706	2693	2695	2700	rVB2	529	349	0.03%	0.003%
66	9.821	2728	2731	2734	rBV	297	224	0.02%	0.002%
67	9.850	2737	2740	2742	rBV2	428	252	0.02%	0.002%
68	9.943	2761	2769	2773	rBV4	885	1266	0.10%	0.012%
69	10.011	2786	2790	2791	rBV	457	274	0.02%	0.003%
70	10.133	2819	2828	2837	rVB3	3848	6574	0.51%	0.063%
71	10.223	2842	2856	2873	rBV	371003	613543	47.63%	5.883%
72	10.458	2926	2929	2934	rVB2	522	410	0.03%	0.004%
73	10.490	2934	2939	2944	rVB3	368	387	0.03%	0.004%
74	10.522	2946	2949	2952	rVB3	279	188	0.01%	0.002%
75	10.541	2952	2955	2957	rBV2	750	534	0.04%	0.005%
76	10.651	2987	2989	2991	rBV3	397	197	0.02%	0.002%

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 ClientSampleId :
 COAT7ME

Integration Parameters: LSCINT.P

Integrator: RTE

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

77	10.741	3014	3017	3020	rBV	329	300	0.02%	0.003%
78	10.805	3034	3037	3042	rBV3	318	312	0.02%	0.003%
79	10.921	3065	3073	3081	rBV5	3563	5964	0.46%	0.057%
80	11.011	3097	3101	3103	rBV	277	213	0.02%	0.002%
81	11.069	3115	3119	3122	rBV	290	197	0.02%	0.002%
82	11.111	3130	3132	3134	rBV	303	211	0.02%	0.002%
83	11.149	3137	3144	3153	rVB7	1733	3095	0.24%	0.030%
84	11.252	3165	3176	3196	rBV	779861	1228620	95.38%	11.781%
85	11.477	3244	3246	3253	rVB5	664	451	0.04%	0.004%
86	11.522	3256	3260	3262	rBV2	466	397	0.03%	0.004%
87	11.628	3281	3293	3315	rBV	644851	1012510	78.60%	9.709%
88	11.934	3386	3388	3391	rVB2	397	216	0.02%	0.002%
89	11.982	3399	3403	3407	rBV3	401	383	0.03%	0.004%
90	12.001	3407	3409	3412	rVB2	419	189	0.01%	0.002%
91	12.056	3424	3426	3428	rBV	607	266	0.02%	0.003%
92	12.233	3474	3481	3482	rBV2	385	374	0.03%	0.004%
93	12.599	3589	3595	3605	rBV5	822	1061	0.08%	0.010%
94	12.715	3630	3631	3638	rVB2	370	326	0.03%	0.003%
95	12.747	3638	3641	3645	rBV	317	275	0.02%	0.003%
96	12.773	3647	3649	3654	rVB	291	188	0.01%	0.002%
97	12.895	3684	3687	3691	rBV2	516	350	0.03%	0.003%
98	13.017	3719	3725	3727	rBV	241	273	0.02%	0.003%
99	13.303	3811	3814	3816	rBV	295	209	0.02%	0.002%
100	14.146	4073	4076	4079	rBV2	722	486	0.04%	0.005%

