

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072821\
 Data File : VV021704.D
 Acq On : 28 Jul 2021 12:54
 Operator : SY/MD
 Sample : VV0728MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VBLK221

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\SFAMVLM071921WMA.M
 Title : VOC Analysis

Signal : TIC: VV021704.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	223260	225700	13.60%	1.745%
2	1.561	155	162	179	rVB	175194	204053	12.29%	1.577%
3	2.105	321	331	364	rVB	373045	556300	33.52%	4.300%
4	2.506	449	456	468	rVB3	6255	9756	0.59%	0.075%
5	2.664	501	505	508	rBV2	430	359	0.02%	0.003%
6	2.709	517	519	521	rBV2	374	163	0.01%	0.001%
7	2.767	531	537	544	rBV9	993	1511	0.09%	0.012%
8	2.950	591	594	596	rVV2	246	132	0.01%	0.001%
9	3.040	615	622	626	rBV3	729	732	0.04%	0.006%
10	3.082	630	635	639	rBV3	371	427	0.03%	0.003%
11	3.204	669	673	675	rBV3	366	227	0.01%	0.002%
12	3.262	690	691	695	rVB2	327	140	0.01%	0.001%
13	3.297	700	702	705	rVB3	402	219	0.01%	0.002%
14	3.378	723	727	730	rVB2	323	230	0.01%	0.002%
15	3.407	730	736	737	rBV2	138	148	0.01%	0.001%
16	3.561	781	784	787	rVB	522	351	0.02%	0.003%
17	3.600	793	796	803	rVB3	424	336	0.02%	0.003%
18	3.645	803	810	815	rBV4	348	399	0.02%	0.003%
19	3.712	829	831	834	rVV	421	251	0.02%	0.002%
20	3.725	834	835	839	rVB	337	145	0.01%	0.001%
21	3.770	845	849	852	rBV	270	206	0.01%	0.002%
22	3.789	852	855	857	rBV	296	182	0.01%	0.001%
23	3.873	870	881	927	rBV	144546	384477	23.16%	2.972%
24	4.349	1012	1029	1053	rBV2	259330	646548	38.95%	4.998%
25	4.661	1123	1126	1127	rBV2	499	259	0.02%	0.002%
26	4.822	1175	1176	1180	rBV2	207	172	0.01%	0.001%
27	4.895	1197	1199	1204	rVB3	261	229	0.01%	0.002%
28	4.921	1204	1207	1209	rBV2	347	158	0.01%	0.001%
29	4.944	1209	1214	1215	rBV2	253	167	0.01%	0.001%
30	4.953	1215	1217	1223	rVB2	379	298	0.02%	0.002%
31	5.047	1223	1246	1285	rBV2	646983	1659799	100.00%	12.830%
32	5.326	1331	1333	1335	rBV2	508	194	0.01%	0.001%
33	5.484	1380	1382	1385	rBV2	195	149	0.01%	0.001%
34	5.529	1394	1396	1399	rVB2	724	296	0.02%	0.002%
35	5.551	1399	1403	1406	rBV3	603	612	0.04%	0.005%
36	5.616	1411	1423	1456	rBV	523810	1053843	63.49%	8.146%

