

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV083121\
 Data File : VV022039.D
 Acq On : 31 Aug 2021 14:07
 Operator : SY/MD
 Sample : M3579-07 10X
 Misc : 6.61g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 GB6A9

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: VV022039.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	115563	117818	11.22%	1.352%
2	1.552	152	159	174	rVB	104869	122340	11.65%	1.404%
3	2.101	321	330	358	rVB	211993	322066	30.67%	3.695%
4	2.503	448	455	465	rVB6	3120	4833	0.46%	0.055%
5	2.716	519	521	524	rVB2	620	251	0.02%	0.003%
6	2.780	537	541	545	rBV2	242	265	0.03%	0.003%
7	2.880	570	572	575	rBV2	298	199	0.02%	0.002%
8	2.989	602	606	608	rBV2	284	236	0.02%	0.003%
9	3.117	644	646	650	rVB	345	198	0.02%	0.002%
10	3.162	656	660	663	rBV2	240	191	0.02%	0.002%
11	3.384	726	729	731	rBV2	395	221	0.02%	0.003%
12	3.542	771	778	781	rBV	281	252	0.02%	0.003%
13	3.712	828	831	837	rVB	306	281	0.03%	0.003%
14	3.799	854	858	861	rBV2	255	235	0.02%	0.003%
15	3.876	872	882	911	rBV	98895	269780	25.69%	3.095%
16	4.294	1009	1012	1013	rBV	403	234	0.02%	0.003%
17	4.349	1013	1029	1060	rVV	155115	418781	39.88%	4.805%
18	4.564	1093	1096	1097	rBV3	274	182	0.02%	0.002%
19	4.613	1107	1111	1114	rBV	209	179	0.02%	0.002%
20	4.638	1115	1119	1120	rBV	389	249	0.02%	0.003%
21	4.677	1128	1131	1133	rBV2	279	234	0.02%	0.003%
22	4.703	1136	1139	1141	rVB2	424	195	0.02%	0.002%
23	4.741	1147	1151	1154	rBV2	411	279	0.03%	0.003%
24	4.789	1163	1166	1171	rVB2	257	232	0.02%	0.003%
25	4.905	1199	1202	1205	rBV2	272	209	0.02%	0.002%
26	4.953	1213	1217	1219	rBV2	450	321	0.03%	0.004%
27	5.047	1229	1246	1281	rBV2	409614	1050164	100.00%	12.048%
28	5.317	1327	1330	1333	rVB3	511	309	0.03%	0.004%
29	5.397	1351	1355	1358	rBV4	501	410	0.04%	0.005%
30	5.494	1383	1385	1387	rVV2	478	212	0.02%	0.002%
31	5.616	1411	1423	1454	rBV	371977	763729	72.72%	8.762%
32	5.908	1502	1514	1534	rBV2	26750	57043	5.43%	0.654%
33	6.072	1551	1565	1590	rBV	236576	486522	46.33%	5.582%
34	6.320	1639	1642	1644	rBV2	358	205	0.02%	0.002%
35	6.346	1647	1650	1653	rBV	276	200	0.02%	0.002%
36	6.394	1663	1665	1670	rVB	542	217	0.02%	0.002%

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Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

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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