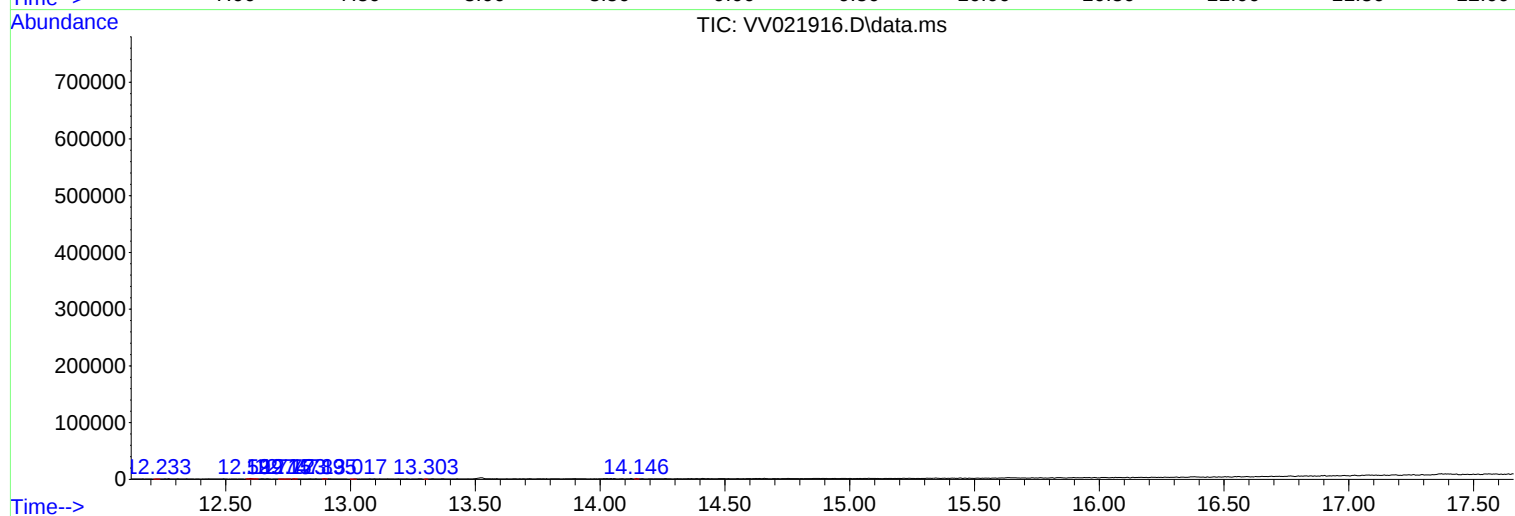
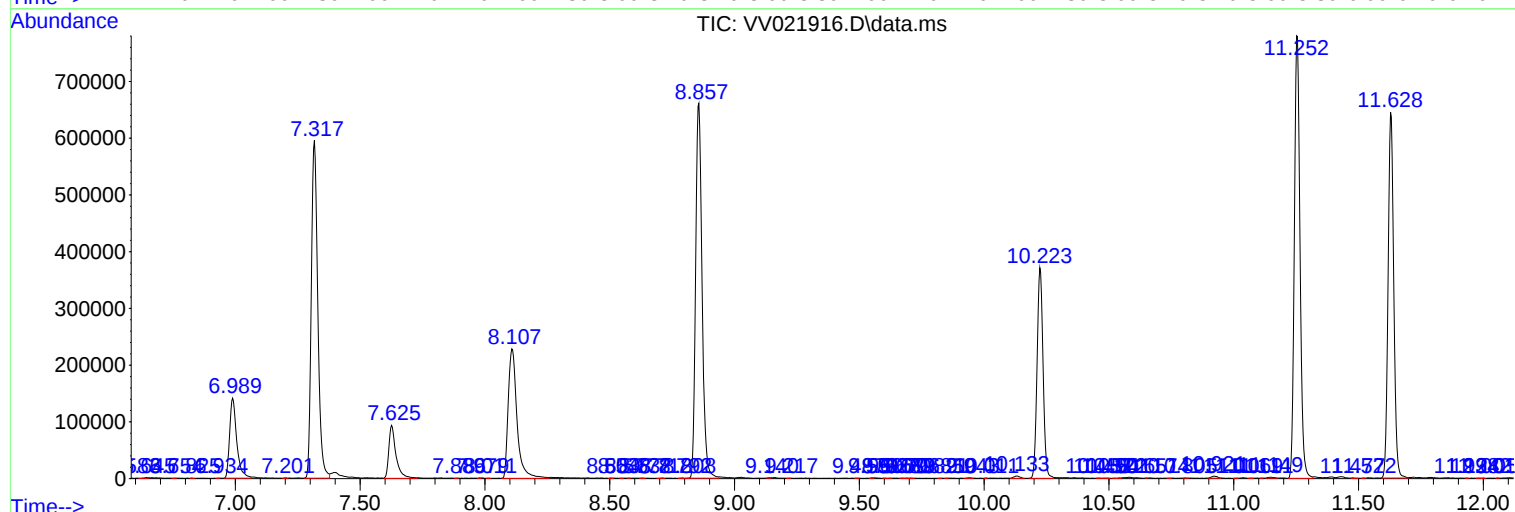
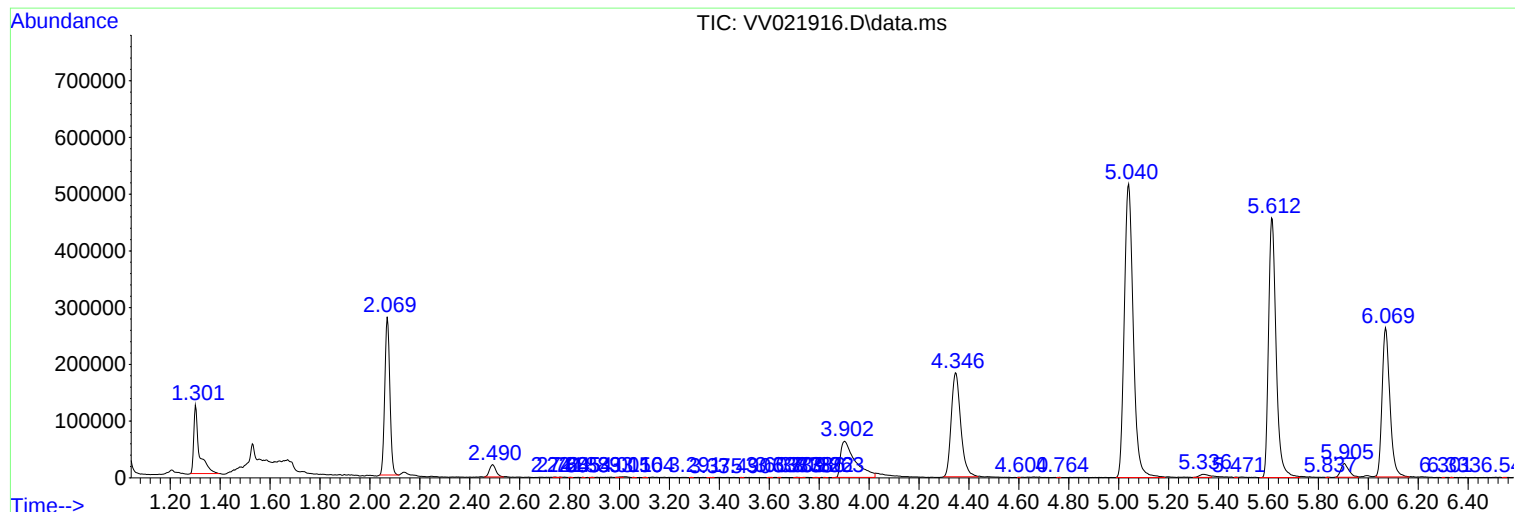
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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AT7ME

