

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV030121\
 Data File : VV020422.D
 Acq On : 01 Mar 2021 11:24
 Operator : SY/MD
 Sample : VV0301MBL01
 Misc : 5.0g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VBLK168

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\SFAMVLM022621WMA.M
 Title : VOC Analysis

Signal : TIC: VV020422.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.307	76	83	99	rVB	214862	217641	12.15%	1.506%
2	1.571	157	165	176	rBV	189007	215717	12.04%	1.492%
3	2.108	321	332	361	rVB	394648	610260	34.07%	4.222%
4	2.230	369	370	373	rVB	419	204	0.01%	0.001%
5	2.298	386	391	398	rVB2	1078	1483	0.08%	0.010%
6	2.326	398	400	407	rVB2	334	292	0.02%	0.002%
7	2.510	451	457	466	rVB5	1630	2323	0.13%	0.016%
8	2.613	486	489	496	rVB2	370	379	0.02%	0.003%
9	2.648	496	500	503	rVB2	322	216	0.01%	0.001%
10	2.667	503	506	508	rBV	281	181	0.01%	0.001%
11	2.809	546	550	551	rBV2	242	163	0.01%	0.001%
12	3.121	642	647	650	rBV	256	196	0.01%	0.001%
13	3.156	650	658	663	rBV2	190	290	0.02%	0.002%
14	3.185	663	667	670	rVB2	242	173	0.01%	0.001%
15	3.352	715	719	724	rVB	235	181	0.01%	0.001%
16	3.642	802	809	811	rBV2	155	171	0.01%	0.001%
17	3.892	876	887	929	rBV	116175	359625	20.08%	2.488%
18	4.352	1012	1030	1065	rBV	290905	732003	40.87%	5.064%
19	4.545	1086	1090	1096	rVB4	396	426	0.02%	0.003%
20	4.619	1111	1113	1115	rVB	360	171	0.01%	0.001%
21	4.828	1174	1178	1181	rBV3	307	249	0.01%	0.002%
22	4.863	1184	1189	1191	rBV	317	229	0.01%	0.002%
23	4.934	1208	1211	1215	rBV2	306	269	0.02%	0.002%
24	5.050	1229	1247	1270	rBV2	709335	1791130	100.00%	12.392%
25	5.455	1367	1373	1376	rBV2	399	507	0.03%	0.004%
26	5.523	1393	1394	1399	rVB2	332	183	0.01%	0.001%
27	5.551	1399	1403	1406	rBV3	297	212	0.01%	0.001%
28	5.622	1411	1425	1466	rBV	608393	1226942	68.50%	8.488%
29	5.854	1494	1497	1498	rBV2	270	175	0.01%	0.001%
30	5.908	1501	1514	1534	rBV2	50797	104899	5.86%	0.726%
31	5.998	1540	1542	1545	rVB3	440	201	0.01%	0.001%
32	6.072	1552	1565	1594	rBV	395964	807217	45.07%	5.585%
33	6.278	1627	1629	1632	rVB2	497	242	0.01%	0.002%
34	6.320	1640	1642	1645	rVB3	425	205	0.01%	0.001%
35	6.410	1667	1670	1676	rVB2	185	177	0.01%	0.001%
36	6.442	1676	1680	1681	rBV2	258	173	0.01%	0.001%

