

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082521\
 Data File : VV021946.D
 Acq On : 25 Aug 2021 13:46
 Operator : SY/MD
 Sample : M3518-12ME
 Misc : 7.54g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0B25ME

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: VV021946.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	88	rBV	113633	125676	9.42%	1.165%
2	2.076	312	322	334	rBV	263693	377168	28.26%	3.497%
3	2.410	424	426	427	rBV2	453	186	0.01%	0.002%
4	2.632	491	495	497	rBV	401	345	0.03%	0.003%
5	2.664	502	505	511	rVB2	610	440	0.03%	0.004%
6	2.728	521	525	533	rBV4	988	1375	0.10%	0.013%
7	2.818	551	553	555	rVB2	476	169	0.01%	0.002%
8	2.899	576	578	580	rBV3	347	190	0.01%	0.002%
9	2.924	583	586	588	rBV2	365	229	0.02%	0.002%
10	2.969	596	600	602	rBV2	229	142	0.01%	0.001%
11	2.982	602	604	606	rBV2	306	180	0.01%	0.002%
12	3.072	631	632	636	rVB2	413	130	0.01%	0.001%
13	3.114	642	645	652	rVB2	539	453	0.03%	0.004%
14	3.236	681	683	685	rBV2	260	157	0.01%	0.001%
15	3.265	690	692	696	rVB3	295	165	0.01%	0.002%
16	3.323	706	710	714	rVB3	401	269	0.02%	0.002%
17	3.378	724	727	729	rBV2	456	283	0.02%	0.003%
18	3.442	745	747	749	rBV2	441	222	0.02%	0.002%
19	3.519	770	771	774	rBV	296	131	0.01%	0.001%
20	3.731	832	837	838	rBV2	1021	924	0.07%	0.009%
21	3.805	858	860	863	rBV2	359	202	0.02%	0.002%
22	3.892	877	887	920	rBV2	68801	261537	19.60%	2.425%
23	4.346	1010	1028	1058	rBV	191860	514721	38.57%	4.772%
24	4.719	1140	1144	1147	rBV3	472	405	0.03%	0.004%
25	4.744	1147	1152	1154	rBV2	751	529	0.04%	0.005%
26	4.828	1176	1178	1182	rVB2	255	167	0.01%	0.002%
27	4.876	1190	1193	1196	rVB2	399	226	0.02%	0.002%
28	4.895	1196	1199	1202	rBV3	596	454	0.03%	0.004%
29	4.921	1205	1207	1209	rVB3	549	217	0.02%	0.002%
30	4.979	1222	1225	1228	rBV	231	166	0.01%	0.002%
31	5.040	1228	1244	1279	rBV2	530193	1334673	100.00%	12.375%
32	5.571	1406	1409	1410	rBV2	438	232	0.02%	0.002%
33	5.616	1410	1423	1457	rBV	428344	902069	67.59%	8.364%
34	5.902	1500	1512	1530	rBV2	31903	71664	5.37%	0.664%
35	6.069	1551	1564	1597	rVB	279606	609100	45.64%	5.648%
36	6.272	1625	1627	1632	rVV4	513	404	0.03%	0.004%

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 ClientSampleId :
 C0B25ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Peak separation: 5

