

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV081721\
 Data File : VV021818.D
 Acq On : 17 Aug 2021 16:34
 Operator : SY/MD
 Sample : M3365-10ME
 Misc : 13.02g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DBKB4ME

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: VV021818.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	111	rVB	134341	190131	13.50%	1.653%
2	2.076	313	322	333	rBV	246660	352410	25.03%	3.063%
3	2.494	441	452	472	rVB	22310	40558	2.88%	0.353%
4	2.741	523	529	531	rBV4	1091	1074	0.08%	0.009%
5	2.815	549	552	553	rBV	358	257	0.02%	0.002%
6	2.918	581	584	586	rBV	520	287	0.02%	0.002%
7	3.201	669	672	676	rBV2	275	189	0.01%	0.002%
8	3.224	676	679	684	rVB	530	381	0.03%	0.003%
9	3.304	702	704	707	rVB	395	202	0.01%	0.002%
10	3.320	707	709	714	rVB2	300	212	0.02%	0.002%
11	3.352	714	719	723	rBV3	466	606	0.04%	0.005%
12	3.413	731	738	741	rVB4	469	432	0.03%	0.004%
13	3.484	754	760	765	rBV2	424	419	0.03%	0.004%
14	3.542	772	778	781	rBV2	254	271	0.02%	0.002%
15	3.622	798	803	807	rBV3	412	338	0.02%	0.003%
16	3.642	807	809	812	rVV	329	248	0.02%	0.002%
17	3.658	812	814	818	rVV2	466	318	0.02%	0.003%
18	3.677	818	820	824	rVB	351	192	0.01%	0.002%
19	3.741	838	840	843	rVB2	498	204	0.01%	0.002%
20	3.773	847	850	854	rBV3	530	503	0.04%	0.004%
21	3.892	877	887	935	rBV2	84147	343140	24.37%	2.983%
22	4.346	1012	1028	1058	rBV	217695	565418	40.15%	4.915%
23	4.568	1095	1097	1099	rBV2	452	270	0.02%	0.002%
24	4.616	1110	1112	1118	rVB5	740	610	0.04%	0.005%
25	4.667	1118	1128	1130	rBV4	980	1259	0.09%	0.011%
26	4.709	1139	1141	1146	rVB3	450	361	0.03%	0.003%
27	4.876	1189	1193	1195	rBV2	428	268	0.02%	0.002%
28	4.892	1195	1198	1200	rVV	374	226	0.02%	0.002%
29	4.902	1200	1201	1205	rVB	588	300	0.02%	0.003%
30	5.040	1226	1244	1277	rBV2	562439	1408115	100.00%	12.241%
31	5.333	1324	1335	1337	rBV6	5319	7662	0.54%	0.067%
32	5.529	1393	1396	1403	rVB4	634	582	0.04%	0.005%
33	5.613	1410	1422	1465	rVV	469544	989039	70.24%	8.598%
34	5.902	1501	1512	1533	rBV2	29765	66846	4.75%	0.581%
35	6.069	1552	1564	1598	rVB	305571	646777	45.93%	5.622%
36	6.297	1631	1635	1640	rVB4	509	477	0.03%	0.004%

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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\SFAMVLM081621WMA.M
 Title : VOC Analysis

