

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082521\
 Data File : VV021942.D
 Acq On : 25 Aug 2021 12:07
 Operator : SY/MD
 Sample : M3518-06ME
 Misc : 4.99g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AY8ME

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: VV021942.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	109	rVB	126418	181214	13.18%	1.645%
2	2.076	312	322	334	rBV	283943	410045	29.81%	3.723%
3	2.674	504	508	511	rBV	350	250	0.02%	0.002%
4	2.725	517	524	526	rBV4	1620	1688	0.12%	0.015%
5	2.780	539	541	543	rBV	380	165	0.01%	0.001%
6	2.828	553	556	558	rBV	259	205	0.01%	0.002%
7	2.860	564	566	568	rVB	328	121	0.01%	0.001%
8	2.892	573	576	578	rBV	265	156	0.01%	0.001%
9	3.011	607	613	615	rBV	912	930	0.07%	0.008%
10	3.076	630	633	635	rVB	456	240	0.02%	0.002%
11	3.230	679	681	685	rVB2	462	194	0.01%	0.002%
12	3.288	696	699	701	rBV2	198	145	0.01%	0.001%
13	3.423	739	741	744	rBV2	408	176	0.01%	0.002%
14	3.458	748	752	755	rBV3	301	296	0.02%	0.003%
15	3.506	764	767	770	rBV	292	203	0.01%	0.002%
16	3.551	778	781	782	rBV	251	136	0.01%	0.001%
17	3.600	794	796	800	rVB	247	122	0.01%	0.001%
18	3.638	805	808	809	rBV	260	128	0.01%	0.001%
19	3.658	812	814	818	rVB3	303	200	0.01%	0.002%
20	3.738	826	839	849	rBV5	2336	5769	0.42%	0.052%
21	3.789	853	855	858	rVB2	170	100	0.01%	0.001%
22	3.822	862	865	867	rVB3	449	237	0.02%	0.002%
23	3.883	874	884	920	rBV	62032	241260	17.54%	2.191%
24	4.339	1009	1026	1059	rBV	191706	536508	39.01%	4.871%
25	4.661	1114	1126	1142	rVB8	4310	10747	0.78%	0.098%
26	4.731	1144	1148	1149	rBV2	828	514	0.04%	0.005%
27	4.892	1190	1198	1199	rBV4	1285	1383	0.10%	0.013%
28	5.034	1224	1242	1276	rBV2	536289	1375326	100.00%	12.488%
29	5.458	1372	1374	1375	rBV	442	146	0.01%	0.001%
30	5.558	1403	1405	1408	rVB	291	94	0.01%	0.001%
31	5.609	1408	1421	1446	rBV	427098	910482	66.20%	8.267%
32	5.899	1500	1511	1531	rBV3	28924	66673	4.85%	0.605%
33	6.066	1550	1563	1596	rVB	279426	643269	46.77%	5.841%
34	6.310	1638	1639	1642	rBV2	403	158	0.01%	0.001%
35	6.362	1648	1655	1660	rVB5	1349	1632	0.12%	0.015%
36	6.426	1671	1675	1676	rBV2	578	297	0.02%	0.003%

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Integration Parameters: LSCINT.P