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

37	6.304	1634	1637	1639	rVB	643	350	0.03%	0.003%
38	6.323	1639	1643	1644	rBV	198	127	0.01%	0.001%
39	6.365	1651	1656	1657	rBV	330	273	0.02%	0.003%
40	6.374	1657	1659	1661	rVB3	576	250	0.02%	0.002%
41	6.503	1697	1699	1701	rBV	220	120	0.01%	0.001%
42	6.567	1715	1719	1722	rBV2	236	242	0.02%	0.002%
43	6.622	1730	1736	1738	rBV2	894	843	0.06%	0.008%
44	6.763	1776	1780	1782	rBV	228	171	0.01%	0.002%
45	6.837	1799	1803	1805	rBV2	322	227	0.02%	0.002%
46	6.911	1819	1826	1828	rBV3	885	913	0.07%	0.008%
47	6.989	1838	1850	1877	rBV	153468	299520	22.44%	2.777%
48	7.207	1915	1918	1921	rBV2	374	293	0.02%	0.003%
49	7.223	1921	1923	1925	rVB2	547	237	0.02%	0.002%
50	7.243	1925	1929	1930	rBV	528	242	0.02%	0.002%
51	7.265	1931	1936	1937	rBV3	1069	897	0.07%	0.008%
52	7.316	1940	1952	1970	rBV	634663	1116694	83.67%	10.354%
53	7.625	2035	2048	2080	rBV	101977	205407	15.39%	1.905%
54	7.879	2123	2127	2130	rBV2	507	355	0.03%	0.003%
55	7.911	2133	2137	2141	rVB	278	219	0.02%	0.002%
56	7.940	2141	2146	2149	rBV3	359	445	0.03%	0.004%
57	7.979	2152	2158	2159	rBV3	551	372	0.03%	0.003%
58	8.046	2175	2179	2182	rBV2	364	273	0.02%	0.003%
59	8.107	2185	2198	2237	rBV2	297479	685434	51.36%	6.355%
60	8.500	2317	2320	2326	rBV4	723	760	0.06%	0.007%
61	8.664	2366	2371	2376	rBV5	678	819	0.06%	0.008%
62	8.686	2376	2378	2383	rVB3	452	241	0.02%	0.002%
63	8.812	2413	2417	2419	rBV2	719	424	0.03%	0.004%
64	8.857	2419	2431	2458	rBV	648950	1133305	84.91%	10.508%
65	9.149	2513	2522	2533	rBV6	3950	7406	0.55%	0.069%
66	9.275	2559	2561	2563	rBV	233	112	0.01%	0.001%
67	9.442	2609	2613	2616	rBV	445	360	0.03%	0.003%
68	9.474	2620	2623	2626	rBV3	694	468	0.04%	0.004%
69	9.516	2633	2636	2638	rBV2	544	280	0.02%	0.003%
70	9.554	2639	2648	2658	rBV5	3467	5402	0.40%	0.050%
71	9.641	2671	2675	2676	rBV	303	174	0.01%	0.002%
72	9.680	2681	2687	2689	rBV3	620	594	0.04%	0.006%
73	9.693	2689	2691	2692	rBV2	722	283	0.02%	0.003%
74	9.760	2709	2712	2714	rVB2	374	173	0.01%	0.002%
75	9.776	2714	2717	2719	rBV2	225	121	0.01%	0.001%
76	9.795	2719	2723	2725	rBV3	769	616	0.05%	0.006%

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 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0B25ME

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	9.831	2731	2734	2736	rBV	464	335	0.03%	0.003%
78	9.918	2758	2761	2763	rBV2	428	222	0.02%	0.002%
79	10.130	2818	2827	2841	rVB4	4271	7787	0.58%	0.072%
80	10.223	2842	2856	2877	rBV	401165	657960	49.30%	6.101%
81	10.426	2917	2919	2921	rVB	346	165	0.01%	0.002%
82	10.673	2994	2996	2998	rBV	389	190	0.01%	0.002%
83	10.725	3010	3012	3014	rBV	379	175	0.01%	0.002%
84	10.741	3014	3017	3019	rBV2	774	533	0.04%	0.005%
85	11.040	3102	3110	3115	rBV4	1083	1733	0.13%	0.016%
86	11.152	3137	3145	3154	rVB8	2684	4743	0.36%	0.044%
87	11.197	3155	3159	3162	rBV3	1174	895	0.07%	0.008%
88	11.252	3164	3176	3199	rBV	810308	1257443	94.21%	11.659%
89	11.628	3282	3293	3316	rVB	746343	1164584	87.26%	10.798%
90	11.792	3336	3344	3351	rBV8	2812	4219	0.32%	0.039%
91	11.918	3381	3383	3385	rBV2	368	191	0.01%	0.002%
92	12.178	3462	3464	3468	rBV3	587	415	0.03%	0.004%
93	12.654	3608	3612	3618	rVB4	794	742	0.06%	0.007%
94	12.776	3646	3650	3651	rBV3	431	350	0.03%	0.003%
95	12.866	3674	3678	3680	rBV3	617	401	0.03%	0.004%
96	12.892	3682	3686	3693	rVB5	2871	3333	0.25%	0.031%
97	13.049	3729	3735	3740	rVB3	941	1137	0.09%	0.011%
98	13.519	3873	3881	3889	rBV4	2290	4454	0.33%	0.041%
99	13.898	3994	3999	4003	rBV6	1609	1988	0.15%	0.018%
100	14.593	4213	4215	4217	rBV	456	246	0.02%	0.002%