37	6.320	1640	1642	1644	rVV	639	339	0.02%	0.003%
38	6.346	1648	1650	1655	rVB2	529	321	0.02%	0.003%
39	6.391	1662	1664	1668	rBV3	325	210	0.01%	0.002%
40	6.535	1704	1709	1712	rBV3	498	408	0.03%	0.004%
41	6.648	1734	1744	1745	rBV5	1906	2441	0.17%	0.021%
42	6.786	1784	1787	1788	rBV2	391	203	0.01%	0.002%
43	6.825	1795	1799	1801	rBV3	431	331	0.02%	0.003%
44	6.850	1803	1807	1812	rVB3	574	635	0.05%	0.006%
45	6.908	1822	1825	1827	rBV2	659	334	0.02%	0.003%
46	6.944	1833	1836	1838	rBV	307	194	0.01%	0.002%
47	6.989	1838	1850	1871	rBV	170944	332839	23.64%	2.893%
48	7.265	1934	1936	1940	rBV3	561	268	0.02%	0.002%
49	7.317	1940	1952	1971	rBV	614050	1101312	78.21%	9.574%
50	7.625	2037	2048	2074	rBV	116980	223315	15.86%	1.941%
51	7.841	2111	2115	2121	rVB6	619	607	0.04%	0.005%
52	7.908	2132	2136	2137	rBV2	297	210	0.01%	0.002%
53	7.937	2143	2145	2146	rBV2	382	200	0.01%	0.002%
54	7.979	2153	2158	2167	rVB6	1455	1813	0.13%	0.016%
55	8.104	2185	2197	2237	rBV2	311949	712379	50.59%	6.193%
56	8.461	2305	2308	2311	rBV2	416	350	0.02%	0.003%
57	8.532	2327	2330	2331	rBV	392	215	0.02%	0.002%
58	8.580	2342	2345	2348	rBV3	381	246	0.02%	0.002%
59	8.677	2373	2375	2379	rVV2	338	186	0.01%	0.002%
60	8.709	2382	2385	2391	rVB3	319	311	0.02%	0.003%
61	8.738	2391	2394	2400	rVB4	457	393	0.03%	0.003%
62	8.854	2419	2430	2457	rBV	701830	1215010	86.29%	10.562%
63	9.259	2552	2556	2558	rBV2	464	310	0.02%	0.003%
64	9.278	2560	2562	2567	rVB	421	300	0.02%	0.003%
65	9.458	2614	2618	2623	rVV2	449	370	0.03%	0.003%
66	9.522	2634	2638	2639	rBV2	350	191	0.01%	0.002%
67	9.548	2639	2646	2648	rBV3	461	511	0.04%	0.004%
68	9.596	2658	2661	2662	rBV2	716	363	0.03%	0.003%
69	9.690	2685	2690	2694	rBV3	353	332	0.02%	0.003%
70	9.863	2740	2744	2745	rBV2	305	206	0.01%	0.002%
71	9.905	2751	2757	2766	rVB6	2677	3446	0.24%	0.030%
72	9.950	2767	2771	2773	rBV3	334	248	0.02%	0.002%
73	10.111	2818	2821	2824	rBV2	730	624	0.04%	0.005%
74	10.169	2837	2839	2843	rBV	574	411	0.03%	0.004%
75	10.223	2843	2856	2879	rVV	478554	780036	55.40%	6.781%
76	10.384	2902	2906	2910	rBV4	593	495	0.04%	0.004%

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Instrument :
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 ClientSampleId :
 DBKB4ME

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

77	10.403	2910	2912	2919	rVB3	365	300	0.02%	0.003%
78	10.487	2935	2938	2944	rVB2	383	292	0.02%	0.003%
79	10.519	2944	2948	2952	rBV	473	378	0.03%	0.003%
80	10.542	2952	2955	2960	rBV3	672	697	0.05%	0.006%
81	10.712	3004	3008	3011	rBV2	325	289	0.02%	0.003%
82	10.809	3036	3038	3042	rBV2	307	268	0.02%	0.002%
83	10.892	3060	3064	3067	rBV2	581	576	0.04%	0.005%
84	10.921	3068	3073	3083	rVB7	2042	3105	0.22%	0.027%
85	11.046	3110	3112	3116	rVB4	512	351	0.02%	0.003%
86	11.075	3116	3121	3122	rBV4	529	270	0.02%	0.002%
87	11.143	3138	3142	3144	rBV3	612	522	0.04%	0.005%
88	11.194	3150	3158	3165	rBV6	2122	2712	0.19%	0.024%
89	11.252	3165	3176	3196	rBV	829020	1278915	90.82%	11.118%
90	11.628	3281	3293	3316	rBV	757758	1200460	85.25%	10.436%
91	12.059	3424	3427	3428	rBV	388	250	0.02%	0.002%
92	12.397	3525	3532	3534	rBV2	549	657	0.05%	0.006%
93	12.532	3572	3574	3576	rVB2	557	234	0.02%	0.002%
94	12.870	3677	3679	3683	rBV2	377	273	0.02%	0.002%
95	13.336	3819	3824	3825	rBV	381	270	0.02%	0.002%
96	13.345	3825	3827	3831	rVV	363	242	0.02%	0.002%
97	13.477	3866	3868	3870	rBV	419	195	0.01%	0.002%
98	13.516	3873	3880	3887	rVV3	4575	6252	0.44%	0.054%
99	14.628	4223	4226	4228	rBV	585	445	0.03%	0.004%
100	15.185	4390	4399	4402	rBV6	1436	2068	0.15%	0.018%

