

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV080621\
 Data File : VV021746.D
 Acq On : 06 Aug 2021 10:36
 Operator : SY/MD
 Sample : VV0806MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VBLK226

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\SFAMVLM080221WMA.M
 Title : VOC Analysis

Signal : TIC: VV021746.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	96	rVB	178769	172833	11.55%	1.517%
2	1.564	156	163	176	rBV	154680	169090	11.30%	1.484%
3	2.105	321	331	356	rBV	284704	419683	28.04%	3.684%
4	2.507	446	456	470	rVB	5062	9236	0.62%	0.081%
5	2.645	496	499	504	rVB	313	280	0.02%	0.002%
6	2.674	504	508	513	rBV2	267	312	0.02%	0.003%
7	2.754	530	533	536	rBV3	687	558	0.04%	0.005%
8	2.812	548	551	553	rBV	254	176	0.01%	0.002%
9	2.941	589	591	594	rVB2	415	163	0.01%	0.001%
10	2.960	596	597	600	rVB2	294	116	0.01%	0.001%
11	2.979	601	603	606	rBV	287	185	0.01%	0.002%
12	3.034	618	620	625	rVB3	541	328	0.02%	0.003%
13	3.076	631	633	635	rBV3	289	196	0.01%	0.002%
14	3.185	664	667	670	rBV2	345	260	0.02%	0.002%
15	3.288	695	699	701	rBV2	408	237	0.02%	0.002%
16	3.323	705	710	714	rBV2	228	215	0.01%	0.002%
17	3.516	768	770	775	rBV2	209	167	0.01%	0.001%
18	3.609	794	799	801	rBV2	228	226	0.02%	0.002%
19	3.722	829	834	838	rBV	280	221	0.01%	0.002%
20	3.825	864	866	869	rBV	249	121	0.01%	0.001%
21	3.880	872	883	922	rBV	122131	360148	24.06%	3.162%
22	4.346	1011	1028	1052	rBV	235521	586629	39.20%	5.150%
23	4.667	1126	1128	1129	rBV	306	105	0.01%	0.001%
24	4.767	1156	1159	1160	rBV	365	203	0.01%	0.002%
25	4.841	1179	1182	1183	rBV	213	115	0.01%	0.001%
26	4.918	1204	1206	1209	rVB	235	128	0.01%	0.001%
27	4.934	1209	1211	1215	rBV3	300	185	0.01%	0.002%
28	4.970	1220	1222	1224	rBV2	204	109	0.01%	0.001%
29	5.043	1228	1245	1277	rBV2	579792	1496690	100.00%	13.139%
30	5.391	1351	1353	1354	rBV	345	126	0.01%	0.001%
31	5.455	1369	1373	1377	rBV2	415	338	0.02%	0.003%
32	5.519	1390	1393	1396	rVB2	280	188	0.01%	0.002%
33	5.539	1396	1399	1400	rBV2	318	207	0.01%	0.002%
34	5.616	1410	1423	1456	rBV	438797	897360	59.96%	7.878%
35	5.905	1501	1513	1532	rBV2	48399	101689	6.79%	0.893%
36	6.069	1550	1564	1598	rBV	333396	678098	45.31%	5.953%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM080221WMA.M
 Title : VOC Analysis