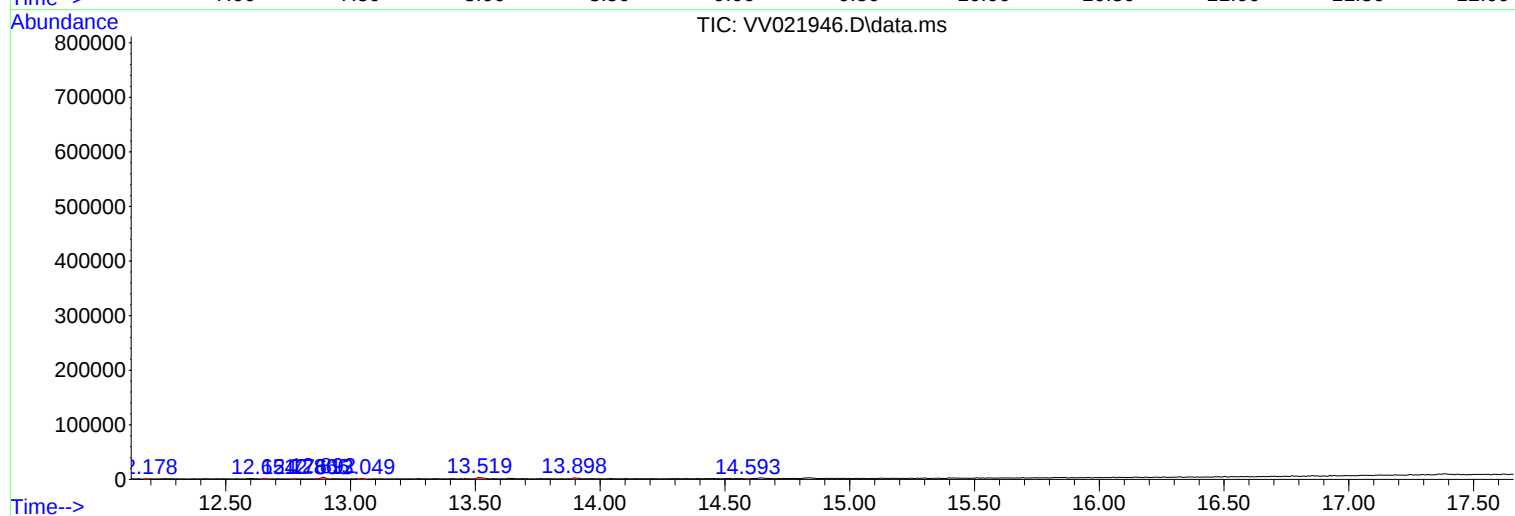
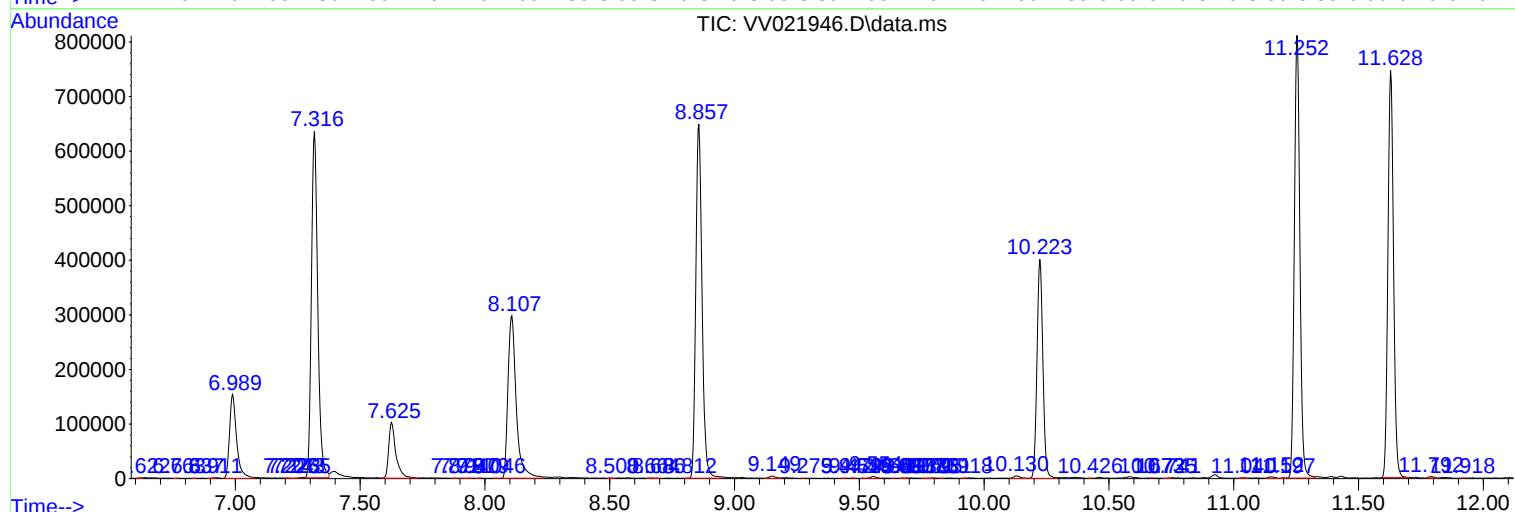
