

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV031122\
 Data File : VV024956.D
 Acq On : 11 Mar 2022 11:49
 Operator : SY/MD
 Sample : N1775-24ME
 Misc : 4.97g/5.0mL/100uL/5mL/MSVOA_V/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DBSC7ME

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\SFAMVLM022822WMA.M
 Title : VOC Analysis

Signal : TIC: VV024956.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	75	82	100	rVB	203806	234790	13.93%	1.906%
2	1.568	156	164	185	rVB	136105	182786	10.84%	1.484%
3	2.089	316	326	340	rBV	379876	539986	32.03%	4.385%
4	2.336	400	403	407	rBV2	258	164	0.01%	0.001%
5	2.429	429	432	434	rBV	320	236	0.01%	0.002%
6	2.500	446	454	470	rVB6	2943	6001	0.36%	0.049%
7	2.642	493	498	500	rBV2	238	215	0.01%	0.002%
8	2.735	523	527	530	rBV2	305	235	0.01%	0.002%
9	3.024	613	617	619	rBV3	1259	1144	0.07%	0.009%
10	3.130	648	650	653	rVB	154	72	0.00%	0.001%
11	3.150	653	656	659	rBV	333	240	0.01%	0.002%
12	3.169	659	662	668	rVV	230	248	0.01%	0.002%
13	3.211	672	675	677	rVV2	175	139	0.01%	0.001%
14	3.243	681	685	688	rBV2	159	125	0.01%	0.001%
15	3.420	737	740	743	rVB	203	110	0.01%	0.001%
16	3.478	753	758	761	rBV2	257	272	0.02%	0.002%
17	3.548	778	780	784	rVB2	171	96	0.01%	0.001%
18	3.574	784	788	791	rBV2	165	140	0.01%	0.001%
19	3.622	800	803	806	rBV	188	110	0.01%	0.001%
20	3.658	811	814	815	rBV2	129	72	0.00%	0.001%
21	3.674	816	819	822	rBV	363	218	0.01%	0.002%
22	3.732	833	837	838	rBV	133	88	0.01%	0.001%
23	3.806	858	860	863	rVB	156	83	0.00%	0.001%
24	3.828	863	867	869	rBV2	153	126	0.01%	0.001%
25	3.899	878	889	935	rBV2	67332	307826	18.26%	2.499%
26	4.339	1011	1026	1057	rVB	264892	655901	38.91%	5.326%
27	4.539	1085	1088	1090	rBV2	247	179	0.01%	0.001%
28	4.606	1106	1109	1116	rVB3	257	301	0.02%	0.002%
29	4.648	1116	1122	1123	rBV2	477	354	0.02%	0.003%
30	4.719	1141	1144	1147	rBV	372	256	0.02%	0.002%
31	4.783	1161	1164	1166	rBV2	122	86	0.01%	0.001%
32	4.863	1184	1189	1192	rBV2	212	211	0.01%	0.002%
33	4.899	1196	1200	1205	rBV4	830	909	0.05%	0.007%
34	5.037	1226	1243	1290	rBV2	673734	1685793	100.00%	13.688%
35	5.336	1323	1336	1352	rBV4	4630	13479	0.80%	0.109%
36	5.455	1371	1373	1375	rBV	360	186	0.01%	0.002%