37	6.317	1638	1641	1646	rBV3	411	299	0.02%	0.003%
38	6.355	1650	1653	1655	rVV3	510	314	0.02%	0.003%
39	6.375	1658	1659	1661	rBV2	302	116	0.01%	0.001%
40	6.461	1681	1686	1690	rBV3	189	174	0.01%	0.002%
41	6.494	1695	1696	1700	rBV	262	194	0.01%	0.002%
42	6.526	1703	1706	1709	rBV2	297	255	0.02%	0.002%
43	6.593	1724	1727	1732	rVB3	377	293	0.02%	0.003%
44	6.632	1735	1739	1741	rBV2	902	748	0.05%	0.007%
45	6.818	1788	1797	1799	rBV3	386	367	0.02%	0.003%
46	6.831	1799	1801	1806	rBV	323	148	0.01%	0.001%
47	6.986	1837	1849	1876	rBV	195232	355189	23.73%	3.118%
48	7.317	1940	1952	1971	rBV	703063	1233013	82.38%	10.824%
49	7.622	2037	2047	2072	rBV	130083	231339	15.46%	2.031%
50	7.998	2163	2164	2167	rVB2	310	113	0.01%	0.001%
51	8.027	2170	2173	2176	rBV2	215	152	0.01%	0.001%
52	8.088	2181	2192	2223	rBV2	383593	769215	51.39%	6.753%
53	8.522	2324	2327	2331	rBV2	390	310	0.02%	0.003%
54	8.690	2376	2379	2381	rBV	458	317	0.02%	0.003%
55	8.725	2388	2390	2393	rBV	213	118	0.01%	0.001%
56	8.767	2401	2403	2406	rVB2	303	132	0.01%	0.001%
57	8.799	2411	2413	2415	rBV	316	158	0.01%	0.001%
58	8.854	2418	2430	2459	rBV	643589	1070749	71.54%	9.400%
59	9.146	2513	2521	2527	rBV3	1506	2343	0.16%	0.021%
60	9.217	2542	2543	2548	rVB2	275	134	0.01%	0.001%
61	9.262	2552	2557	2562	rBV4	378	394	0.03%	0.003%
62	9.374	2591	2592	2595	rVB2	261	108	0.01%	0.001%
63	9.403	2596	2601	2604	rBV2	295	271	0.02%	0.002%
64	9.458	2614	2618	2620	rBV	256	146	0.01%	0.001%
65	9.474	2621	2623	2629	rVV3	328	340	0.02%	0.003%
66	9.497	2629	2630	2633	rVV2	296	122	0.01%	0.001%
67	9.725	2699	2701	2706	rVB	232	137	0.01%	0.001%
68	9.889	2749	2752	2756	rVB	239	168	0.01%	0.001%
69	9.905	2756	2757	2761	rBV	215	183	0.01%	0.002%
70	9.931	2761	2765	2767	rBV2	560	460	0.03%	0.004%
71	9.969	2775	2777	2782	rVB2	212	115	0.01%	0.001%
72	10.046	2798	2801	2804	rBV2	315	212	0.01%	0.002%
73	10.085	2811	2813	2818	rVB	253	140	0.01%	0.001%
74	10.130	2819	2827	2834	rBV5	2803	4092	0.27%	0.036%
75	10.217	2842	2854	2877	rBV	405418	642225	42.91%	5.638%
76	10.474	2932	2934	2935	rBV	311	118	0.01%	0.001%

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 Title : VOC Analysis

77	10.538	2949	2954	2956	rBV3	820	788	0.05%	0.007%
78	10.667	2991	2994	2995	rBV	285	127	0.01%	0.001%
79	10.844	3045	3049	3051	rBV4	570	422	0.03%	0.004%
80	10.924	3065	3074	3082	rBV5	3281	5394	0.36%	0.047%
81	10.992	3094	3095	3100	rVB2	261	122	0.01%	0.001%
82	11.098	3126	3128	3133	rBV2	158	108	0.01%	0.001%
83	11.146	3139	3143	3152	rBV3	1086	1500	0.10%	0.013%
84	11.191	3152	3157	3164	rBV4	1417	2038	0.14%	0.018%
85	11.249	3164	3175	3196	rBV	660787	1031931	68.95%	9.059%
86	11.477	3245	3246	3248	rBV	304	150	0.01%	0.001%
87	11.625	3280	3292	3319	rBV	717844	1109111	74.10%	9.736%
88	11.828	3352	3355	3359	rBV	481	484	0.03%	0.004%
89	12.001	3406	3409	3412	rBV2	380	302	0.02%	0.003%
90	12.062	3425	3428	3433	rBV3	317	355	0.02%	0.003%
91	12.133	3449	3450	3452	rBV	300	109	0.01%	0.001%
92	12.284	3494	3497	3498	rBV	380	176	0.01%	0.002%
93	12.474	3554	3556	3558	rBV	287	142	0.01%	0.001%
94	12.484	3558	3559	3563	rVB	574	214	0.01%	0.002%
95	12.554	3579	3581	3584	rVB	292	108	0.01%	0.001%
96	12.654	3605	3612	3624	rBV6	2807	4285	0.29%	0.038%
97	12.773	3647	3649	3651	rBV	393	218	0.01%	0.002%
98	13.271	3797	3804	3811	rBV4	3255	4392	0.29%	0.039%
99	13.516	3872	3880	3890	rVB2	6154	10131	0.68%	0.089%
100	13.754	3946	3954	3963	rVB5	4180	6325	0.42%	0.056%