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 Title : VOC Analysis

37	6.519	1699	1704	1707	rBV	208	179	0.01%	0.001%
38	6.555	1713	1715	1719	rVB	275	177	0.01%	0.001%
39	6.635	1736	1740	1744	rVV3	506	426	0.02%	0.003%
40	6.661	1744	1748	1752	rVV3	487	468	0.03%	0.003%
41	6.680	1752	1754	1757	rVV	455	182	0.01%	0.001%
42	6.706	1757	1762	1765	rVV4	338	340	0.02%	0.002%
43	6.886	1813	1818	1820	rBV2	261	216	0.01%	0.001%
44	6.992	1838	1851	1877	rBV	207592	382008	21.33%	2.643%
45	7.265	1933	1936	1940	rBV2	437	350	0.02%	0.002%
46	7.320	1940	1953	1988	rBV	853889	1471612	82.16%	10.181%
47	7.590	2033	2037	2038	rBV2	376	219	0.01%	0.002%
48	7.625	2038	2048	2072	rBV	149639	259666	14.50%	1.796%
49	7.838	2112	2114	2118	rVB2	500	292	0.02%	0.002%
50	7.860	2118	2121	2123	rVB2	508	256	0.01%	0.002%
51	7.924	2136	2141	2145	rBV2	406	373	0.02%	0.003%
52	7.982	2154	2159	2165	rBV3	1031	1386	0.08%	0.010%
53	8.095	2183	2194	2238	rBV2	405124	821456	45.86%	5.683%
54	8.333	2265	2268	2275	rVB6	613	534	0.03%	0.004%
55	8.374	2279	2281	2282	rBV	443	182	0.01%	0.001%
56	8.394	2286	2287	2293	rVB3	779	619	0.03%	0.004%
57	8.429	2293	2298	2300	rBV3	307	282	0.02%	0.002%
58	8.770	2401	2404	2409	rBV2	387	269	0.02%	0.002%
59	8.857	2419	2431	2462	rBV	940090	1535043	85.70%	10.620%
60	9.149	2518	2522	2524	rBV2	634	501	0.03%	0.003%
61	9.198	2534	2537	2539	rBV	290	181	0.01%	0.001%
62	9.294	2564	2567	2570	rVV	217	160	0.01%	0.001%
63	9.320	2572	2575	2578	rVV	252	211	0.01%	0.001%
64	9.339	2578	2581	2585	rVB	274	188	0.01%	0.001%
65	9.397	2594	2599	2601	rBV2	217	221	0.01%	0.002%
66	9.551	2645	2647	2649	rBV2	331	198	0.01%	0.001%
67	9.564	2649	2651	2655	rVB2	499	266	0.01%	0.002%
68	9.654	2676	2679	2682	rBV2	281	154	0.01%	0.001%
69	9.953	2766	2772	2777	rBV3	289	419	0.02%	0.003%
70	10.014	2788	2791	2794	rBV	196	173	0.01%	0.001%
71	10.223	2843	2856	2879	rBV	538743	845072	47.18%	5.846%
72	10.635	2980	2984	2988	rBV2	215	192	0.01%	0.001%
73	10.847	3043	3050	3053	rBV2	255	323	0.02%	0.002%
74	10.979	3088	3091	3094	rVB2	333	229	0.01%	0.002%
75	11.011	3094	3101	3103	rBV2	229	192	0.01%	0.001%
76	11.172	3148	3151	3152	rBV	580	267	0.01%	0.002%

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 Title : VOC Analysis

77	11.255	3165	3177	3204	rBV	1000695	1521870	84.97%	10.529%
78	11.493	3248	3251	3254	rBV2	240	158	0.01%	0.001%
79	11.509	3254	3256	3261	rVB3	228	164	0.01%	0.001%
80	11.551	3266	3269	3271	rBV2	334	234	0.01%	0.002%
81	11.632	3281	3294	3318	rBV	984135	1519139	84.81%	10.510%
82	11.805	3346	3348	3351	rBV2	359	160	0.01%	0.001%
83	11.821	3351	3353	3357	rVV2	266	180	0.01%	0.001%
84	11.992	3403	3406	3408	rBV	289	178	0.01%	0.001%
85	12.050	3421	3424	3428	rBV	268	221	0.01%	0.002%
86	12.349	3513	3517	3522	rVB	203	189	0.01%	0.001%
87	12.525	3570	3572	3577	rVB2	365	280	0.02%	0.002%
88	12.657	3606	3613	3618	rBV3	1461	2025	0.11%	0.014%
89	12.886	3682	3684	3690	rVB3	326	192	0.01%	0.001%
90	12.914	3690	3693	3697	rBV	564	397	0.02%	0.003%
91	13.181	3773	3776	3780	rVB	359	233	0.01%	0.002%
92	13.271	3800	3804	3813	rBV4	1286	1788	0.10%	0.012%
93	13.339	3822	3825	3827	rBV	271	191	0.01%	0.001%
94	13.381	3836	3838	3840	rBV	257	168	0.01%	0.001%
95	13.525	3875	3883	3889	rBV3	1542	2131	0.12%	0.015%
96	13.696	3931	3936	3938	rBV	581	518	0.03%	0.004%
97	13.757	3949	3955	3962	rVB3	1807	2398	0.13%	0.017%
98	13.934	4007	4010	4017	rBV3	425	491	0.03%	0.003%
99	14.165	4080	4082	4086	rVB2	504	213	0.01%	0.001%
100	15.162	4390	4392	4394	rBV2	717	343	0.02%	0.002%