37	6.532	1705	1708	1717	rVB2	505	551	0.05%	0.006%
38	6.574	1717	1721	1728	rBV2	452	473	0.05%	0.005%
39	6.622	1728	1736	1739	rBV4	454	626	0.06%	0.007%
40	6.645	1739	1743	1746	rBV3	719	618	0.06%	0.007%
41	6.686	1754	1756	1762	rVB3	431	379	0.04%	0.004%
42	6.715	1762	1765	1768	rBV3	251	189	0.02%	0.002%
43	6.731	1768	1770	1773	rBV2	396	194	0.02%	0.002%
44	6.786	1784	1787	1790	rVV2	296	214	0.02%	0.002%
45	6.815	1794	1796	1800	rVB2	389	178	0.02%	0.002%
46	6.841	1800	1804	1807	rBV2	296	216	0.02%	0.002%
47	6.873	1812	1814	1817	rVB	401	185	0.02%	0.002%
48	6.915	1823	1827	1831	rVB3	195	215	0.02%	0.002%
49	6.989	1838	1850	1874	rBV	122171	226439	21.56%	2.598%
50	7.317	1938	1952	1971	rBV	490229	845267	80.49%	9.698%
51	7.625	2037	2048	2064	rBV	83246	147965	14.09%	1.698%
52	7.821	2106	2109	2113	rBV	309	281	0.03%	0.003%
53	7.956	2148	2151	2153	rBV2	336	201	0.02%	0.002%
54	7.985	2153	2160	2168	rVB5	2473	3674	0.35%	0.042%
55	8.043	2176	2178	2180	rBV5	488	199	0.02%	0.002%
56	8.092	2182	2193	2226	rBV2	288234	552128	52.58%	6.334%
57	8.619	2351	2357	2358	rBV4	691	651	0.06%	0.007%
58	8.651	2363	2367	2370	rBV2	304	270	0.03%	0.003%
59	8.706	2380	2384	2387	rVB2	242	181	0.02%	0.002%
60	8.741	2393	2395	2398	rBV2	318	198	0.02%	0.002%
61	8.854	2418	2430	2456	rBV	580349	942848	89.78%	10.817%
62	9.069	2495	2497	2502	rVB3	479	255	0.02%	0.003%
63	9.117	2507	2512	2513	rBV2	320	212	0.02%	0.002%
64	9.300	2565	2569	2572	rBV	385	221	0.02%	0.003%
65	9.365	2586	2589	2592	rBV2	400	255	0.02%	0.003%
66	9.445	2609	2614	2617	rVB3	275	214	0.02%	0.002%
67	9.857	2738	2742	2743	rBV2	349	185	0.02%	0.002%
68	9.892	2750	2753	2758	rBV2	303	303	0.03%	0.003%
69	9.956	2770	2773	2780	rBV2	316	289	0.03%	0.003%
70	10.001	2785	2787	2790	rBV2	361	220	0.02%	0.003%
71	10.130	2819	2827	2829	rBV3	1230	1536	0.15%	0.018%
72	10.220	2843	2855	2880	rBV	326486	521093	49.62%	5.978%
73	10.632	2976	2983	2986	rBV3	288	292	0.03%	0.003%
74	10.677	2995	2997	2999	rBV	336	174	0.02%	0.002%
75	10.805	3034	3037	3040	rBV2	243	180	0.02%	0.002%
76	10.886	3059	3062	3063	rBV2	442	216	0.02%	0.002%

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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
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77	10.921	3067	3073	3080	rBV6	1548	2057	0.20%	0.024%
78	11.014	3099	3102	3104	rBV2	262	171	0.02%	0.002%
79	11.027	3104	3106	3108	rBV2	443	204	0.02%	0.002%
80	11.194	3156	3158	3162	rBV3	390	202	0.02%	0.002%
81	11.252	3164	3176	3198	rBV	614566	977170	93.05%	11.211%
82	11.432	3228	3232	3242	rVB5	1420	1803	0.17%	0.021%
83	11.542	3264	3266	3267	rBV	593	225	0.02%	0.003%
84	11.625	3280	3292	3316	rBV	551318	860450	81.93%	9.872%
85	11.911	3377	3381	3384	rBV	216	175	0.02%	0.002%
86	11.976	3398	3401	3405	rBV4	250	175	0.02%	0.002%
87	12.101	3437	3440	3441	rBV	470	232	0.02%	0.003%
88	12.188	3461	3467	3470	rBV3	376	387	0.04%	0.004%
89	12.252	3484	3487	3491	rVB3	426	232	0.02%	0.003%
90	12.390	3528	3530	3532	rBV2	332	186	0.02%	0.002%
91	12.471	3552	3555	3559	rVB2	242	173	0.02%	0.002%
92	12.493	3559	3562	3566	rBV2	524	457	0.04%	0.005%
93	12.660	3611	3614	3617	rVB2	432	256	0.02%	0.003%
94	12.754	3636	3643	3644	rBV	393	415	0.04%	0.005%
95	13.259	3795	3800	3803	rBV	477	419	0.04%	0.005%
96	13.310	3814	3816	3821	rVB3	520	347	0.03%	0.004%
97	13.355	3826	3830	3835	rBV	511	450	0.04%	0.005%
98	13.519	3877	3881	3883	rBV4	487	342	0.03%	0.004%
99	13.885	3993	3995	3998	rBV2	345	241	0.02%	0.003%
100	14.561	4202	4205	4207	rVB2	502	237	0.02%	0.003%