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Integrator: RTE

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 Title : VOC Analysis

37	5.539	1395	1399	1401	rBV2	344	273	0.02%	0.002%
38	5.609	1409	1421	1466	rBV	441710	898958	53.33%	7.299%
39	5.902	1500	1512	1533	rBV	29237	63040	3.74%	0.512%
40	6.063	1549	1562	1597	rVB	361917	745662	44.23%	6.055%
41	6.397	1663	1666	1670	rBV	212	134	0.01%	0.001%
42	6.529	1702	1707	1709	rBV2	298	268	0.02%	0.002%
43	6.545	1709	1712	1715	rVB2	320	213	0.01%	0.002%
44	6.567	1715	1719	1721	rVB	191	115	0.01%	0.001%
45	6.593	1721	1727	1729	rBV	121	124	0.01%	0.001%
46	6.641	1733	1742	1754	rBV7	2229	5079	0.30%	0.041%
47	6.738	1770	1772	1774	rBV	253	131	0.01%	0.001%
48	6.844	1801	1805	1810	rVB2	180	174	0.01%	0.001%
49	6.873	1810	1814	1816	rBV	254	194	0.01%	0.002%
50	6.982	1837	1848	1876	rBV	195825	369249	21.90%	2.998%
51	7.310	1938	1950	1969	rBV	787138	1386967	82.27%	11.262%
52	7.619	2036	2046	2076	rBV	121995	241153	14.31%	1.958%
53	7.799	2098	2102	2104	rBV2	374	309	0.02%	0.003%
54	7.863	2119	2122	2125	rBV2	323	248	0.01%	0.002%
55	7.940	2143	2146	2151	rBV2	158	131	0.01%	0.001%
56	8.114	2184	2200	2238	rBV	198831	697600	41.38%	5.664%
57	8.477	2311	2313	2316	rBV	115	80	0.00%	0.001%
58	8.526	2326	2328	2330	rBV2	205	101	0.01%	0.001%
59	8.616	2350	2356	2357	rBV2	375	282	0.02%	0.002%
60	8.696	2375	2381	2383	rBV	82	90	0.01%	0.001%
61	8.731	2389	2392	2395	rBV2	231	180	0.01%	0.001%
62	8.802	2408	2414	2417	rBV2	244	282	0.02%	0.002%
63	8.850	2417	2429	2461	rBV	631550	1137650	67.48%	9.237%
64	9.127	2512	2515	2516	rBV	294	163	0.01%	0.001%
65	9.149	2518	2522	2523	rBV2	570	417	0.02%	0.003%
66	9.220	2540	2544	2546	rBV2	170	128	0.01%	0.001%
67	9.333	2577	2579	2582	rBV	141	95	0.01%	0.001%
68	9.391	2594	2597	2599	rBV	178	90	0.01%	0.001%
69	9.407	2599	2602	2605	rVB2	169	82	0.00%	0.001%
70	9.497	2626	2630	2632	rBV2	213	178	0.01%	0.001%
71	9.551	2645	2647	2649	rBV	203	120	0.01%	0.001%
72	9.587	2655	2658	2660	rBV2	142	93	0.01%	0.001%
73	9.619	2665	2668	2670	rBV2	198	120	0.01%	0.001%
74	9.673	2682	2685	2688	rBV2	261	198	0.01%	0.002%
75	9.767	2709	2714	2720	rBV2	186	240	0.01%	0.002%
76	9.895	2751	2754	2756	rBV2	199	129	0.01%	0.001%

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Instrument :
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 ClientSampleId :
 DBSC7ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

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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\SFAMVLM022822WMA.M
 Title : VOC Analysis

77	9.989	2780	2783	2786	rBV2	135	92	0.01%	0.001%
78	10.127	2816	2826	2837	rVB3	5672	8770	0.52%	0.071%
79	10.175	2838	2841	2842	rBV2	161	93	0.01%	0.001%
80	10.220	2842	2855	2873	rBV	431848	740461	43.92%	6.012%
81	10.548	2952	2957	2959	rBV2	551	409	0.02%	0.003%
82	10.580	2959	2967	2982	rVB7	3693	6746	0.40%	0.055%
83	10.747	3016	3019	3021	rBV	180	113	0.01%	0.001%
84	10.770	3024	3026	3027	rBV	185	90	0.01%	0.001%
85	10.821	3039	3042	3045	rBV2	462	364	0.02%	0.003%
86	10.915	3065	3071	3084	rVB4	4058	6083	0.36%	0.049%
87	11.034	3102	3108	3114	rVB3	959	1143	0.07%	0.009%
88	11.143	3136	3142	3151	rVB4	2465	3696	0.22%	0.030%
89	11.249	3163	3175	3195	rBV	735921	1136257	67.40%	9.226%
90	11.464	3239	3242	3243	rBV	412	254	0.02%	0.002%
91	11.525	3259	3261	3263	rBV2	197	75	0.00%	0.001%
92	11.567	3268	3274	3278	rBV4	431	547	0.03%	0.004%
93	11.625	3279	3292	3311	rBV	789249	1221707	72.47%	9.920%
94	11.786	3336	3342	3349	rVB5	1560	1909	0.11%	0.016%
95	11.844	3355	3360	3364	rBV4	878	1045	0.06%	0.008%
96	11.972	3398	3400	3405	rBV2	182	132	0.01%	0.001%
97	12.355	3513	3519	3522	rBV5	1077	1339	0.08%	0.011%
98	12.538	3571	3576	3579	rBV2	253	260	0.02%	0.002%
99	12.641	3605	3608	3610	rBV	159	92	0.01%	0.001%
100	14.246	4104	4107	4109	rBV	291	154	0.01%	0.001%

