

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV081721\
 Data File : VV021821.D
 Acq On : 17 Aug 2021 18:11
 Operator : SY/MD
 Sample : M3365-14ME
 Misc : 11.82g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DBKCOME

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: VV021821.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	98	rVB	183190	183299	12.91%	1.619%
2	1.558	154	161	175	rVB	146579	169849	11.97%	1.500%
3	2.105	321	331	345	rBV	267400	393601	27.73%	3.475%
4	2.288	383	388	397	rVB2	3397	4796	0.34%	0.042%
5	2.323	397	399	400	rVV	281	89	0.01%	0.001%
6	2.333	400	402	405	rVB	271	131	0.01%	0.001%
7	2.439	431	435	436	rBV2	519	376	0.03%	0.003%
8	2.503	445	455	469	rVB	15286	25717	1.81%	0.227%
9	2.555	469	471	474	rBV2	154	120	0.01%	0.001%
10	2.606	485	487	488	rBV	328	124	0.01%	0.001%
11	2.635	494	496	500	rVB3	597	299	0.02%	0.003%
12	2.699	512	516	521	rVB3	432	470	0.03%	0.004%
13	2.764	524	536	545	rBV7	1999	3669	0.26%	0.032%
14	2.857	562	565	569	rBV2	254	164	0.01%	0.001%
15	2.873	569	570	573	rBV2	208	116	0.01%	0.001%
16	2.957	594	596	603	rVB	445	258	0.02%	0.002%
17	2.998	603	609	610	rBV2	321	238	0.02%	0.002%
18	3.043	617	623	626	rVB3	438	355	0.03%	0.003%
19	3.108	640	643	647	rVB2	155	107	0.01%	0.001%
20	3.143	650	654	656	rBV2	137	106	0.01%	0.001%
21	3.207	672	674	676	rVB	219	76	0.01%	0.001%
22	3.227	676	680	682	rBV2	545	291	0.02%	0.003%
23	3.249	685	687	688	rBV	273	98	0.01%	0.001%
24	3.333	709	713	714	rBV2	269	174	0.01%	0.002%
25	3.387	727	730	732	rBV	392	173	0.01%	0.002%
26	3.439	743	746	749	rBV2	349	241	0.02%	0.002%
27	3.458	749	752	756	rVB2	554	340	0.02%	0.003%
28	3.523	769	772	774	rBV	243	136	0.01%	0.001%
29	3.600	794	796	798	rBV2	297	161	0.01%	0.001%
30	3.642	806	809	812	rBV2	319	252	0.02%	0.002%
31	3.873	871	881	915	rBV	138910	361184	25.45%	3.189%
32	4.349	1015	1029	1060	rVB	231831	570133	40.17%	5.034%
33	4.825	1174	1177	1179	rBV	377	226	0.02%	0.002%
34	4.924	1205	1208	1212	rVB2	565	388	0.03%	0.003%
35	5.047	1227	1246	1281	rBV2	551490	1419393	100.00%	12.533%
36	5.342	1335	1338	1340	rBV2	765	422	0.03%	0.004%