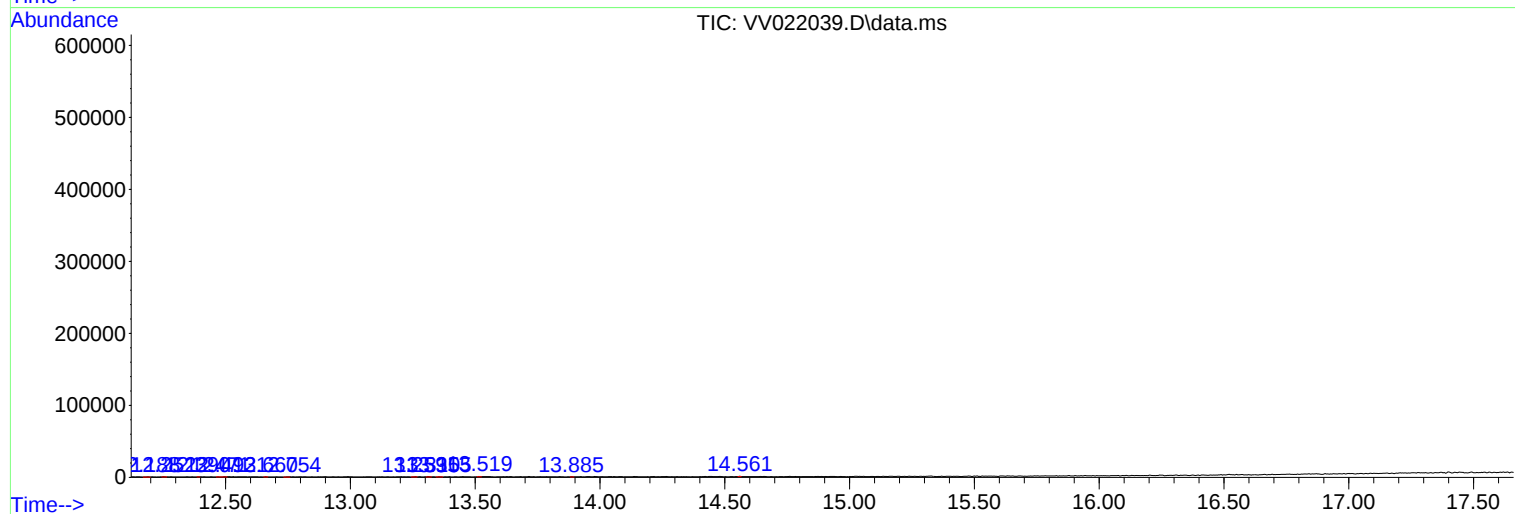
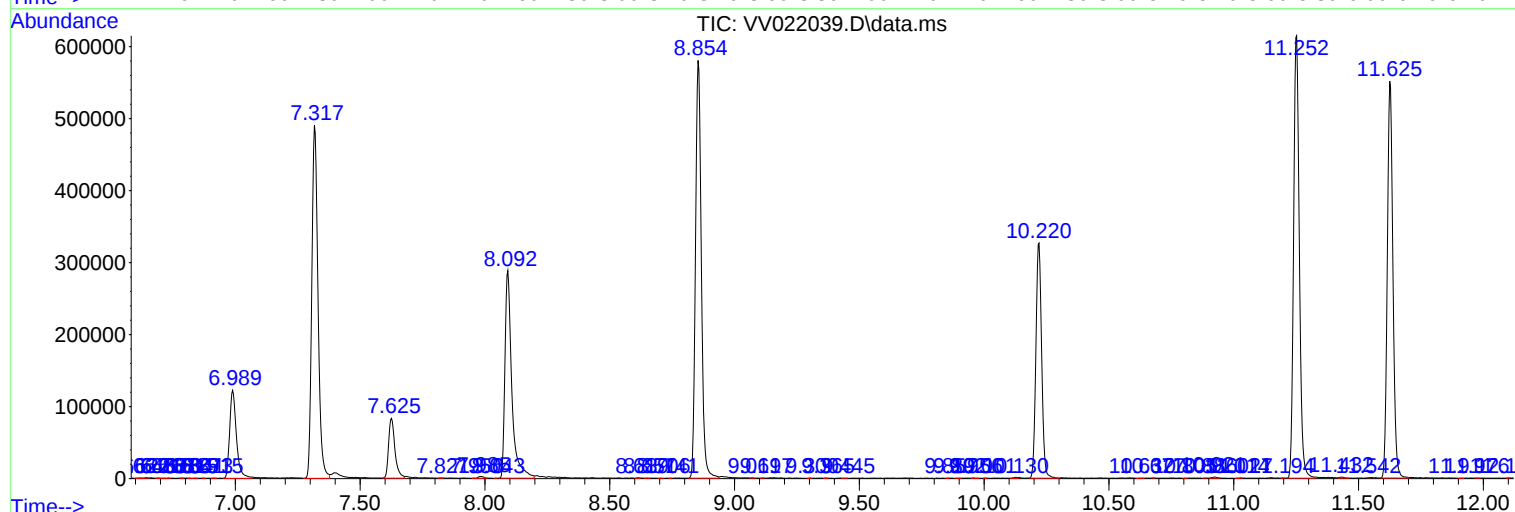