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 Title : VOC Analysis

37	5.905	1502	1513	1530	rBV2	35646	74649	4.50%	0.577%
38	6.008	1544	1545	1550	rBV3	527	322	0.02%	0.002%
39	6.069	1550	1564	1596	rBV	366397	746864	45.00%	5.773%
40	6.349	1647	1651	1657	rBV3	512	539	0.03%	0.004%
41	6.375	1657	1659	1663	rVB	317	200	0.01%	0.002%
42	6.394	1663	1665	1668	rBV	330	236	0.01%	0.002%
43	6.481	1690	1692	1694	rBV2	350	185	0.01%	0.001%
44	6.632	1734	1739	1744	rBV4	956	1475	0.09%	0.011%
45	6.757	1776	1778	1783	rVB2	535	415	0.03%	0.003%
46	6.783	1783	1786	1788	rBV2	226	186	0.01%	0.001%
47	6.815	1792	1796	1800	rBV3	129	133	0.01%	0.001%
48	6.860	1808	1810	1815	rVB	312	167	0.01%	0.001%
49	6.892	1815	1820	1823	rBV2	270	185	0.01%	0.001%
50	6.985	1835	1849	1869	rBV	216667	394184	23.75%	3.047%
51	7.317	1940	1952	1970	rBV	783724	1365582	82.27%	10.555%
52	7.622	2037	2047	2068	rBV	150404	258316	15.56%	1.997%
53	7.828	2107	2111	2114	rVB4	592	409	0.02%	0.003%
54	7.873	2121	2125	2128	rVB2	423	316	0.02%	0.002%
55	7.931	2139	2143	2144	rBV	300	165	0.01%	0.001%
56	7.985	2156	2160	2164	rBV5	681	778	0.05%	0.006%
57	8.024	2168	2172	2175	rVB2	276	203	0.01%	0.002%
58	8.088	2181	2192	2231	rBV	428391	826909	49.82%	6.392%
59	8.419	2293	2295	2299	rVB2	417	257	0.02%	0.002%
60	8.599	2349	2351	2354	rBV3	475	293	0.02%	0.002%
61	8.616	2354	2356	2358	rVV	359	166	0.01%	0.001%
62	8.651	2364	2367	2369	rBV	316	190	0.01%	0.001%
63	8.680	2373	2376	2379	rBV2	471	282	0.02%	0.002%
64	8.718	2385	2388	2391	rBV	394	220	0.01%	0.002%
65	8.776	2404	2406	2409	rBV	343	248	0.01%	0.002%
66	8.854	2417	2430	2459	rBV	763975	1262370	76.06%	9.758%
67	9.085	2498	2502	2504	rBV4	316	254	0.02%	0.002%
68	9.146	2516	2521	2522	rBV3	1420	977	0.06%	0.008%
69	9.223	2539	2545	2548	rBV2	373	354	0.02%	0.003%
70	9.313	2570	2573	2575	rBV2	306	213	0.01%	0.002%
71	9.400	2598	2600	2605	rVB2	261	166	0.01%	0.001%
72	9.506	2631	2633	2636	rBV	341	215	0.01%	0.002%
73	9.542	2641	2644	2646	rBV2	674	494	0.03%	0.004%
74	9.673	2683	2685	2689	rBV3	266	224	0.01%	0.002%
75	9.857	2739	2742	2745	rBV2	322	179	0.01%	0.001%
76	9.905	2753	2757	2761	rBV2	311	292	0.02%	0.002%

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Title : VOC Analysis

77	9.931	2762	2765	2767	rBV2	571	426	0.03%	0.003%
78	10.050	2800	2802	2806	rVB	315	147	0.01%	0.001%
79	10.072	2806	2809	2812	rBV2	181	155	0.01%	0.001%
80	10.104	2816	2819	2820	rBV	440	210	0.01%	0.002%
81	10.133	2820	2828	2839	rBV6	3482	5755	0.35%	0.044%
82	10.217	2842	2854	2873	rBV	464661	733141	44.17%	5.667%
83	10.452	2925	2927	2930	rBV3	510	274	0.02%	0.002%
84	10.548	2946	2957	2961	rBV4	1441	2329	0.14%	0.018%
85	10.664	2988	2993	2995	rBV2	429	437	0.03%	0.003%
86	10.722	3007	3011	3015	rVB2	520	339	0.02%	0.003%
87	10.751	3015	3020	3023	rBV2	386	435	0.03%	0.003%
88	10.828	3041	3044	3047	rBV2	462	452	0.03%	0.003%
89	10.921	3064	3073	3083	rBV4	4787	7727	0.47%	0.060%
90	11.024	3103	3105	3108	rBV2	484	334	0.02%	0.003%
91	11.114	3130	3133	3134	rBV	377	175	0.01%	0.001%
92	11.249	3164	3175	3201	rBV	791925	1234519	74.38%	9.542%
93	11.625	3280	3292	3310	rBV	765577	1213273	73.10%	9.378%
94	11.876	3368	3370	3373	rVB2	435	212	0.01%	0.002%
95	11.966	3395	3398	3401	rBV3	381	288	0.02%	0.002%
96	12.654	3605	3612	3620	rBV8	4344	6540	0.39%	0.051%
97	12.889	3683	3685	3687	rBV2	514	247	0.01%	0.002%
98	13.268	3796	3803	3813	rBV5	5963	9107	0.55%	0.070%
99	13.512	3871	3879	3890	rBV	12259	19432	1.17%	0.150%
100	13.750	3945	3953	3965	rVB4	7772	12321	0.74%	0.095%