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

37	5.381	1347	1350	1353	rBV3	603	428	0.03%	0.004%
38	5.400	1353	1356	1361	rBV5	632	698	0.05%	0.006%
39	5.477	1378	1380	1382	rBV	430	301	0.02%	0.003%
40	5.619	1411	1424	1455	rBV	483554	979578	69.01%	8.650%
41	5.905	1502	1513	1532	rBV2	39834	86413	6.09%	0.763%
42	6.072	1551	1565	1593	rBV	318514	660103	46.51%	5.829%
43	6.333	1644	1646	1648	rBV3	537	203	0.01%	0.002%
44	6.371	1656	1658	1659	rBV	281	116	0.01%	0.001%
45	6.455	1682	1684	1685	rBV	375	136	0.01%	0.001%
46	6.490	1692	1695	1696	rBV	265	146	0.01%	0.001%
47	6.526	1702	1706	1708	rBV	641	542	0.04%	0.005%
48	6.751	1774	1776	1780	rVB2	426	236	0.02%	0.002%
49	6.780	1783	1785	1788	rBV	246	171	0.01%	0.002%
50	6.847	1802	1806	1808	rBV3	321	229	0.02%	0.002%
51	6.892	1818	1820	1823	rVB2	341	161	0.01%	0.001%
52	6.908	1823	1825	1827	rBV	245	102	0.01%	0.001%
53	6.928	1827	1831	1833	rBV2	218	159	0.01%	0.001%
54	6.989	1839	1850	1878	rBV	180288	332989	23.46%	2.940%
55	7.317	1941	1952	1972	rBV	620602	1085081	76.45%	9.581%
56	7.625	2038	2048	2073	rBV	122138	213746	15.06%	1.887%
57	7.892	2129	2131	2134	rBV3	428	263	0.02%	0.002%
58	7.940	2145	2146	2148	rVB	229	68	0.00%	0.001%
59	7.956	2148	2151	2153	rBV	285	180	0.01%	0.002%
60	7.982	2153	2159	2166	rVB7	2173	3119	0.22%	0.028%
61	8.053	2177	2181	2182	rBV	248	134	0.01%	0.001%
62	8.091	2182	2193	2234	rBV2	343374	682155	48.06%	6.023%
63	8.580	2343	2345	2347	rBV2	483	173	0.01%	0.002%
64	8.619	2355	2357	2363	rVB3	767	558	0.04%	0.005%
65	8.735	2389	2393	2394	rBV	287	150	0.01%	0.001%
66	8.808	2414	2416	2418	rBV2	275	124	0.01%	0.001%
67	8.854	2418	2430	2458	rBV	705589	1153997	81.30%	10.190%
68	9.300	2567	2569	2570	rBV	324	128	0.01%	0.001%
69	9.378	2591	2593	2598	rVB3	316	168	0.01%	0.001%
70	9.413	2602	2604	2608	rBV	362	350	0.02%	0.003%
71	9.506	2631	2633	2634	rVB	338	82	0.01%	0.001%
72	9.516	2634	2636	2637	rVB	282	81	0.01%	0.001%
73	9.554	2640	2648	2650	rBV4	1974	2153	0.15%	0.019%
74	9.702	2692	2694	2697	rBV2	245	115	0.01%	0.001%
75	9.760	2710	2712	2715	rBV2	273	138	0.01%	0.001%
76	9.943	2760	2769	2776	rBV6	2144	3247	0.23%	0.029%

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Peak Location: TOP

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

77	10.024	2791	2794	2796	rBV2	265	167	0.01%	0.001%
78	10.056	2801	2804	2809	rVV	336	201	0.01%	0.002%
79	10.111	2819	2821	2822	rBV	222	96	0.01%	0.001%
80	10.220	2842	2855	2879	rBV	435161	698769	49.23%	6.170%
81	10.410	2912	2914	2918	rVB2	556	372	0.03%	0.003%
82	10.548	2950	2957	2963	rBV4	2636	3235	0.23%	0.029%
83	10.886	3061	3062	3065	rBV	234	113	0.01%	0.001%
84	10.921	3065	3073	3081	rBV3	5023	7384	0.52%	0.065%
85	11.079	3120	3122	3127	rBV2	424	257	0.02%	0.002%
86	11.191	3150	3157	3164	rBV7	3684	5587	0.39%	0.049%
87	11.252	3164	3176	3200	rBV	717277	1114795	78.54%	9.844%
88	11.554	3267	3270	3274	rVB2	346	210	0.01%	0.002%
89	11.625	3281	3292	3311	rBV	683313	1084761	76.42%	9.578%
90	11.918	3379	3383	3386	rBV2	393	351	0.02%	0.003%
91	12.271	3491	3493	3495	rBV2	373	170	0.01%	0.002%
92	12.606	3595	3597	3600	rBV2	535	256	0.02%	0.002%
93	12.654	3604	3612	3623	rVB3	5982	9467	0.67%	0.084%
94	12.741	3637	3639	3644	rBV3	410	459	0.03%	0.004%
95	13.091	3746	3748	3752	rVB2	527	273	0.02%	0.002%
96	13.107	3752	3753	3758	rBV	260	169	0.01%	0.001%
97	13.271	3796	3804	3815	rVB4	8022	11899	0.84%	0.105%
98	13.512	3871	3879	3889	rVB	15826	24814	1.75%	0.219%
99	13.750	3944	3953	3966	rVB3	9468	14190	1.00%	0.125%
100	13.959	4015	4018	4023	rBV2	582	544	0.04%	0.005%