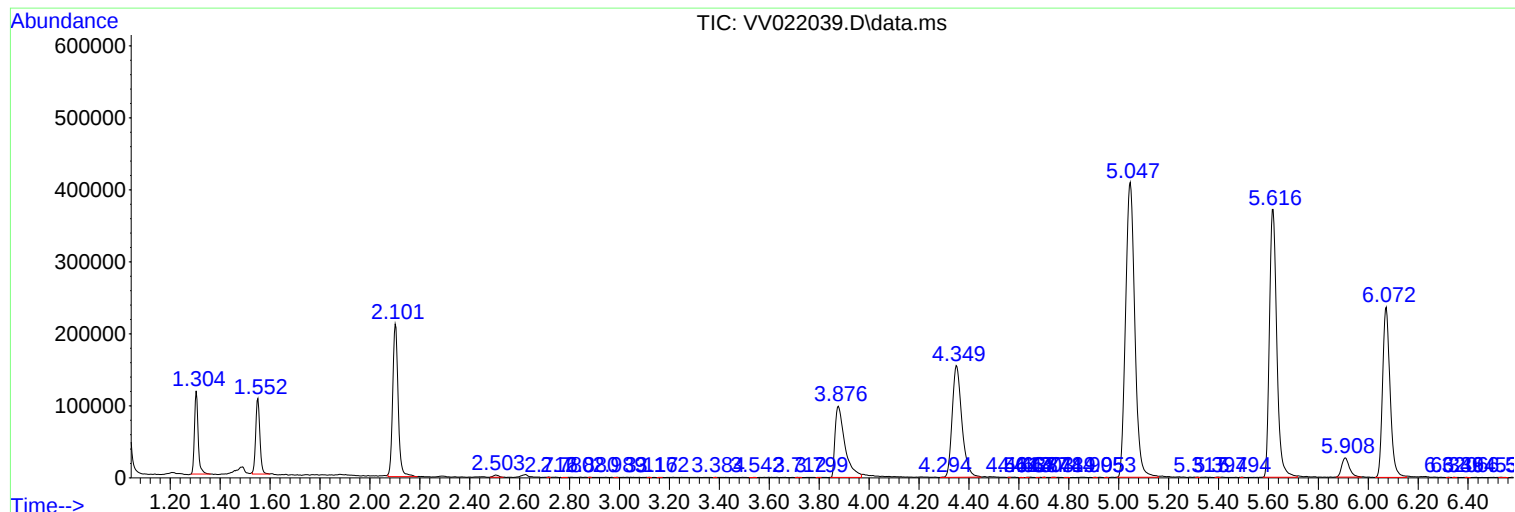
Sum of corrected areas: 8716263