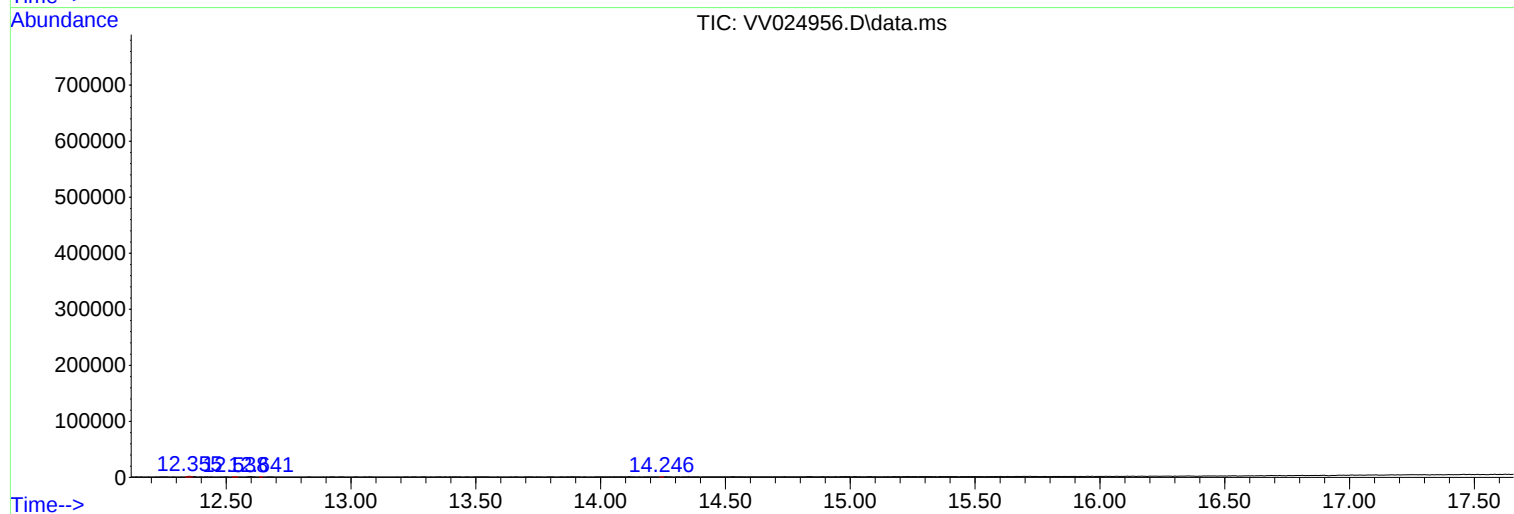
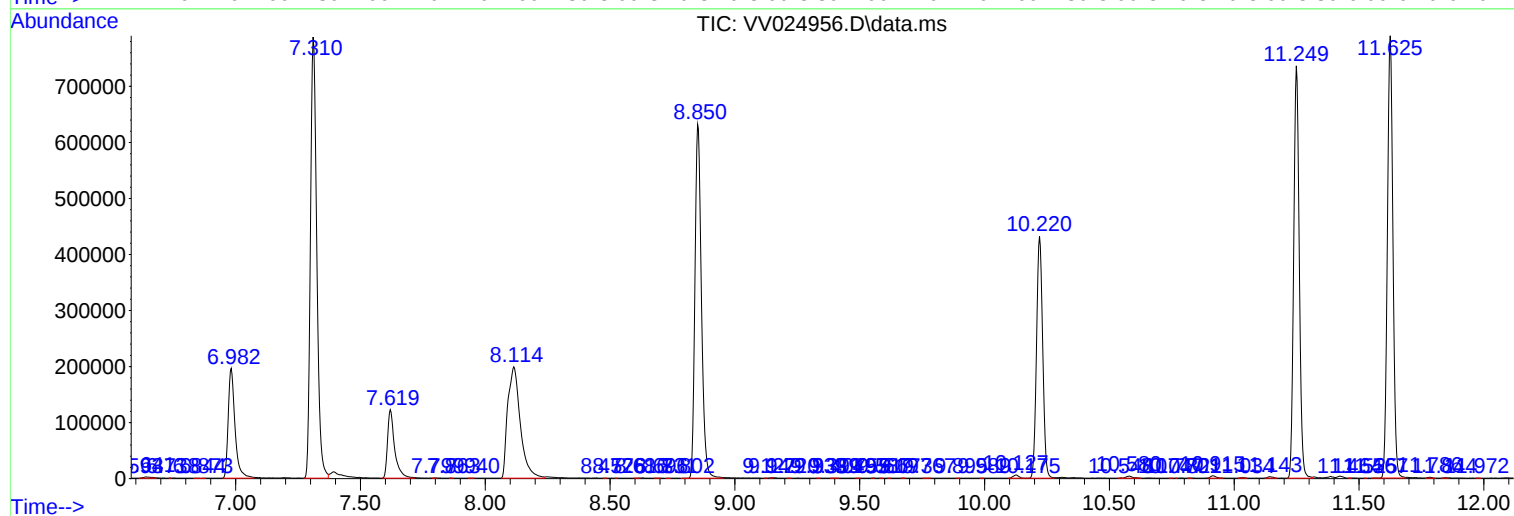