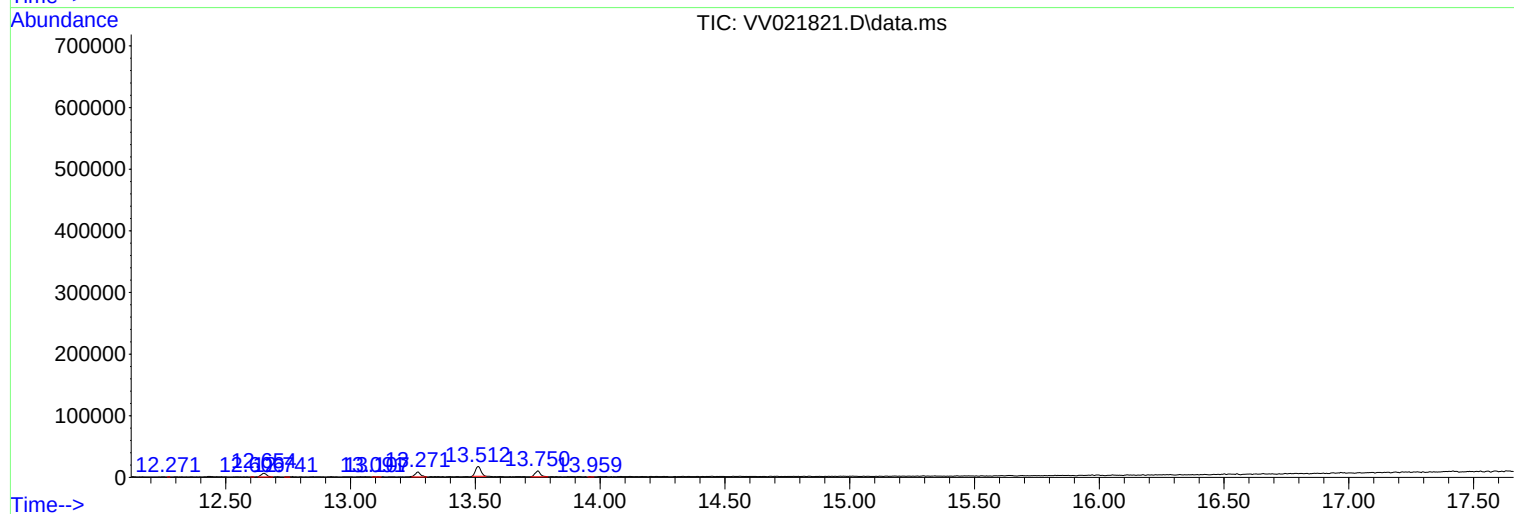
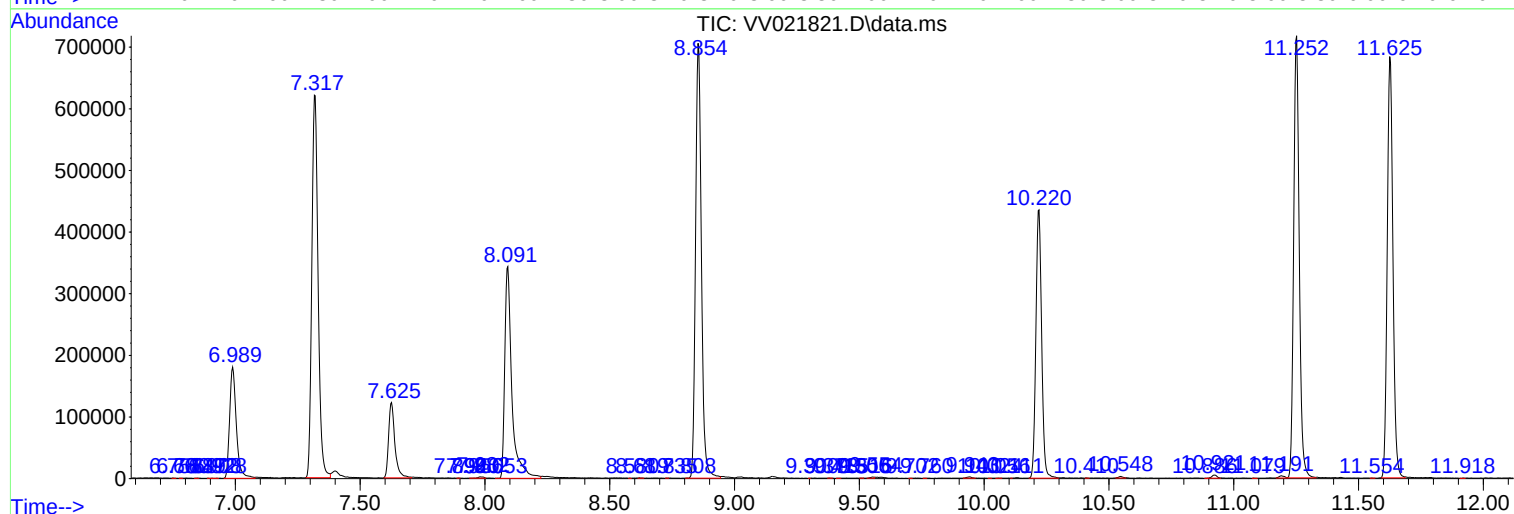