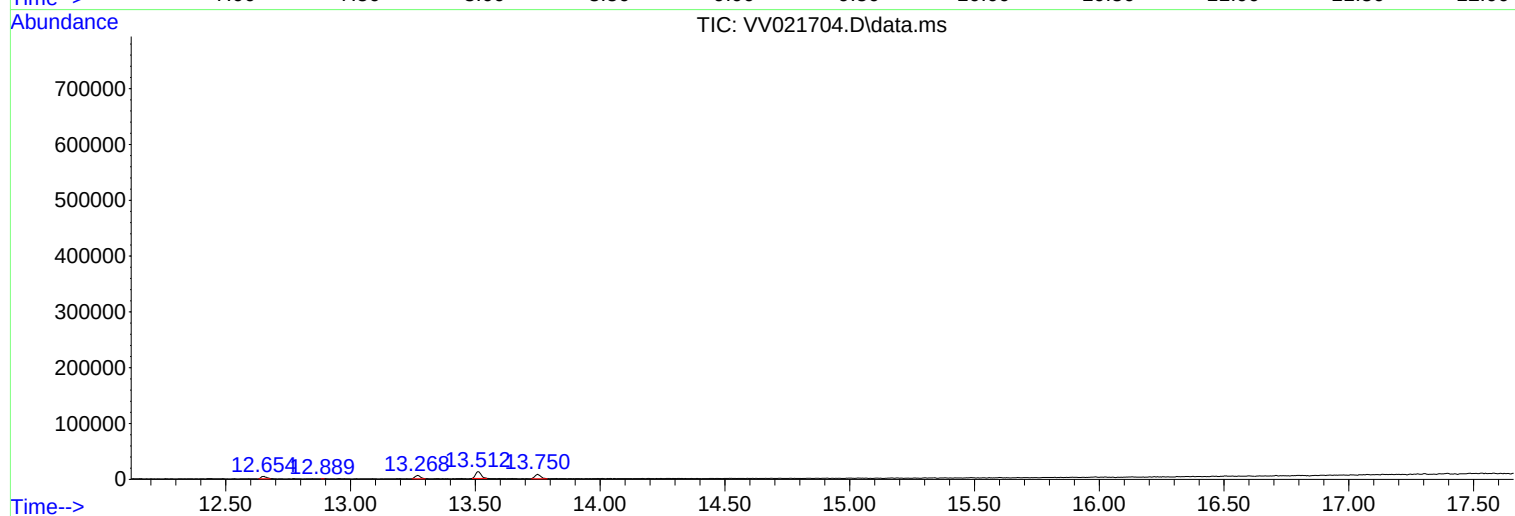
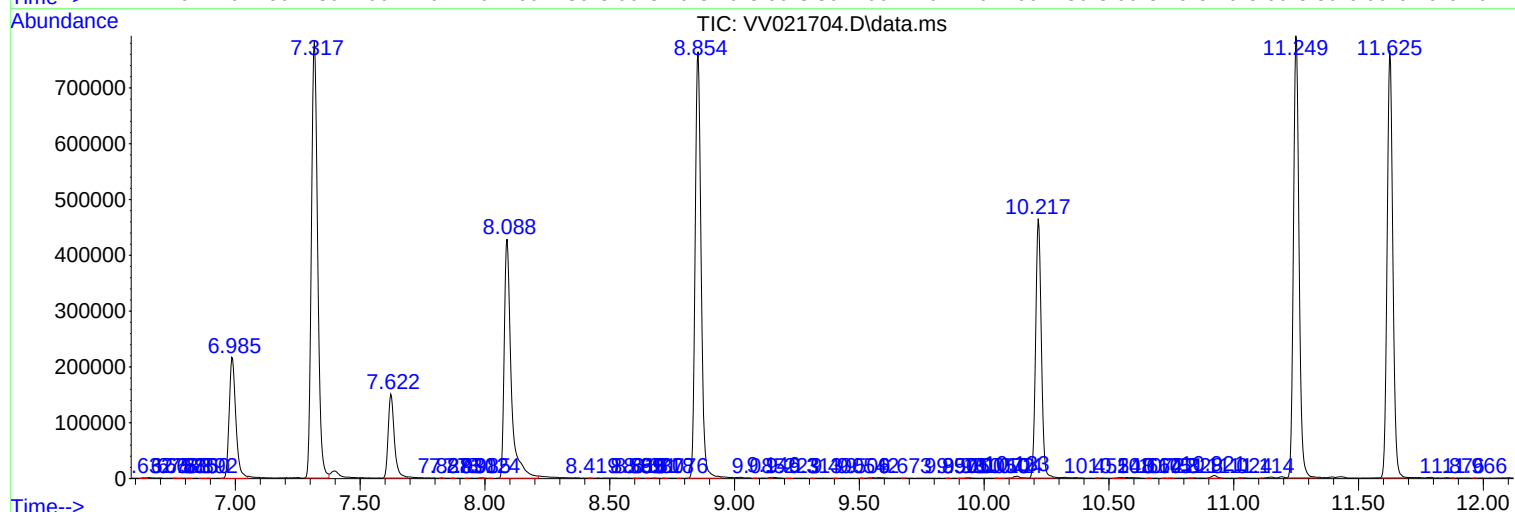