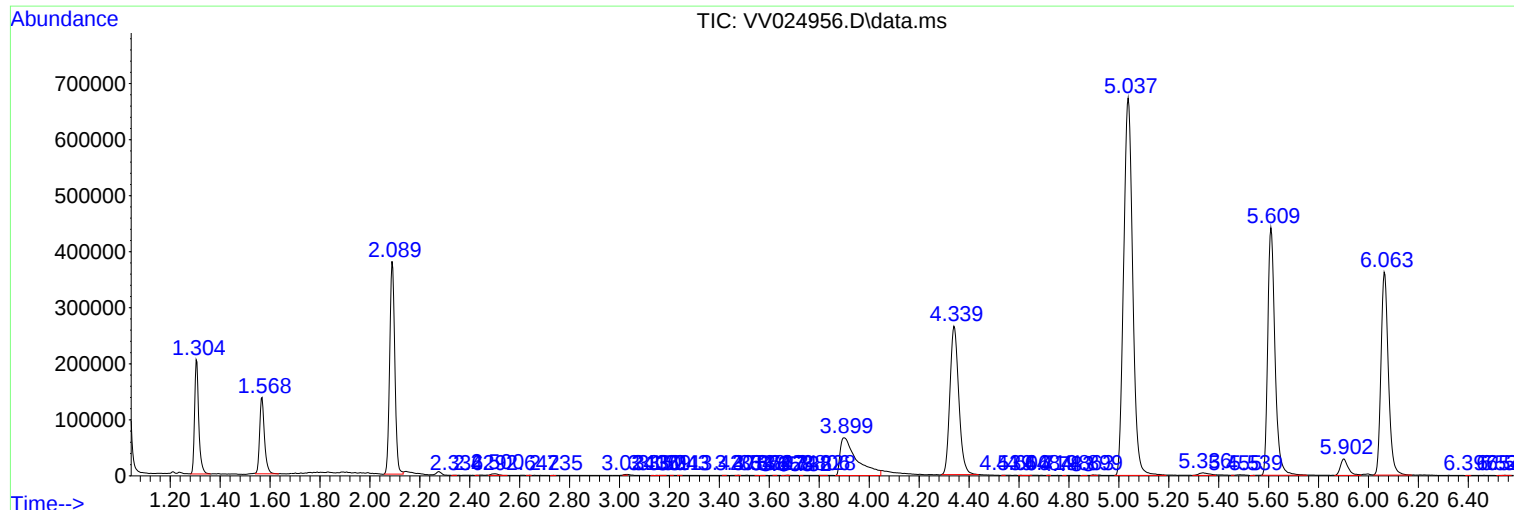
Sum of corrected areas: 12315748