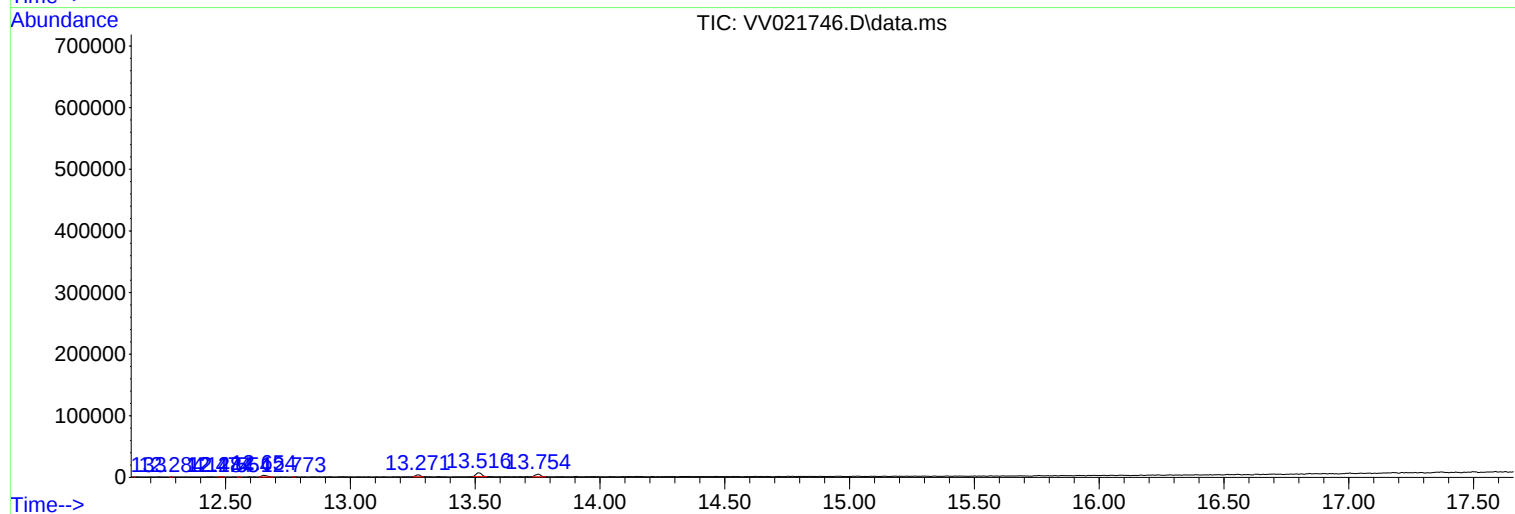
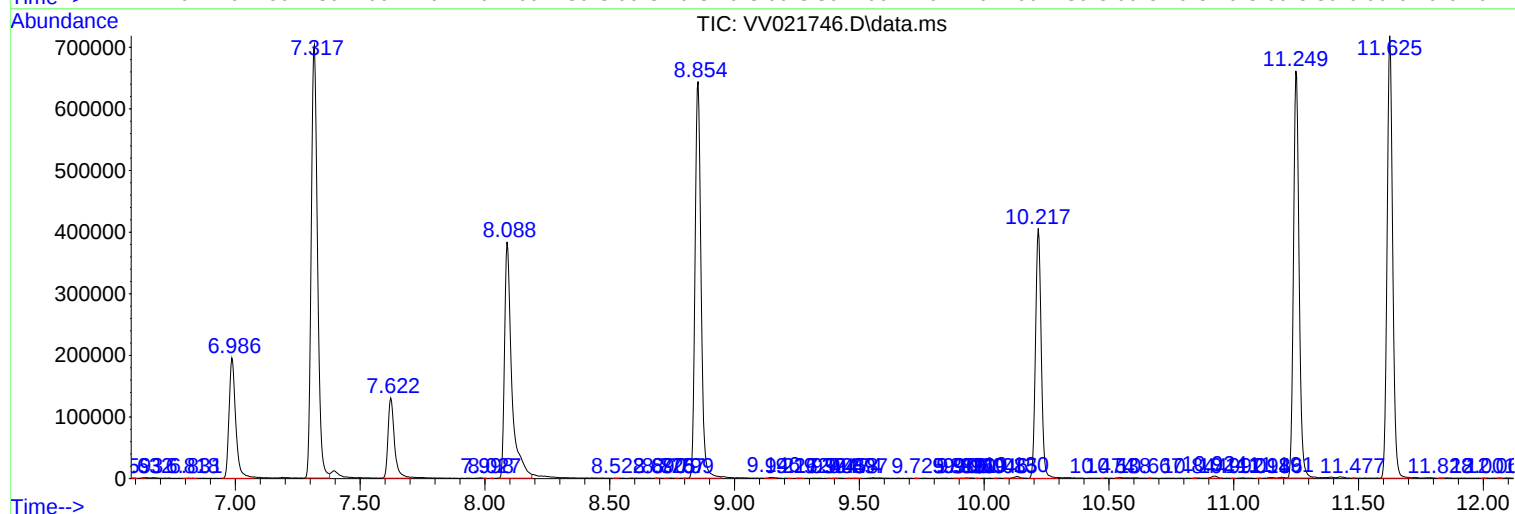