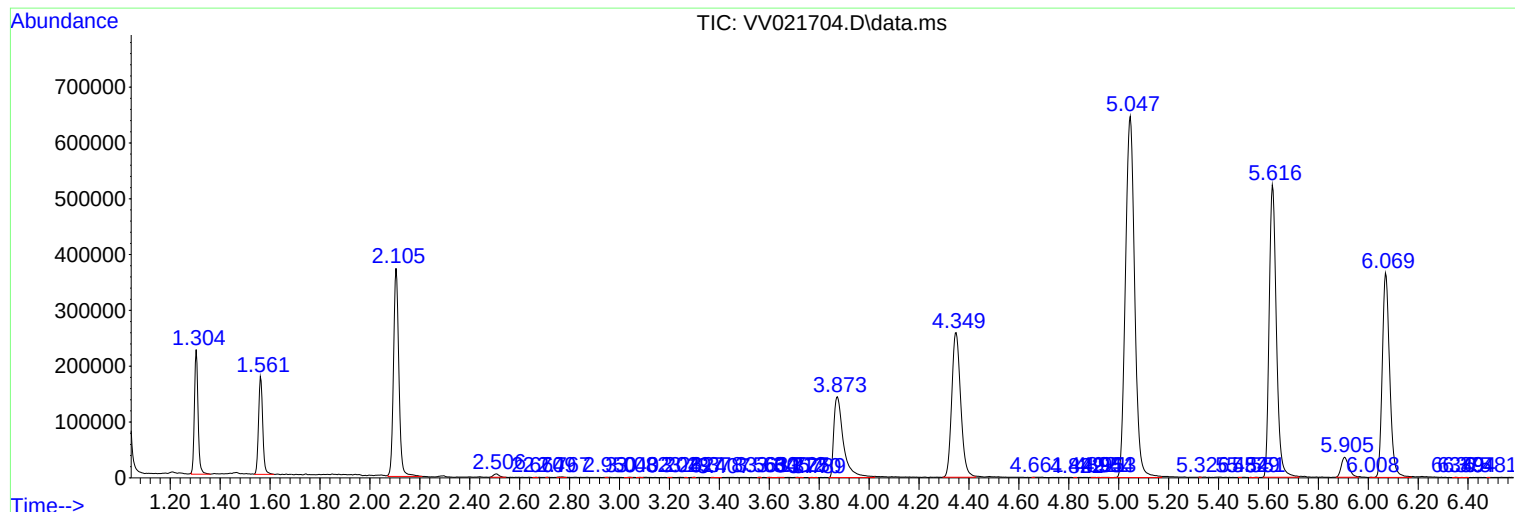
Sum of corrected areas: 12937255