Integrator: RTE

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

37	6.500	1695	1698	1700	rBV	274	201	0.01%	0.002%
38	6.513	1700	1702	1705	rBV2	249	166	0.01%	0.002%
39	6.583	1720	1724	1727	rVB	260	180	0.01%	0.002%
40	6.632	1727	1739	1742	rBV5	2110	3890	0.28%	0.035%
41	6.834	1798	1802	1805	rVB4	456	367	0.03%	0.003%
42	6.870	1811	1813	1816	rBV	274	161	0.01%	0.001%
43	6.911	1820	1826	1832	rBV5	1487	1876	0.14%	0.017%
44	6.985	1837	1849	1874	rBV2	155704	319611	23.24%	2.902%
45	7.259	1927	1934	1936	rBV4	2771	3050	0.22%	0.028%
46	7.313	1939	1951	1970	rBV	640037	1156758	84.11%	10.503%
47	7.622	2037	2047	2074	rBV	104195	215852	15.69%	1.960%
48	7.786	2093	2098	2113	rVB7	1705	2920	0.21%	0.027%
49	7.847	2113	2117	2119	rBV2	391	281	0.02%	0.003%
50	7.895	2126	2132	2133	rBV	445	366	0.03%	0.003%
51	7.924	2139	2141	2142	rBV	316	147	0.01%	0.001%
52	7.979	2154	2158	2162	rVV3	778	656	0.05%	0.006%
53	8.021	2169	2171	2173	rBV	246	117	0.01%	0.001%
54	8.104	2183	2197	2229	rBV2	260253	624417	45.40%	5.670%
55	8.509	2318	2323	2327	rBV4	722	672	0.05%	0.006%
56	8.535	2327	2331	2332	rBV	345	209	0.02%	0.002%
57	8.667	2369	2372	2374	rBV2	528	323	0.02%	0.003%
58	8.718	2384	2388	2391	rBV	338	243	0.02%	0.002%
59	8.747	2394	2397	2399	rBV	221	113	0.01%	0.001%
60	8.760	2399	2401	2402	rBV	297	99	0.01%	0.001%
61	8.853	2418	2430	2450	rBV	652691	1145043	83.26%	10.397%
62	9.146	2515	2521	2534	rVV4	5902	10311	0.75%	0.094%
63	9.204	2534	2539	2548	rVB8	2429	4120	0.30%	0.037%
64	9.304	2566	2570	2573	rVB3	236	213	0.02%	0.002%
65	9.345	2580	2583	2585	rVB2	221	109	0.01%	0.001%
66	9.368	2586	2590	2592	rVB2	246	135	0.01%	0.001%
67	9.413	2598	2604	2607	rBV2	333	259	0.02%	0.002%
68	9.548	2637	2646	2659	rBV2	7235	12138	0.88%	0.110%
69	9.615	2665	2667	2670	rBV2	292	140	0.01%	0.001%
70	9.673	2680	2685	2688	rBV4	1431	1685	0.12%	0.015%
71	9.799	2718	2724	2733	rBV5	1976	3226	0.23%	0.029%
72	9.940	2760	2768	2774	rBV3	2726	3198	0.23%	0.029%
73	9.979	2774	2780	2781	rVB3	480	422	0.03%	0.004%
74	9.992	2781	2784	2788	rBV2	335	226	0.02%	0.002%
75	10.014	2788	2791	2793	rBV2	573	387	0.03%	0.004%
76	10.223	2843	2856	2873	rBV	387153	639515	46.50%	5.807%

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 ClientSampleId :
 C0AY8ME

Integration Parameters: LSCINT.P

Integrator: RTE

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Peak separation: 5

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

77	10.513	2944	2946	2951	rBV4	626	485	0.04%	0.004%
78	10.548	2951	2957	2960	rBV3	1318	1611	0.12%	0.015%
79	10.718	3007	3010	3011	rBV	342	174	0.01%	0.002%
80	10.747	3011	3019	3026	rVV4	2404	3220	0.23%	0.029%
81	10.879	3053	3060	3065	rBV4	1703	2467	0.18%	0.022%
82	10.992	3092	3095	3098	rBV2	257	163	0.01%	0.001%
83	11.197	3154	3159	3165	rVB6	1644	1741	0.13%	0.016%
84	11.252	3165	3176	3196	rBV	813068	1255531	91.29%	11.400%
85	11.535	3261	3264	3266	rBV3	546	394	0.03%	0.004%
86	11.628	3280	3293	3312	rBV	760008	1188572	86.42%	10.792%
87	11.792	3335	3344	3350	rBV8	3231	5848	0.43%	0.053%
88	11.902	3375	3378	3379	rBV	524	339	0.02%	0.003%
89	11.947	3390	3392	3393	rBV	597	228	0.02%	0.002%
90	11.979	3400	3402	3405	rVB2	447	251	0.02%	0.002%
91	11.998	3405	3408	3409	rBV	257	136	0.01%	0.001%
92	12.008	3409	3411	3413	rBV	590	314	0.02%	0.003%
93	12.300	3499	3502	3503	rBV	360	174	0.01%	0.002%
94	12.371	3521	3524	3525	rBV	499	248	0.02%	0.002%
95	12.557	3578	3582	3585	rBV4	579	468	0.03%	0.004%
96	12.606	3594	3597	3598	rBV	624	347	0.03%	0.003%
97	12.869	3677	3679	3680	rBV	546	252	0.02%	0.002%
98	12.889	3680	3685	3692	rVB3	2838	3546	0.26%	0.032%
99	13.278	3801	3806	3811	rVB4	1587	1584	0.12%	0.014%
100	13.577	3897	3899	3903	rBV	549	313	0.02%	0.003%