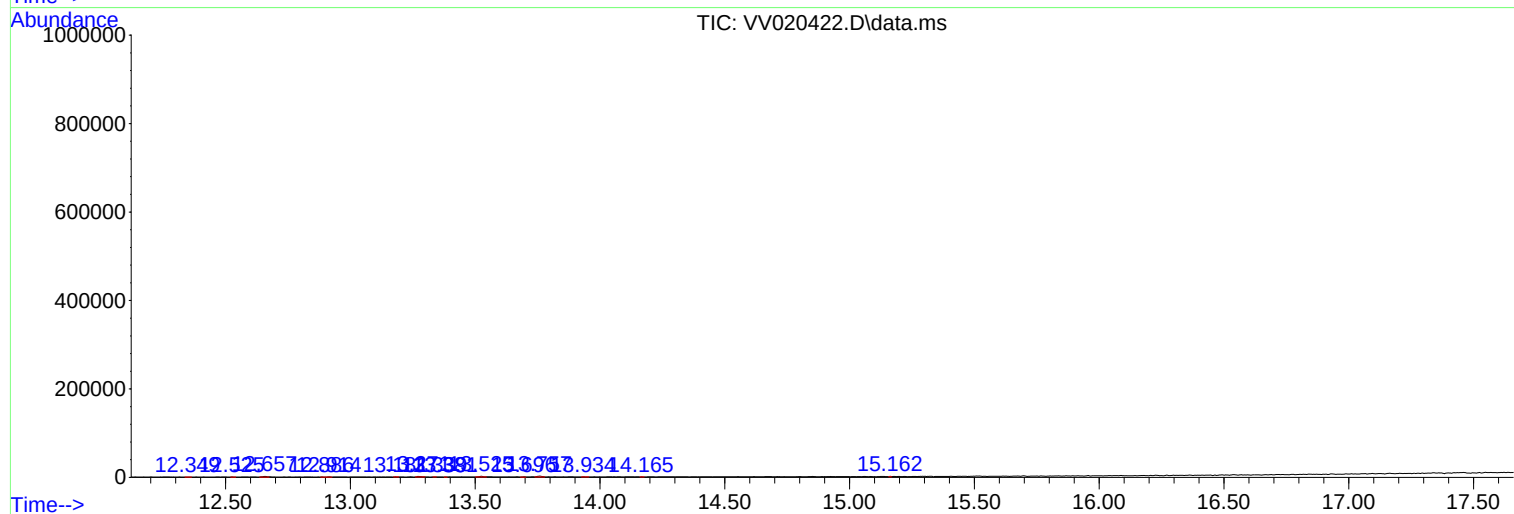
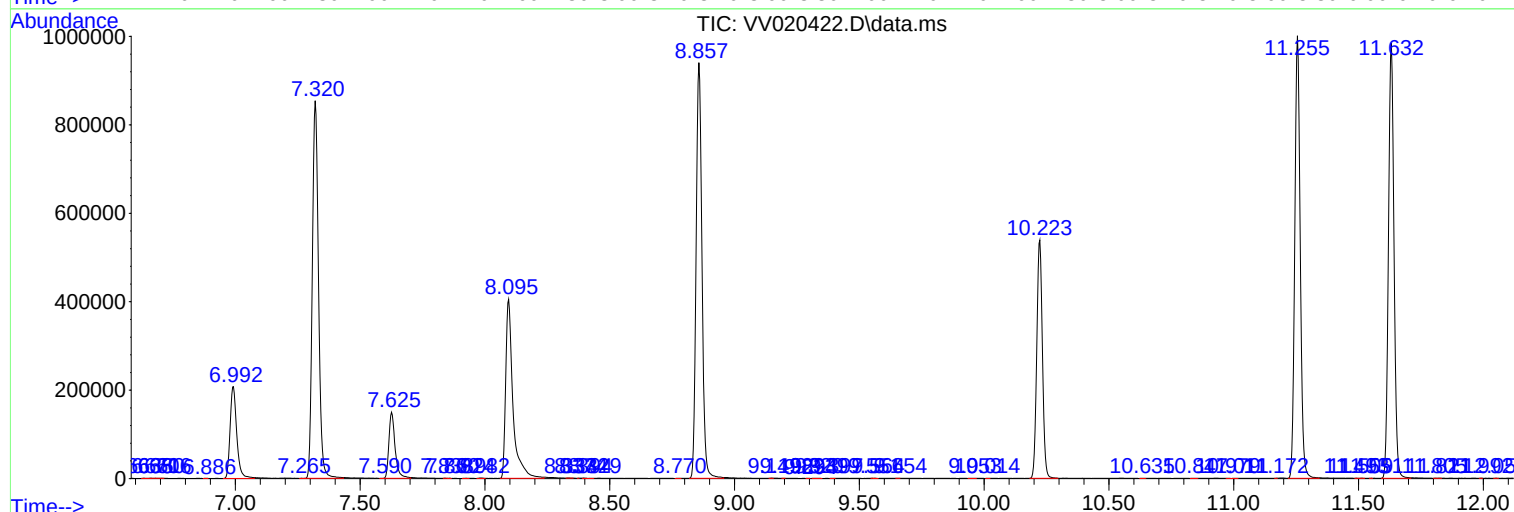