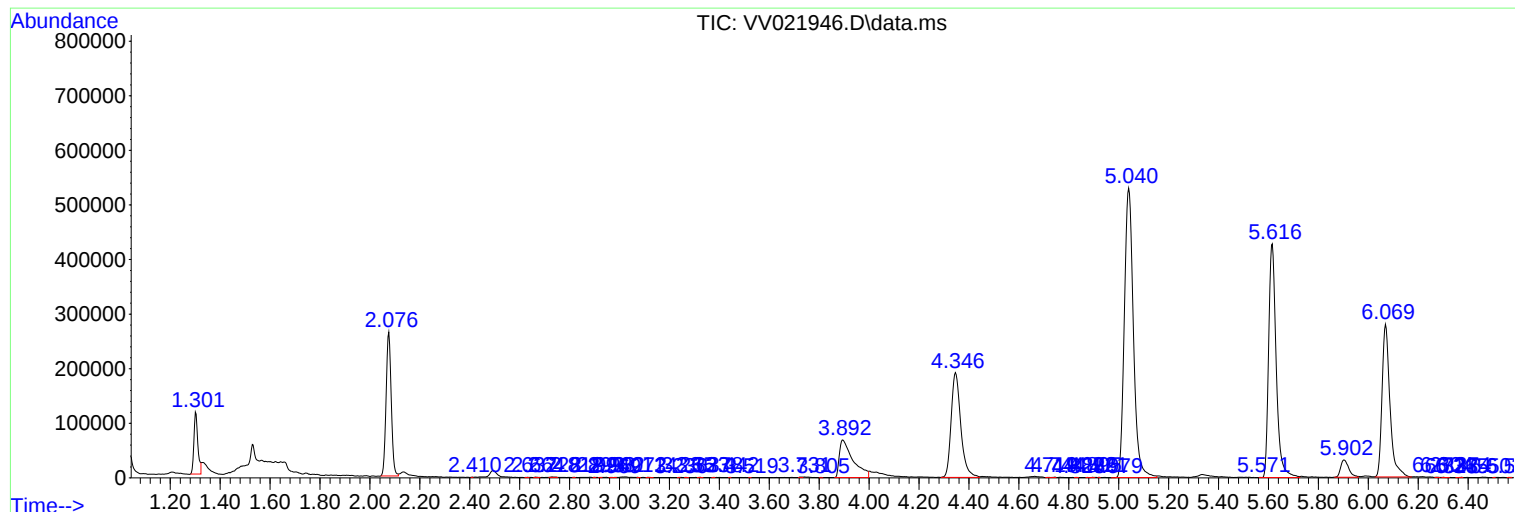
Sum of corrected areas: 10785283