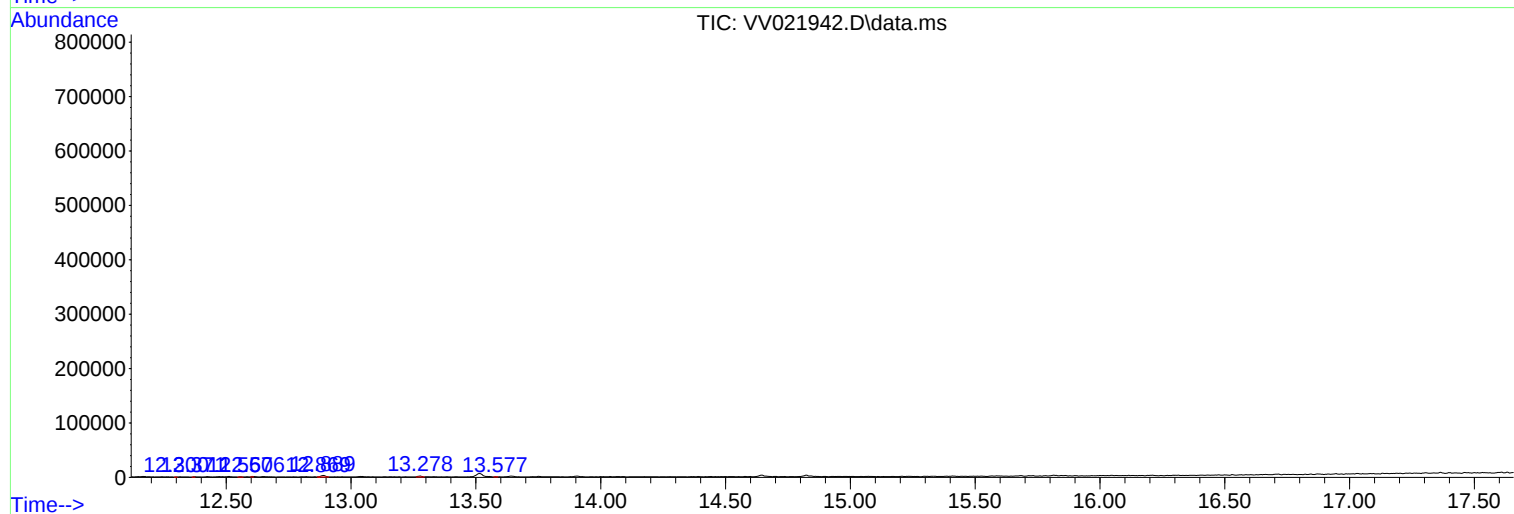
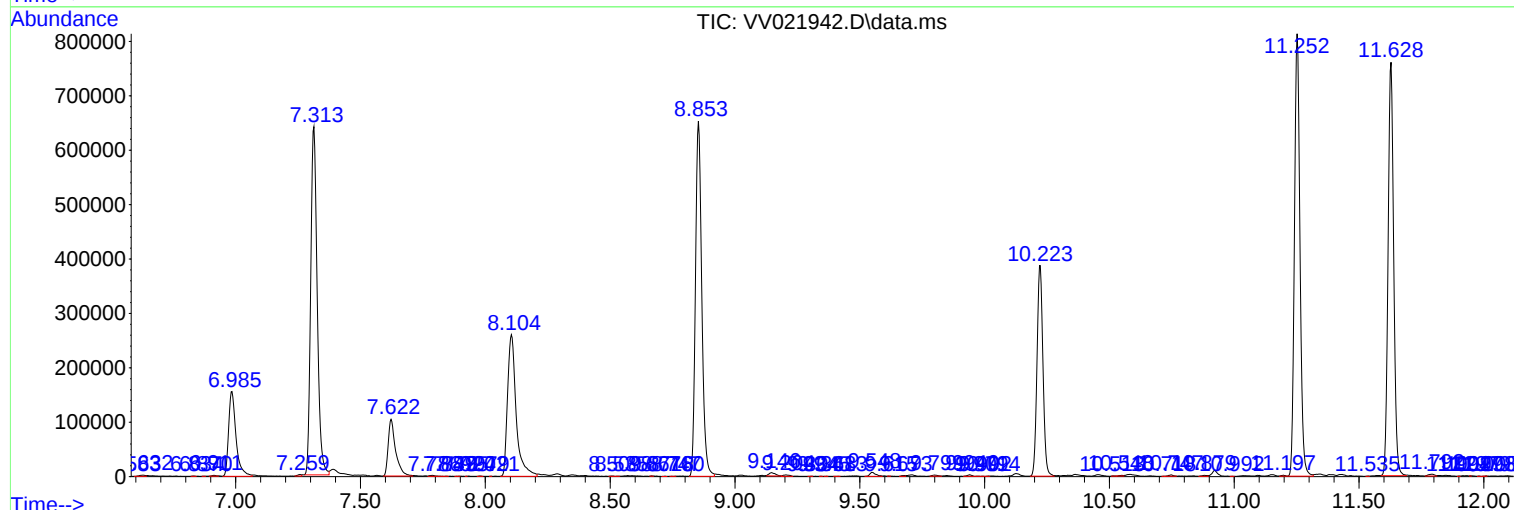
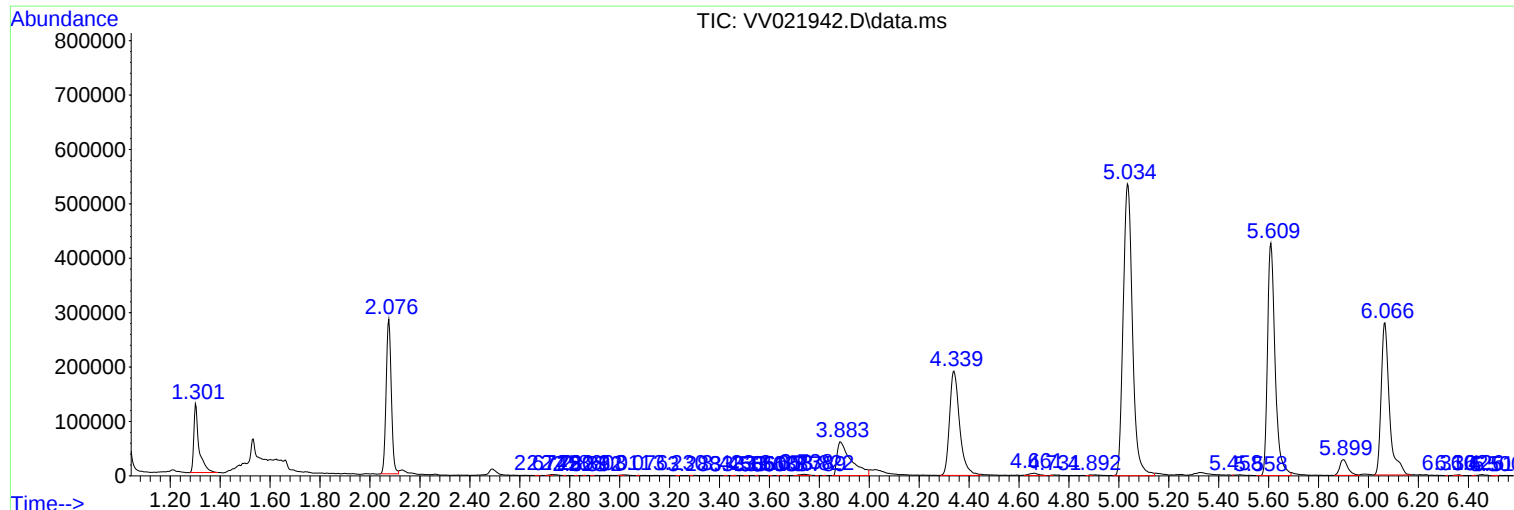
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ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY8ME