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Instrument :
MSVOA_V
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM071921WMA.M
Quant Title : VOC Analysis

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



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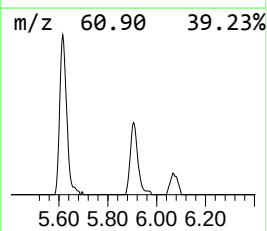
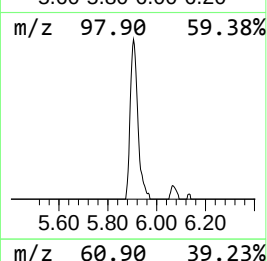
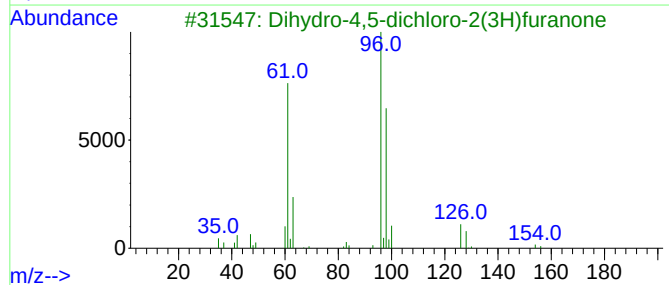
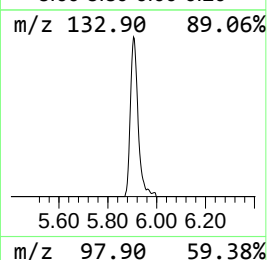
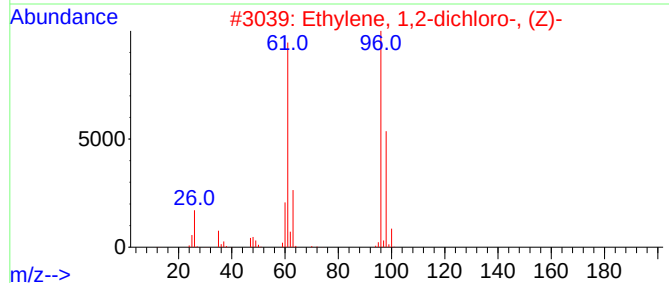
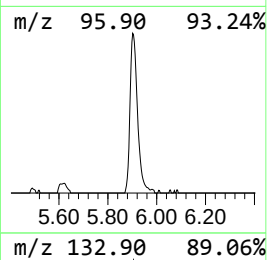
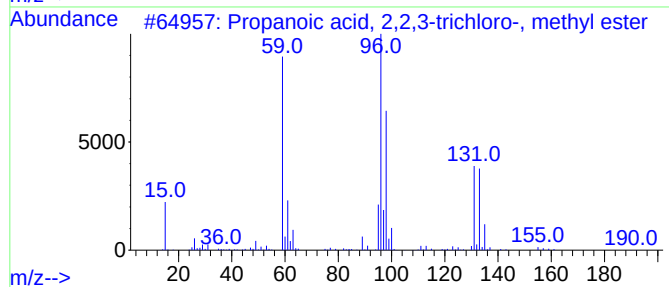
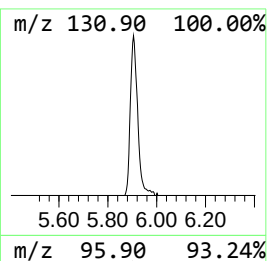
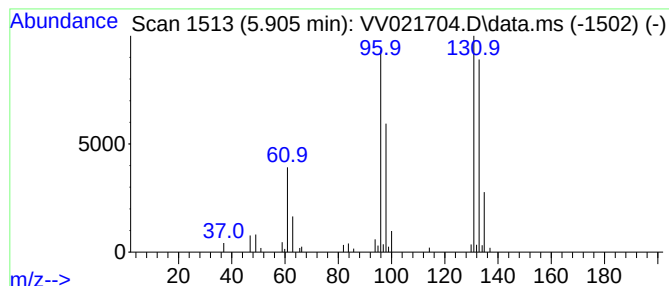
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM071921WMA.M
Quant Title : VOC Analysis

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	3.54 ug/L	74649	1,4-Difluorobenzene	5.616

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	32
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
unknown-01	5.905	3.5	ug/L	74649	1	5.616	1053840	50.0