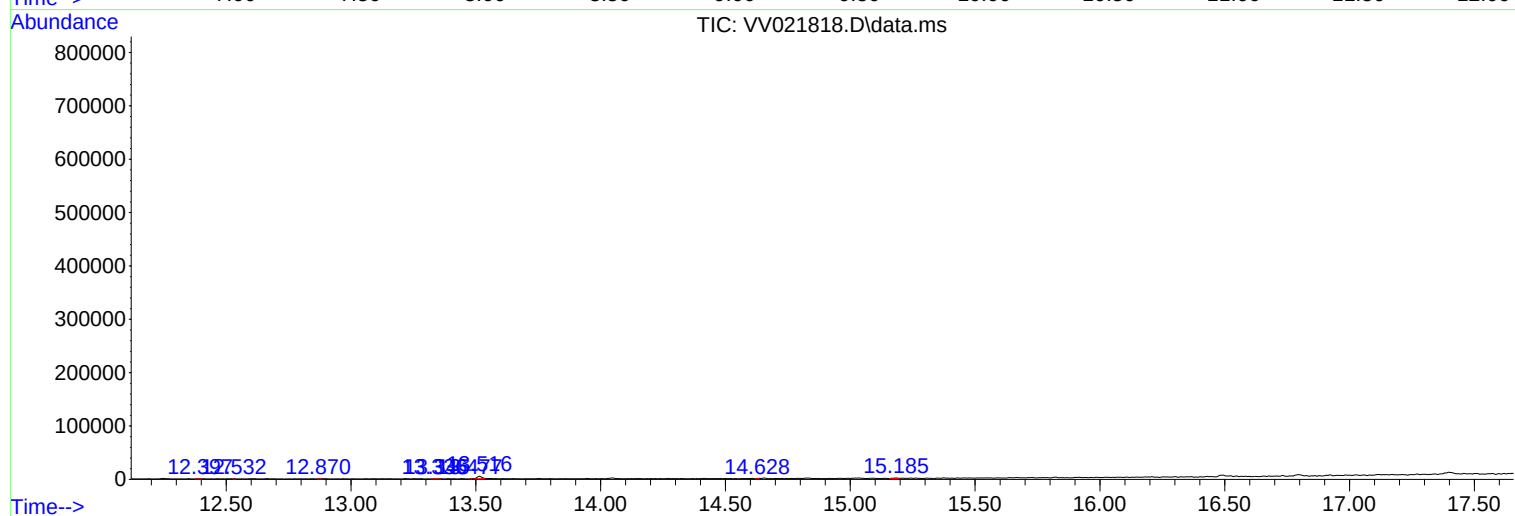
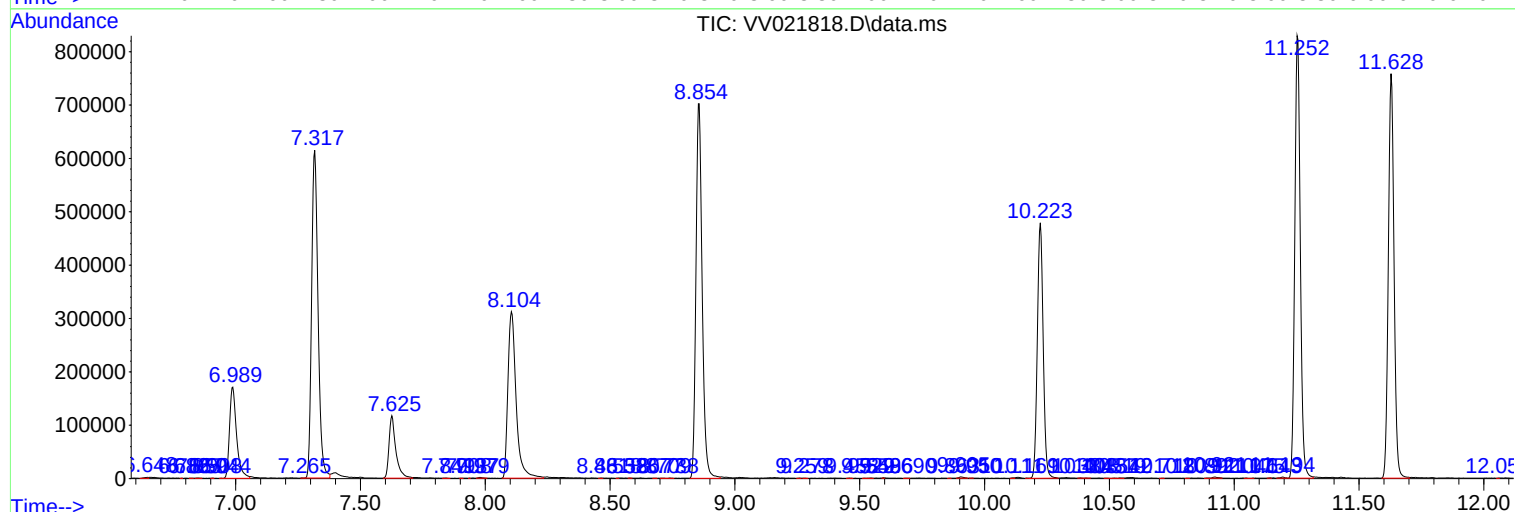