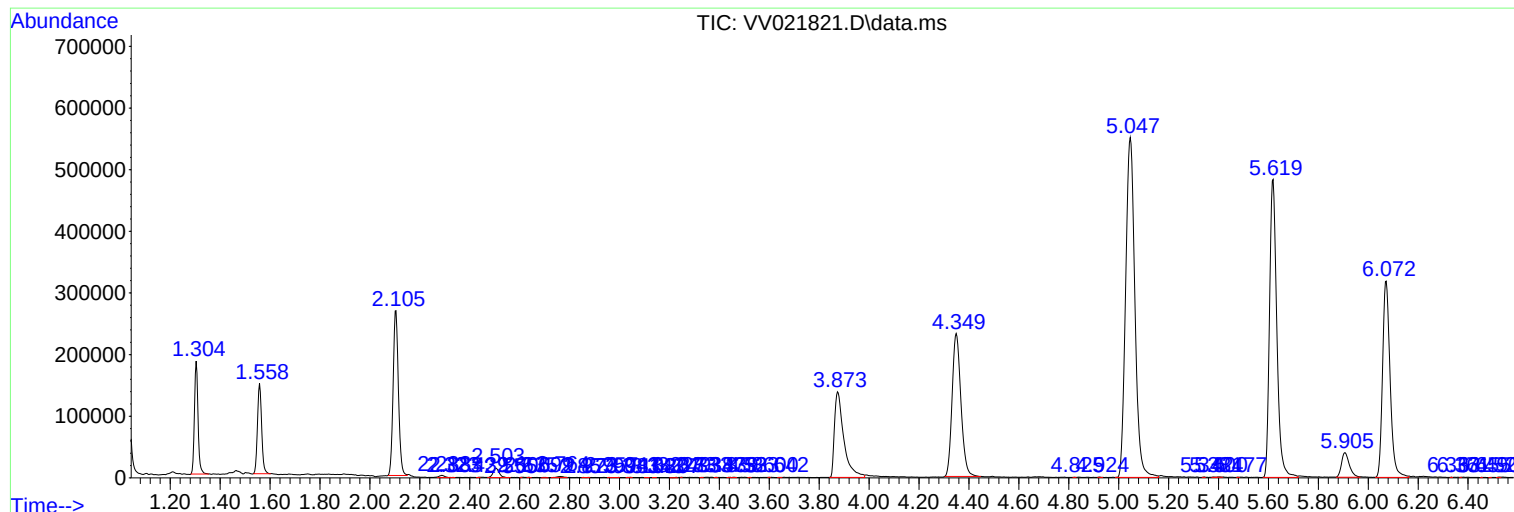
Sum of corrected areas: 11325032