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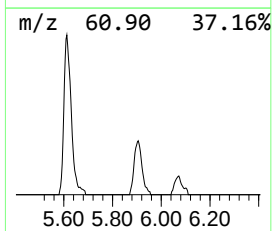
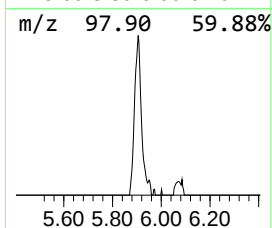
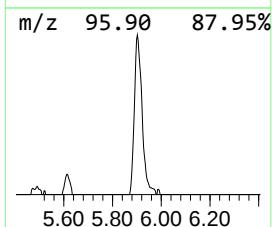
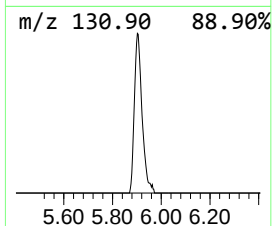
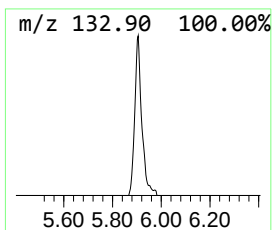
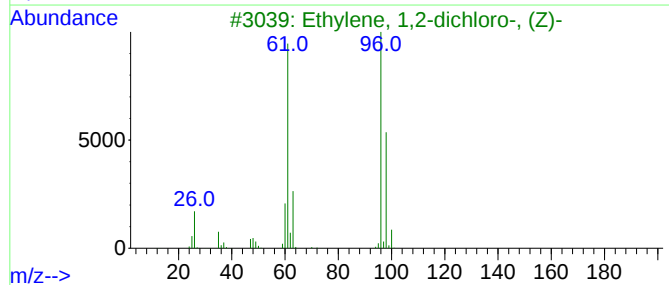
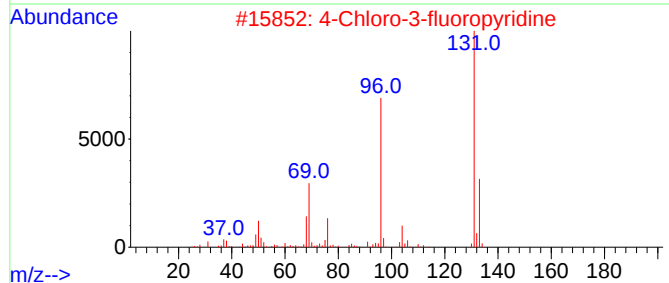
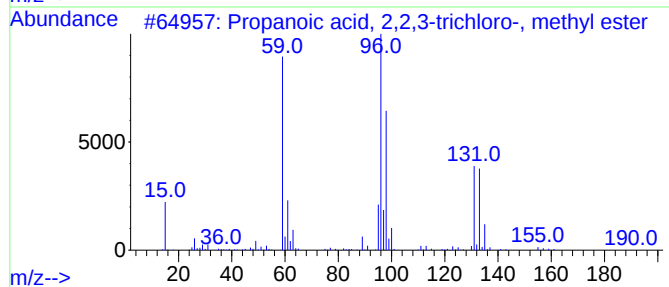
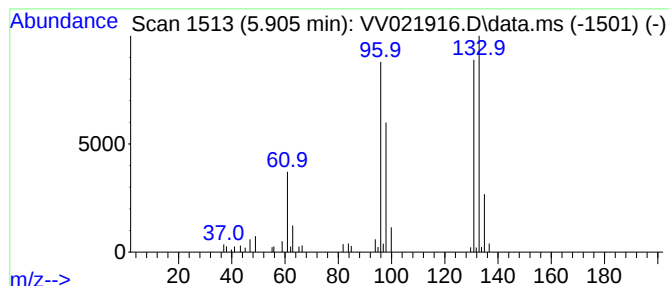
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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	2.76 ug/L	53470	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	64
2			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	38
3			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	30
4			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	27
5			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	23



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	5.905	2.8	ug/L	53470	1	5.612	968614	50.0