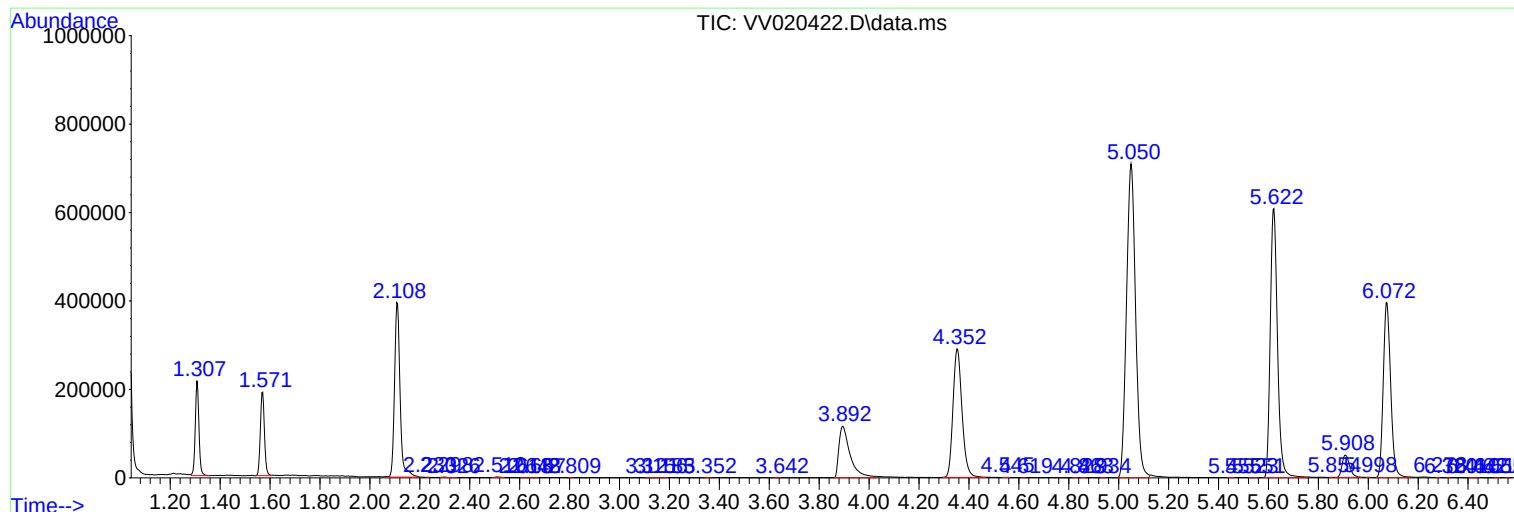
Sum of corrected areas: 14454448