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MSVOA_V
ClientSampleId :
DBKCOME

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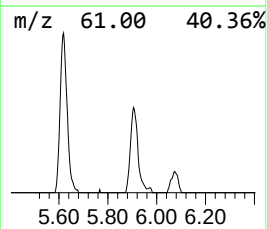
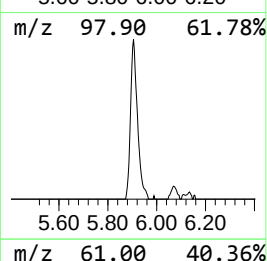
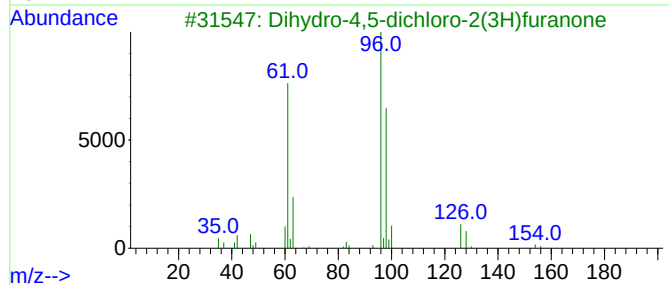
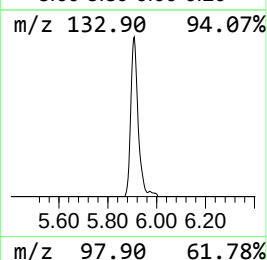
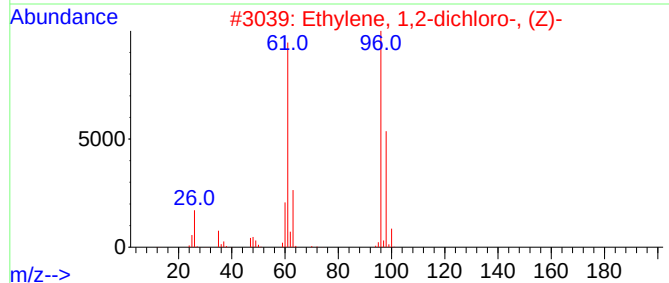
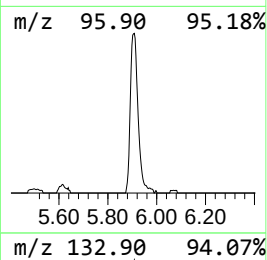
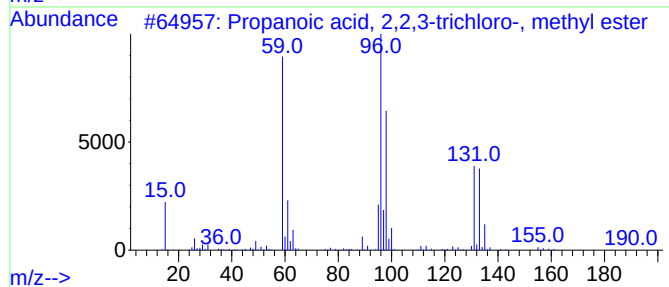
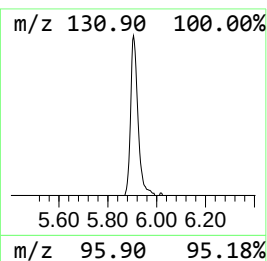
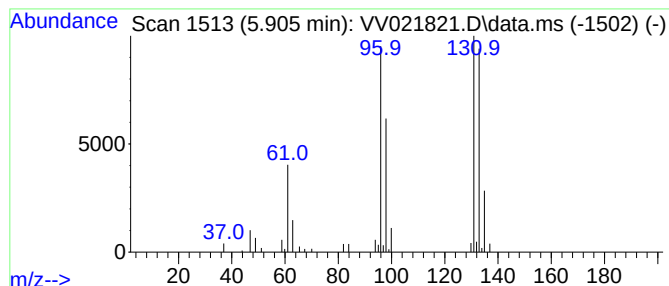
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.905	4.41 ug/L	86413	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	37
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			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	27
5			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	23



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	5.905	4.4	ug/L	86413	1	5.619	979578	50.0