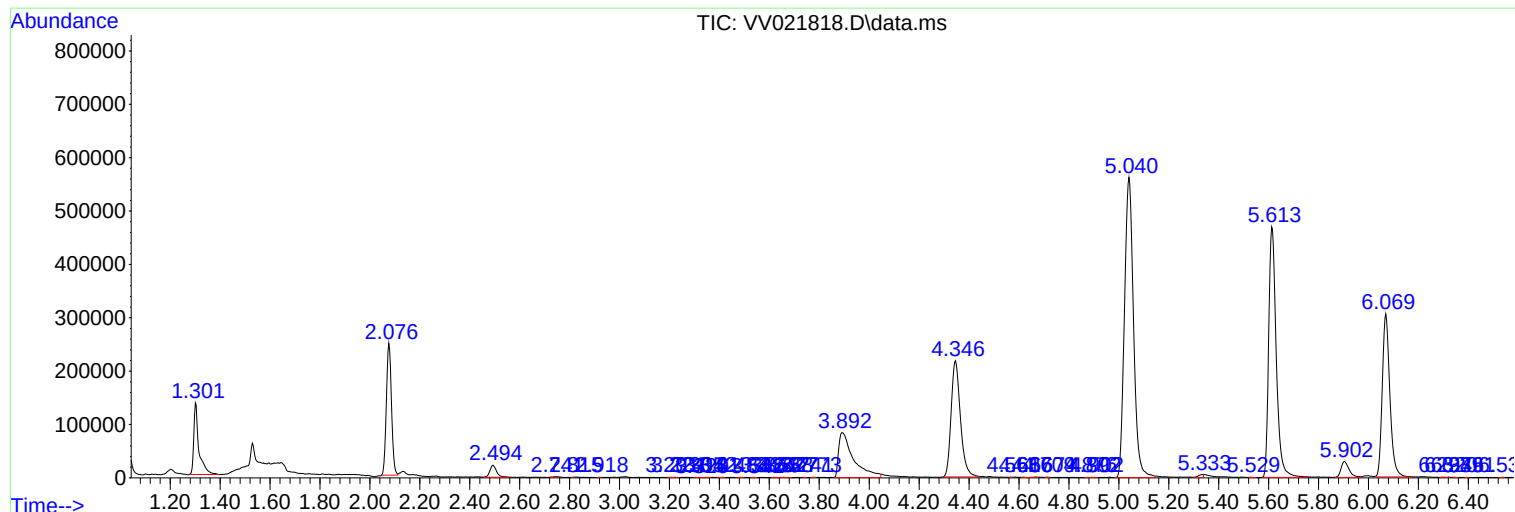
Sum of corrected areas: 11503516