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM022621WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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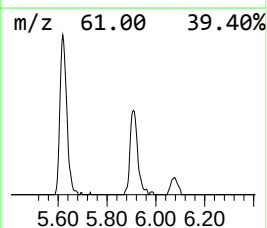
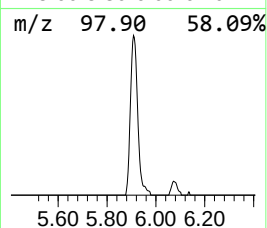
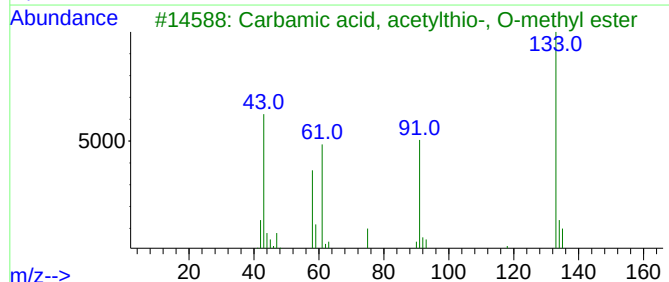
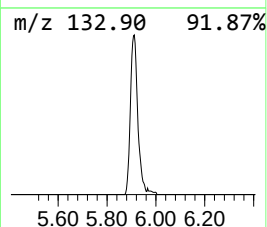
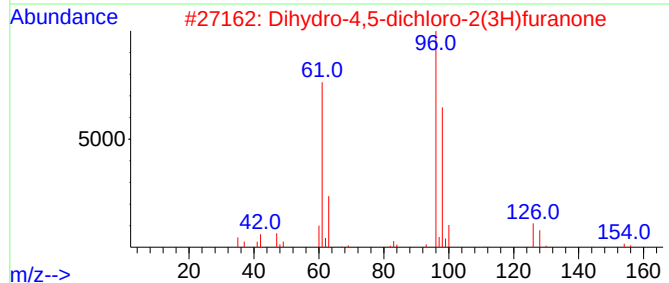
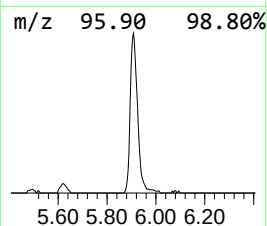
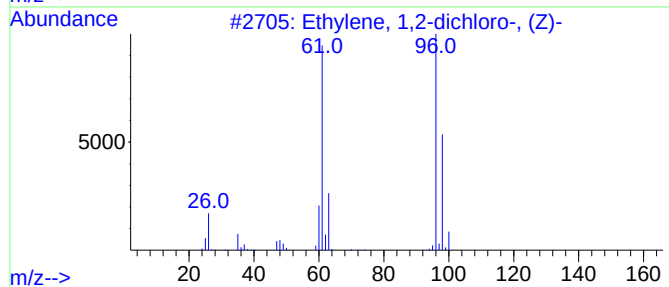
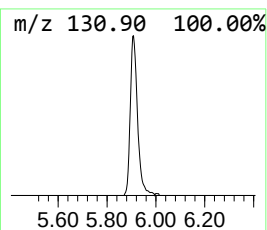
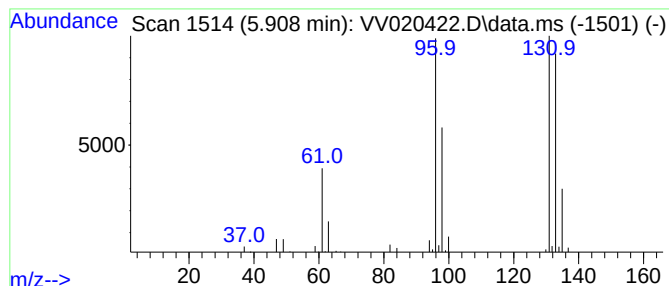
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM022621WMA.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.908	4.27 ug/L	104899	1,4-Difluorobenzene	5.622

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
2			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	25
3			Carbamic acid, acetylthio-, O-me...	133	C4H7NO2S	016696-87-0	9
4			4(1H)-Pyrimidinone	96	C4H4N2O	004562-27-0	9
5			Benzonitrile, 4-methoxy-	133	C8H7NO	000874-90-8	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	5.908	4.3	ug/L	104899	1	5.622	1226940	50.0