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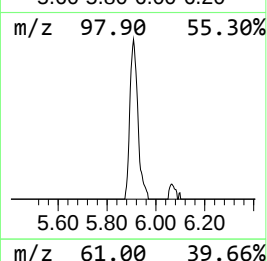
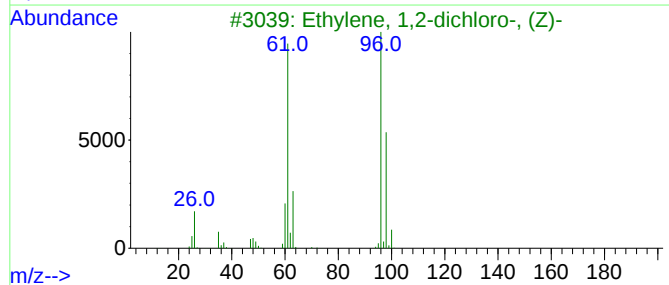
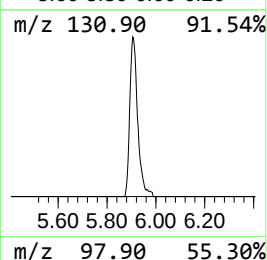
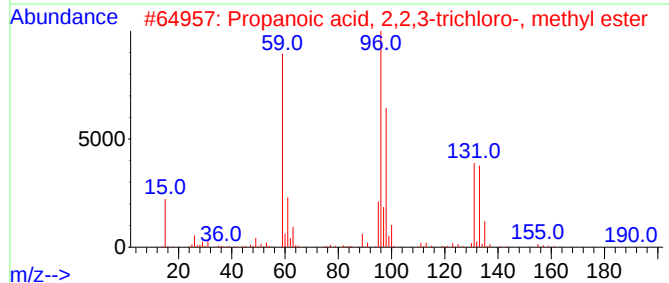
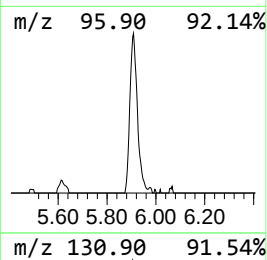
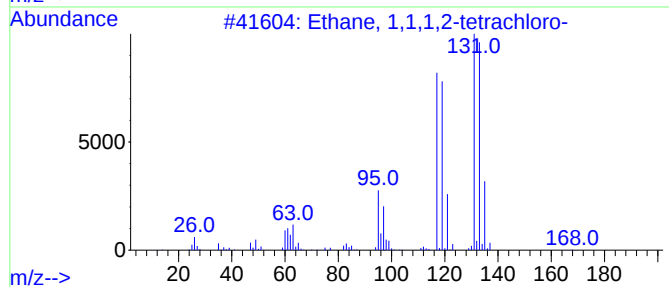
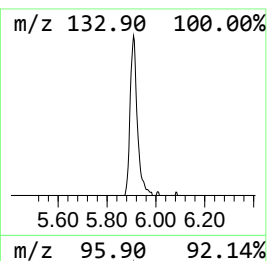
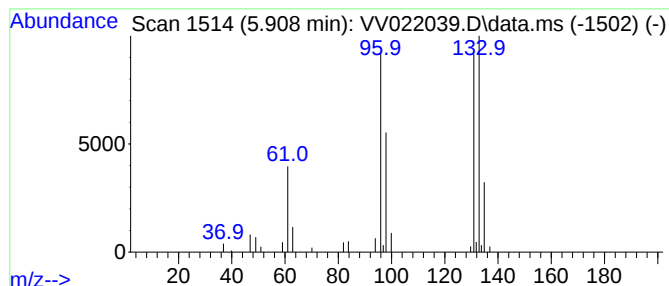
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082721WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.908	3.73 ug/L	57043	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	43
2			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	37
3			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	35
4			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	27
5			2-Chloro-5-methylthiazole	133	C4H4ClNS	033342-65-3	16



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	5.908	3.7	ug/L	57043	1	5.619	763729	50.0