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ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBSC7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM022822WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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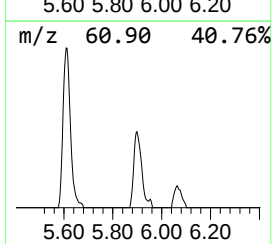
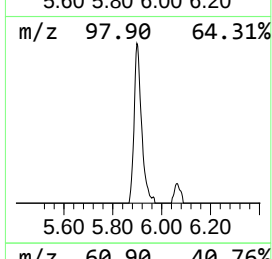
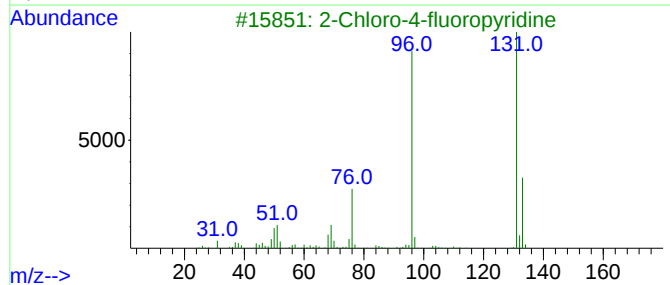
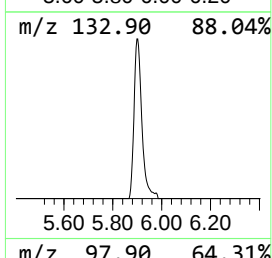
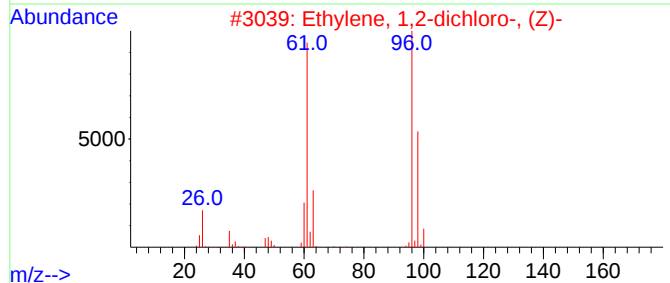
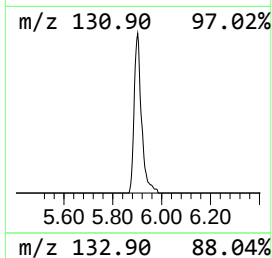
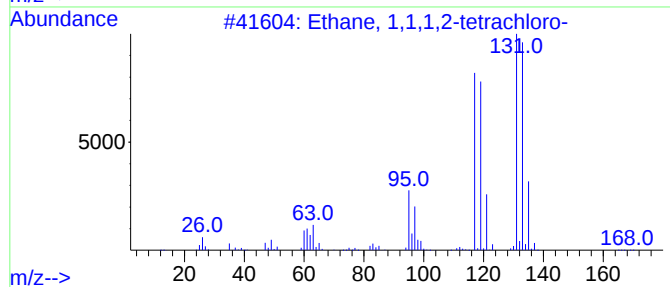
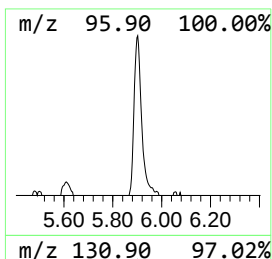
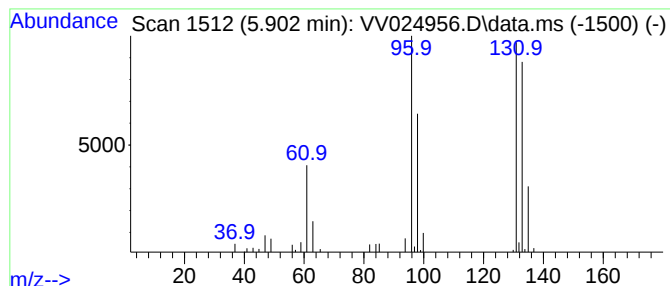
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM022822WMA.M
Quant Title : VOC Analysis

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	3.51 ug/L	63040	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			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
3			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	38
4			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	37
5			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	5.902	3.5	ug/L	63040	1	5.609	898958	50.0