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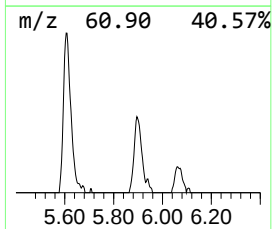
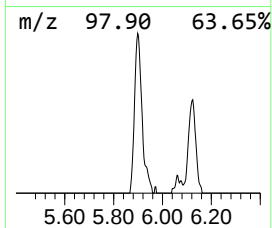
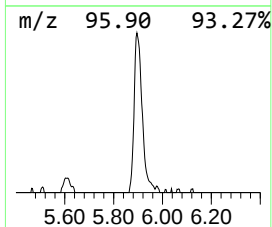
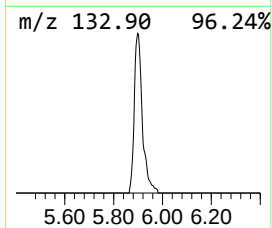
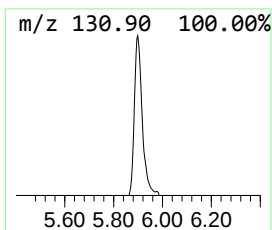
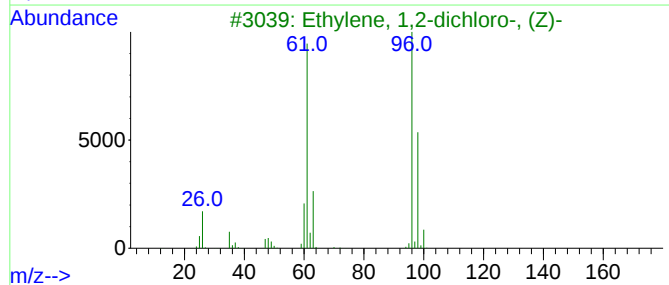
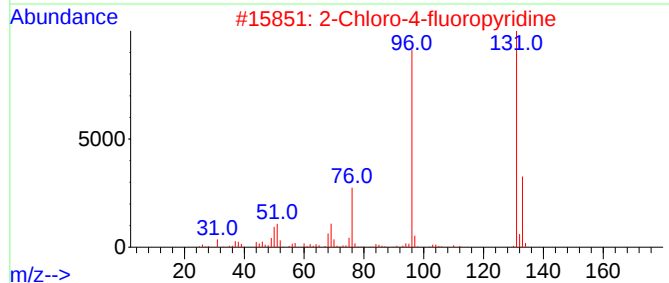
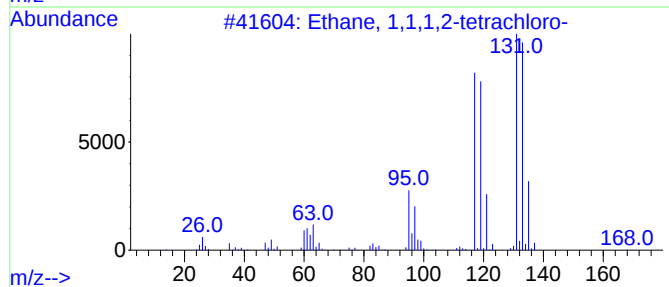
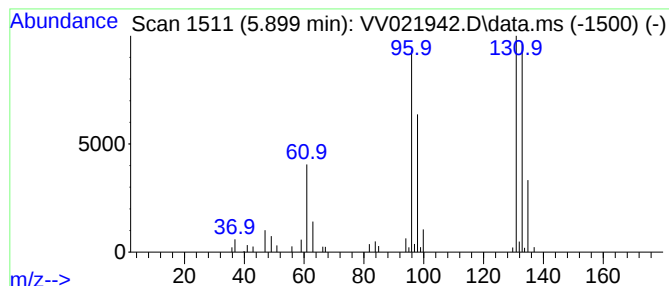
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.899	3.66 ug/L	66673	1,4-Difluorobenzene	5.609

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	43
2			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	38
3			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
4			2-Chloro-5-methylthiazole	133	C4H4ClNS	033342-65-3	27
5			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	5.899	3.7	ug/L	66673	1	5.609	910482	50.0