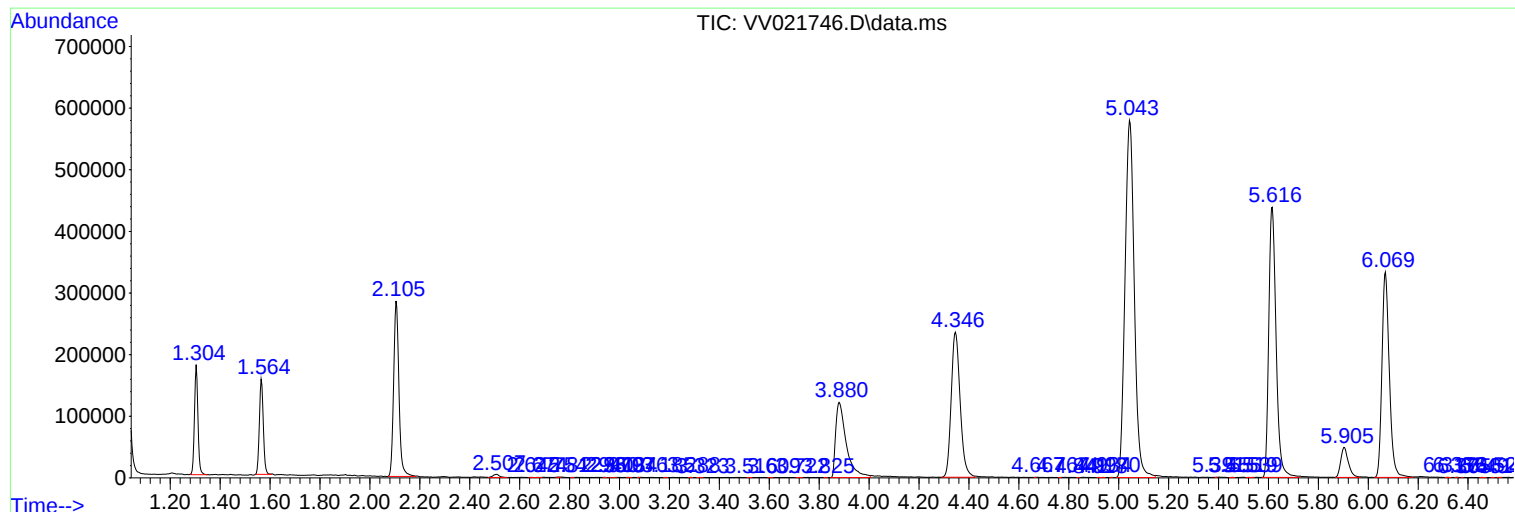
Sum of corrected areas: 11391274