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082521\
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Misc : 7.54g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0B25ME

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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C0B25ME

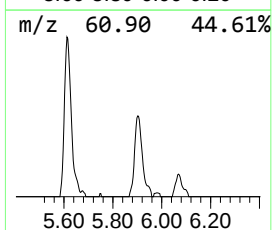
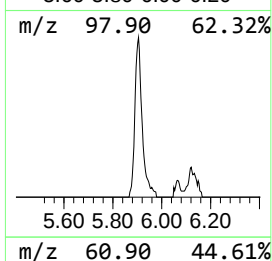
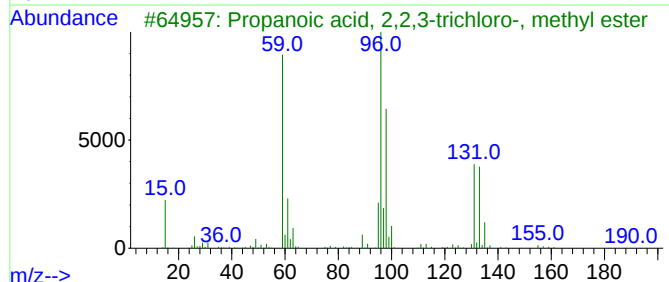
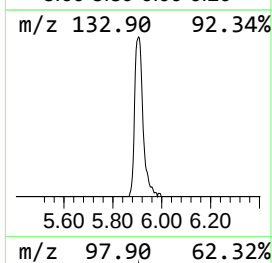
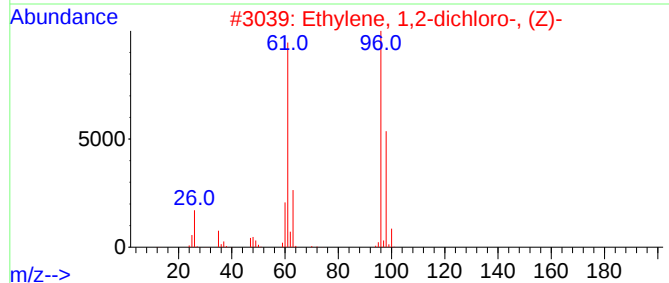
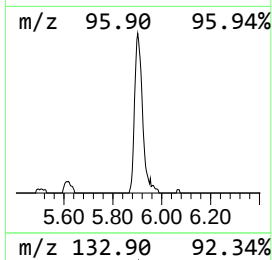
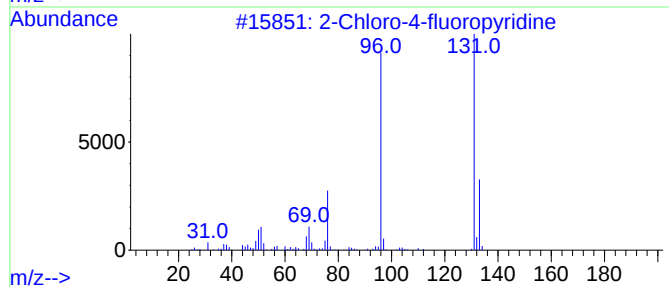
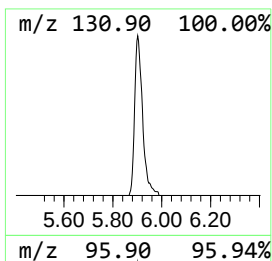
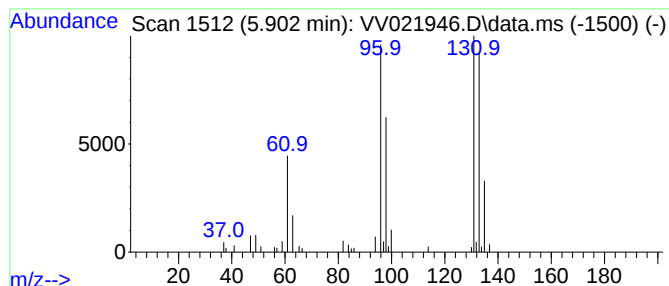
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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	3.97 ug/L	71664	1,4-Difluorobenzene	5.616

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	38
3			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	37
4			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	35
5			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	30



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	5.902	4.0	ug/L	71664	1	5.616	902069	50.0