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV081721\
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Instrument :
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ClientSampleId :
DBKB4ME

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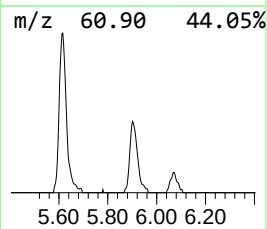
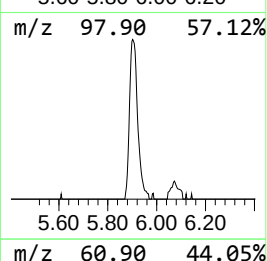
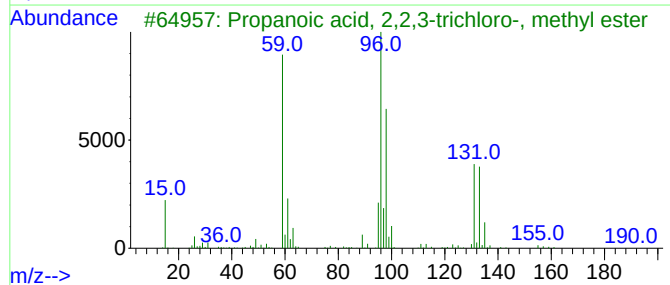
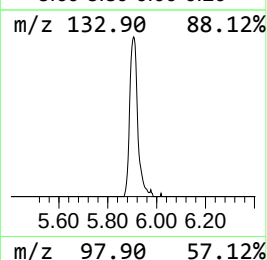
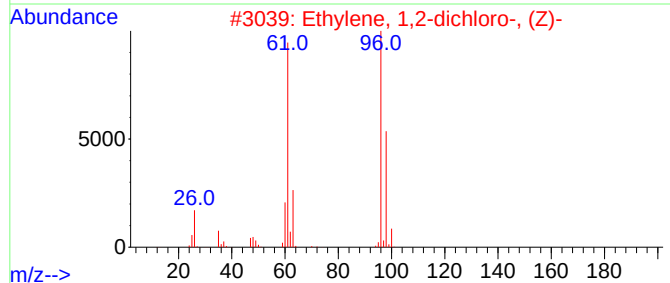
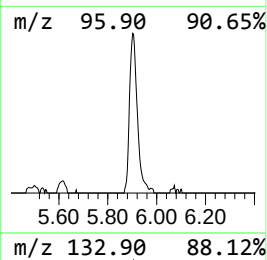
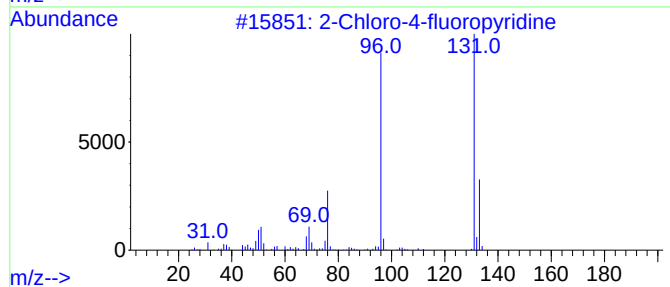
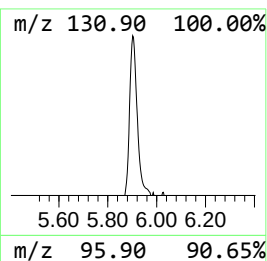
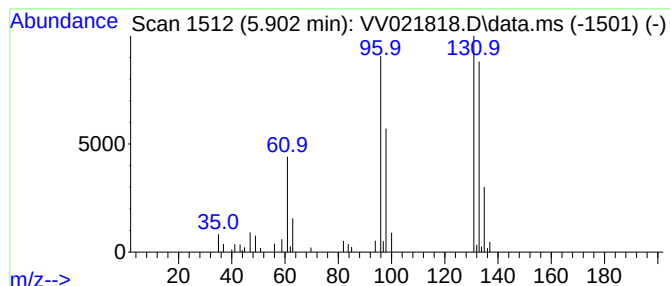
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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.
5.902	3.38 ug/L	66846	1,4-Difluorobenzene	5.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	38
2			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	35
3			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	32
4			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	32
5			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	5.902	3.4	ug/L	66846	1	5.613	989039	50.0