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ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VBLK226

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM080221WMA.M
Quant Title : VOC Analysis

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



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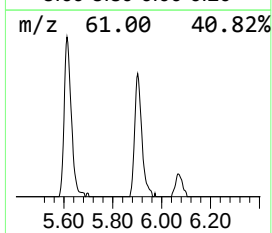
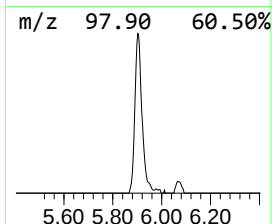
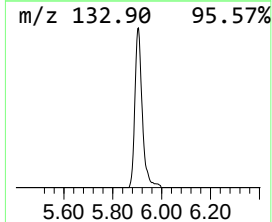
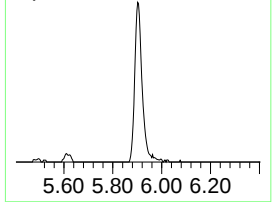
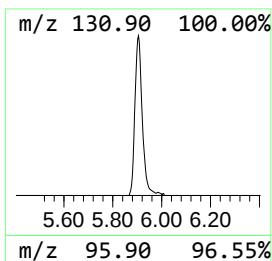
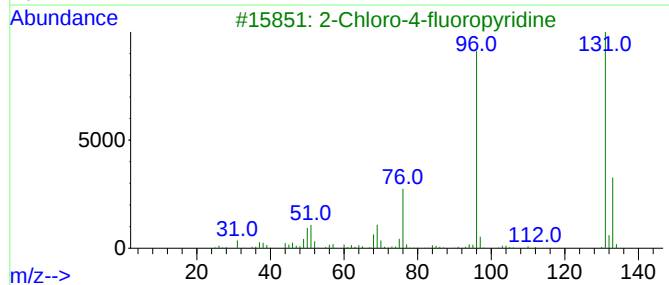
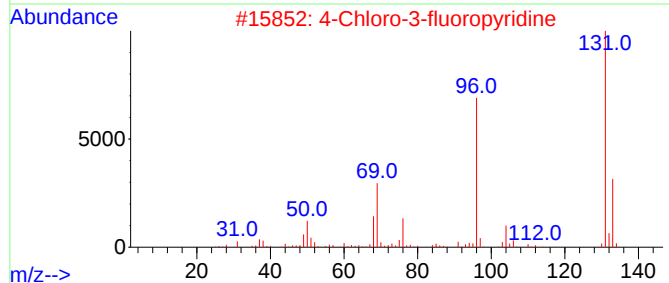
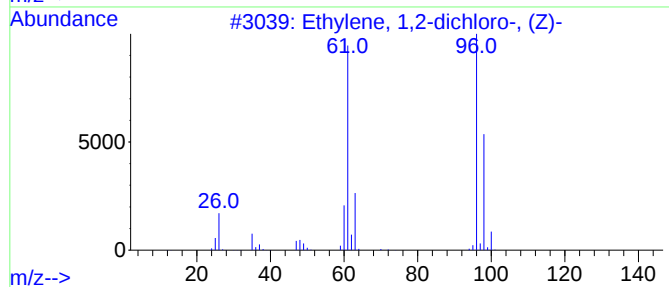
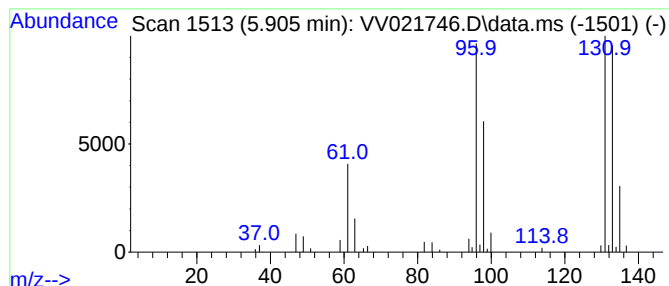
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM080221WMA.M
Quant Title : VOC Analysis

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	5.67 ug/L	101689	1,4-Difluorobenzene	5.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
2			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	32
3			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	23
4			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	23
5			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	12



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	5.905	5.7	ug/L	101689	1	5.616	897360	50.0